Errata in "Principles of Quantum Mechanics", by Ramamurti Shankar

April 15, 2006

Page	Line	Erratum	Correction
xi	30	quite easy so adapt	quite easy to adapt
xii	15	cost were born	cost was born
3	9	do not purposely use	purposely do not use
43	6	$M^iM^i = -M^jM^i$ for $i \neq j$	$M^iM^j = -M^jM^i$ for $i \neq j$
54	24	$e^{\Omega} = \sum_{n=1}^{\infty}$	$e^{\Omega} = \sum_{n=0}^{\infty}$
66	-8	$\int_0^{L+\Delta}$	$\int_{L}^{L+\Delta}$
68	12	$\int_{-\infty}^{\infty} < k\|x >< k\|f > dk$	$\int_{-\infty}^{\infty} < x\|k >< k\|f > dk$
81	8	$\rho = (x^2 + y)^{1/2}$	$\rho = (x^2 + y^2)^{1/2}$
119	10	$P(\lambda) = \| < \lambda\|\psi > \|^2$	$P(\lambda) \propto \| < \lambda\|\psi > \|^2$
131	9	vice vesa	vice versa
167	21	by dotted lines in the figure.	by the dotted line in Figure 5.2.
191	1	The last terms suggests	The last term suggests
191	15	from the atomic physics to cosmology	from atomic physics to cosmology
220	19	asuming for simplicity	assuming for simplicity
252	14	$X_2^{(1)\otimes(2)}$	$X_1^{(1)\otimes(2)}$
255	12	the energy eigenvalues	the energy eigenvectors
296	-5	which does not change with time	which does change with time
317	20	$n = 2$	$n = 1$
317	-9	of charge q	of mass μ and charge q
320	16	$e^{-\theta\cdot\mathbf{L}/\hbar}$	$e^{-i\theta\cdot\mathbf{L}/\hbar}$
336	20	linear combination of each other	linear combinations of each other
337	13	Legendre Polynomial	*Legendre Polynomial*
339	6	$z\ cos\theta_x + y\ sin\theta_x$	$z\ cos\theta_x - y\ sin\theta_x$
339	10	$z\ cos\theta_x - y\ sin\theta_x$	$z\ cos\theta_x + y\ sin\theta_x$
350	3	$(pr\ cos\theta)\hbar$	$(pr\ cos\theta)/\hbar$
393	-2	$B <<< B_0$	$B \ll B_0$
394	-2	$\mathbf{M} = n\mu\mathbf{k}$	$\mathbf{M} = N\mu\mathbf{k}$
399	-2	1000kG	1000kG
415	13	project operators	projection operators
415	13	$j = 2j_1 = 1$	$j = 2j_1 - 1$

Page	Line	Erratum	Correction
418	24	$T_k^q \vert jm >$	$T_k^q \vert \alpha jm >$
419	-1	$\mp(J_x \pm J_y)/2^{1/2}$	$\mp(J_x \pm iJ_y)/2^{1/2}$
429	-1	minimun	minimum
430	-8	but is utility	but its utility
432	17	whose minimum lies at	whose minimum lies not at
434	22	wil	will
439	16	$\psi_n^*(X')$	$\psi_n^*(x')$
446	17	from	nor
456	8	shifted ay	shifted by
471	2	$\left\langle \frac{\lambda}{r^3} \right\rangle$	$\left\langle \frac{\lambda}{r^2} \right\rangle$
480	3	keep one only	keep only the first
485	-3	we did	we get
496	-1	path of least actions	path of least action
502	9	appropximate	approximate
507	30	coordinaters	coordinates
519	6	$+\varepsilon_1^1$	ε_1^1
533	3	$r_0 = 1\mu_0$	$r_0 = 1/\mu_0$
539	30	$\simeq r\left(1 - 2\frac{\mathbf{r}\cdot\mathbf{r}'}{r^2}\right)^{1/2} + O\left[\left(\frac{r'}{r}\right)^2\right] r$	$\simeq r\left(1 - 2\frac{\mathbf{r}\cdot\mathbf{r}'}{r^2}\right)^{1/2}$
564	-7	$\left(\frac{mc^2}{\hbar}\right)^2$	$\left(\frac{mc}{\hbar}\right)^2$
572	1	terms makes	terms make
573	3	$[\mathbf{P} \cdot [\mathbf{P}, v]]$	$[\mathbf{P}, [\mathbf{P}, v]]$
586	13	$\sum_{i=1}^{N}$	$\sum_{n=1}^{N}$
604	11	these coordinate	these coordinates
609	4	$e^{-z_2^* z_2}$	$e^{-z_2^* z_1}$
609	8	$e^{-z_2^* z_1}$	$e^{-z^* z}$
610	15	$e^{-z^* z}$	$e^{-z'^* z}$
614	2	$-\hbar\frac{d}{d\tau}\vert\psi(t)>= H\vert\psi(\tau)>$	$-\hbar\frac{d}{d\tau}\vert\psi(\tau)>= H\vert\psi(\tau)>$
614	-8	$\prod_{0}^{N-1}$	$\prod_{1}^{N-1}$
616	15	for the case a = 1.	for the case a = 1 and A = 1.
619	28	limitis	limits
620	1	costs	causes
620	11	$< -a\vert U(\tau)\vert a >$	$< a\vert U(\tau)\vert -a >$
637	14	so when one usually	usually so when one
662	15	pole as z	pole at z
673	-		Legendre polynomial 337

The items on pages 119 and 564 were submitted by Daniel Keren.

VECTOR SPACES & LINEAR INDEPENDENCE - SOME EXAMPLES

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

References: Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Exercises 1.1.1 - 1.1.5.

Post date: 3 Nov 2016

Here are a few examples of vector space problems.

Given the axioms of a vector space, we can derive a few more properties. I'll use Shankar's notation for vectors, which is essentially Dirac's bra-ket notation.

Theorem 1. *The additive identity* 0 *is unique.*

Proof. Proof: (by contradiction). Suppose there are two distinct additive identities $|0\rangle$ and $|0'\rangle$. Then

$$\begin{aligned} |0'\rangle &= |0'\rangle + |0\rangle \text{ (since } |0\rangle \text{is an additive identity)} && (1)\\ &= |0\rangle + |0'\rangle \text{ (commutative addition)} && (2)\\ &= |0\rangle \text{ (since } |0'\rangle \text{is an additive identity)} && (3) \end{aligned}$$

□

Theorem 2. *Multiplication of any vector by the zero scalar gives the zero vector.*

Proof. We wish to show that $0\,|v\rangle = |0\rangle$ for all $v \in V$. We have

$$\begin{aligned} |0\rangle &= (0+1)\,|v\rangle + |-v\rangle && (4)\\ &= 0\,|v\rangle + |v\rangle + |-v\rangle && (5)\\ &= 0\,|v\rangle + |0\rangle && (6)\\ &= 0\,|v\rangle && (7) \end{aligned}$$

where the third line follows because $|-v\rangle$ is the additive inverse of $|v\rangle$ and the last line follows because $|0\rangle$ is the additive identity vector. □

Theorem 3. $|-v\rangle = -\,|v\rangle$. *That is,* $-\,|v\rangle$ *is the additive inverse of* $|v\rangle$.

Proof. The negative of a vector v is multiplication of v by the scalar -1, so

$$|v\rangle + (-|v\rangle) = (1+(-1))|v\rangle \tag{8}$$
$$= 0|v\rangle \tag{9}$$
$$= |0\rangle \tag{10}$$

by theorem 2. Thus $-|v\rangle$ is an additive inverse of $|v\rangle$, so $-|v\rangle = |-v\rangle$. □

Theorem 4. *The additive inverse $|-v\rangle$ is unique.*

Proof. Suppose there is another vector $|w\rangle$ for which $|v\rangle + |w\rangle = |0\rangle$. By theorem 1, $|0\rangle$ is unique, so we must have $|v\rangle + |w\rangle = |v\rangle + |-v\rangle$. By theorem 3, this gives

$$|v\rangle - |v\rangle + |w\rangle = |-v\rangle \tag{11}$$
$$|0\rangle + |w\rangle = |-v\rangle \tag{12}$$
$$|w\rangle = |-v\rangle \tag{13}$$

where the third line follows because $|0\rangle$ is the additive identity. □

Example 5. Consider the set of all entities (a,b,c) where the entries are real numbers. Addition and scalar multiplication are defined as

$$(a,b,c) + (d,e,f) \equiv (a+d, b+e, c+f) \tag{14}$$
$$\alpha(a,b,c) \equiv (\alpha a, \alpha b, \alpha c) \tag{15}$$

The null vector is

$$|0\rangle = (0,0,0) \tag{16}$$

The inverse of (a,b,c) is $(-a,-b,-c)$. As the set is closed under addition and scalar multiplication it is a vector space. However, a subset such as $(a,b,1)$ is *not* a vector space since it is not closed under addition or scalar multiplication:

$$(a,b,1) + (d,e,1) = (a+d, b+e, 2) \tag{17}$$
$$2(a,b,1) = (2a, 2b, 2) \tag{18}$$

Neither of the vectors on the RHS are of the form $(a,b,1)$ so they don't lie in the set.

Example 6. The set of all functions $f(x)$ defined on an interval $0 \leq x \leq L$ form a vector space if we define addition as pointwise addition $f+g = f(x)+g(x)$ for all x, and scalar multiplication by a as $af(x)$.

Some subsets of this vector space are also vector spaces. For example the set of all functions that satsify $f(0) = f(L) = 0$ is a vector space, because the sum of any two such functions also satisfies $(f+g)(0) = (f+g)(L) = 0$, and scalar multiplication leaves the endpoints at 0 as well.

The subset of periodic functions $f(0) = f(L)$ (not necessarily equal to 0) is also a vector space. Adding any two functions from this subset gives a sum such that

$$\begin{aligned} f(0)+g(0) &= f(L)+g(L) && (19)\\ (f+g)(0) &= (f+g)(L) && (20) \end{aligned}$$

Multiplying by a scalar gives

$$\begin{aligned} a(f(0)+g(0)) &= a(f(L)+g(L)) && (21)\\ a(f+g)(0) &= a(f+g)(L) && (22) \end{aligned}$$

However, a subset such as all functions with $f(0) = 4$ is not a vector space, since adding two such functions gives a sum with $(f+g)(0) = 8$, and multiplying by a scalar gives a function with $af(0) = 4a$, neither of which is in the subset.

Now a couple of examples of linear independence.

Example 7. We have three vectors from the vector space of real 2×2 matrices:

$$\begin{aligned} |1\rangle &= \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} && (23)\\ |2\rangle &= \begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix} && (24)\\ |3\rangle &= \begin{bmatrix} -2 & -1 \\ 0 & -2 \end{bmatrix} && (25) \end{aligned}$$

These are not linearly independent, because $|3\rangle = |1\rangle - 2|2\rangle$.

Example 8. We have 3 row vectors

$$\begin{aligned} |1\rangle &= \begin{bmatrix} 1 & 1 & 0 \end{bmatrix} && (26)\\ |2\rangle &= \begin{bmatrix} 1 & 0 & 1 \end{bmatrix} && (27)\\ |3\rangle &= \begin{bmatrix} 3 & 2 & 1 \end{bmatrix} && (28) \end{aligned}$$

These are linearly dependent, since $|3\rangle = 2|1\rangle + |2\rangle$.

Now we look at the 3 vectors

$$|1\rangle = \begin{bmatrix} 1 & 1 & 0 \end{bmatrix} \tag{29}$$
$$|2\rangle = \begin{bmatrix} 1 & 0 & 1 \end{bmatrix} \tag{30}$$
$$|3\rangle = \begin{bmatrix} 0 & 1 & 1 \end{bmatrix} \tag{31}$$

We can show that these are linearly independent by attempting to solve the equation

$$0 = a|1\rangle + b|2\rangle + c|3\rangle \tag{32}$$

Looking at each component, we have

$$a+b = 0 \tag{33}$$
$$a+c = 0 \tag{34}$$
$$b+c = 0 \tag{35}$$

Solving the last two equations for a and b in terms of c and substituting into the first equation, we get

$$-2c = 0 \tag{36}$$
$$c = 0 \tag{37}$$

Thus we find that the only solution is $a = b = c = 0$, which proves linear independence.

PINGBACKS

Pingback: Vector spaces: span, linear independence and basis

GRAM-SCHMIDT ORTHOGONALIZATION - A COUPLE OF EXAMPLES

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

References: Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Exercises 1.3.1 - 1.3.2.

Post date: 4 Nov 2016

Here are a couple of examples of the Gram-Schmidt orthogonalization procedure. The recipe for generating an orthonormal basis e_i from a general set of linearly independent vectors v_i is as follows.

The first vector e_1 in the orthonormal basis is defined by

$$e_1 = \frac{v_1}{|v_1|} \tag{1}$$

where v_1 is the first vector (well, any vector, really) in the non-orthonormal basis.

Given vector e_{j-1} in the orthonormal basis, we can form e_j from the formula

$$e_j = \frac{v_j - \sum_{i=1}^{j-1} \langle e_i, v_j \rangle e_i}{\left| v_j - \sum_{i=1}^{j-1} \langle e_i, v_j \rangle e_i \right|} \tag{2}$$

Example 1. Given $v_1 = (3,4)$ and $v_2 = (2,-6)$ we can form an orthonormal basis in two ways. Starting with v_1 we have

$$e_1 = \frac{v_1}{|v_1|} = \left(\frac{3}{5}, \frac{4}{5} \right) \tag{3}$$

$$e_2 = \frac{v_2 - \langle e_1, v_2 \rangle e_1}{|v_2 - \langle e_1, v_2 \rangle e_1|} \tag{4}$$

To evaluate e_2, we have

$$\langle e_1, v_2\rangle = \frac{6}{5} - \frac{24}{5} = -\frac{18}{5} \tag{5}$$

$$v_2 - \langle e_1, v_2\rangle e_1 = (2,-6) + \frac{18}{5}\left(\frac{3}{5}, \frac{4}{5}\right) \tag{6}$$

$$= \frac{1}{25}(104,-78) \tag{7}$$

$$|v_2 - \langle e_1, v_2\rangle e_1| = \frac{130}{25} \tag{8}$$

$$e_2 = \frac{1}{130}(104,-78) \tag{9}$$

As a check,

$$\langle e_1, e_2\rangle = \frac{1}{650}(312-312) = 0 \tag{10}$$

$$\langle e_1, e_1\rangle = \frac{1}{25}(9+16) = 1 \tag{11}$$

$$\langle e_2, e_2\rangle = \frac{1}{16900}(10816+6084) = 1 \tag{12}$$

We could also start with v_2, giving

$$e_1 = \frac{v_2}{|v_2|} = \frac{1}{2\sqrt{10}}(2,-6) \tag{13}$$

$$e_2 = \frac{v_1 - \langle e_1, v_1\rangle e_1}{|v_1 - \langle e_1, v_1\rangle e_1|} \tag{14}$$

$$\langle e_1, v_1\rangle = \frac{1}{2\sqrt{10}}(6-24) = -\frac{9}{\sqrt{10}} \tag{15}$$

$$v_1 - \langle e_1, v_1\rangle e_1 = (3,4) + \frac{9}{20}(2,-6) \tag{16}$$

$$= \frac{1}{20}(78,26) \tag{17}$$

$$|v_1 - \langle e_1, v_1\rangle e_1| = \frac{\sqrt{6760}}{20} \tag{18}$$

$$e_2 = \frac{1}{\sqrt{6760}}(78,26) \tag{19}$$

Checking, we get

$$\langle e_1, e_2 \rangle = \frac{1}{2\sqrt{67600}} (156 - 156) = 0 \tag{20}$$

$$\langle e_1, e_1 \rangle = \frac{1}{40} (4 + 36) = 1 \tag{21}$$

$$\langle e_2, e_2 \rangle = \frac{1}{6760} (6084 + 676) = 1 \tag{22}$$

Example 2. We're now given 3 vectors in 3-d space:

$$v_1 = (3,0,0) \tag{23}$$
$$v_2 = (0,1,2) \tag{24}$$
$$v_3 = (0,2,5) \tag{25}$$

The problem is to generate linear combinations of these 3 vectors to give the orthonormal basis

$$e_1 = (1,0,0) \tag{26}$$
$$e_2 = \frac{1}{\sqrt{5}} (0,1,2) \tag{27}$$
$$e_3 = \frac{1}{\sqrt{5}} (0,-2,1) \tag{28}$$

We could use the Gram-Schmidt procedure, but it's probably easier to just solve the equations. We have

$$e_1 = \frac{v_1}{3} \tag{29}$$
$$e_2 = \frac{v_2}{\sqrt{5}} \tag{30}$$
$$e_3 = Av_1 + Bv_2 + Cv_3 \tag{31}$$

Writing out the last equation using components, we have

$$0 = A \tag{32}$$
$$-\frac{2}{\sqrt{5}} = B + 2C \tag{33}$$
$$\frac{1}{\sqrt{5}} = 2B + 5C \tag{34}$$

The solution is

$$C = \frac{5}{\sqrt{5}} = \sqrt{5} \tag{35}$$

$$B = -\frac{12}{\sqrt{5}} \tag{36}$$

Thus we have

$$e_1 = \frac{v_1}{3} \tag{37}$$

$$e_2 = \frac{v_2}{\sqrt{5}} \tag{38}$$

$$e_3 = -\frac{12}{\sqrt{5}} v_2 + \sqrt{5} v_3 \tag{39}$$

TRIANGLE INEQUALITY AS AN EQUALITY

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References: Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Exercises 1.3.3 - 1.3.4.

Post date: 5 Nov 2016

We've already proved the triangle inequality for vectors, but it's worth adding a note on when the inequality becomes an equality. The triangle inequality states that for all $u, v \in V$

$$|u+v| \leq |u| + |v| \tag{1}$$

To make this an equality, we need to look back at the proof. The last step in the proof invokes the Schwarz inequality to state that

$$|u+v|^2 \leq |u|^2 + |v|^2 + 2|u||v| \tag{2}$$

Looking at the proof for the Schwarz inequality, we see that it becomes an equality if the component w of u that is orthogonal to v is zero, that is, if $u = \alpha v$ for some (possibly complex) scalar α. If that is the case, then

$$|u+v| = |\alpha v + v| = |1+\alpha||v| \tag{3}$$

$$|u| + |v| = |\alpha v| + |v| = (1+|\alpha|)|v| \tag{4}$$

Thus the triangle inequality becomes an equality if

$$|1+\alpha| = 1 + |\alpha| \tag{5}$$

which occurs if α is real and $\alpha \geq 0$. In terms of vectors as arrows in 3-d space, this condition is equivalent to the two vectors being parallel and pointing in the same direction (rather than in opposite directions).

To see that equality doesn't happen if α is complex, suppose $\alpha = 1 + i$. Then

$$|1+\alpha| = |2+i| = \sqrt{5} \tag{6}$$

$$1 + |\alpha| = 1 + \sqrt{2} \tag{7}$$

VECTOR SPACES - NUMBER OF DIMENSIONS

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References: Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Exercises 1.4.1 - 1.4.2.

Post date: 5 Nov 2016

Here are a couple of theorems that arise from the subspace theorem we proved earlier, which is:

If U is a subspace of V, then $V = U \oplus U^{\perp}$. (Recall the direct sum.) Here, the orthogonal complement $U^{\perp}$ of U is the set of all vectors that are orthogonal to all vectors $u \in U$.

First, we can show that:

Theorem 1. *The dimensionality of a vector space is $n_{\perp}$, the maximum number of mutually orthogonal vectors in the space.*

Proof. The set of mutually orthogonal vectors is linearly independent, and since it is the largest such set, any vector $v \in V$ can be written as a linear combination of them. Thus the dimension of the space cannot be greater than $n_{\perp}$. Since the set is linearly dependent, no member of the set can be written as a linear combination of the remaining members of the set, so the dimension can't be less than $n_{\perp}$. Thus the dimension must be equal to $n_{\perp}$. □

Now we look at a couple of other theorems.

Theorem 2. *In a vector space V^n of dimension n, the set $V_{\perp}$ of all vectors orthogonal to any specific vector $v \neq |0\rangle$ forms a subspace V^{n-1} of dimension $n-1$.*

Proof. From the subspace theorem above, if we take U to be the subspace spanned by v, then $U^{\perp}$ is the orthogonal subspace. Since the dimension of U is 1 and $V^n = U \oplus U^{\perp}$, the dimension of $U^{\perp} = V^{n-1}$ is $n-1$. □

Theorem 3. *Given two subspaces $V_1^{n_1}$ and $V_2^{n_2}$ such that every vector $v_1 \in V_1$ is orthogonal to every vector $v_2 \in V_2$, the dimension of $V_1 \oplus V_2$ is $n_1 + n_2$.*

Proof. An orthonormal basis of V_1 consists of n_1 mutually orthogonal vectors in V_1, and similarly, an orthonormal basis of V_2 consists of n_2 mutually orthogonal vectors in V_2. These bases consist of the maximum number of mutually orthogonal vectors in their respective spaces. In the direct sum $V_1 \oplus V_2$, we therefore have a set of $n_1 + n_2$ mutually orthogonal vectors,

which is the maximum number of such vectors in $V_1 \oplus V_2$. This follows because a vector $w \in V_1 \oplus V_2$ must be a linear combination of a vector $v_1 \in V_1$ and a vector $v_2 \in V_2$, where v_i is, in turn, a linear combination of the basis of space V_i. Thus $w = v_1 + v_2$ must be a linear combination of vectors from the two bases combined. Hence the dimension of $V_1 \oplus V_2$ is $n_1 + n_2$. $\square$

ROTATION MATRICES - MATRIX ELEMENTS

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References: Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Exercise 1.6.1.

Post date: 5 Nov 2016

We can represent a linear operator $\mathbf{\Omega}$ by its matrix representation in a given basis. If the basis e_i is orthonormal then the matrix elements are given by

$$\mathbf{\Omega}_{ij} = \langle e_i | \mathbf{\Omega} | e_j \rangle \tag{1}$$

The rotation operator $R\left(\frac{\pi}{2}\mathbf{i}\right)$ that rotates vectors by $\frac{\pi}{2}$ about the x axis can be written in terms of the orthonormal basis consisting of the unit vectors $|1\rangle, |2\rangle, |3\rangle$ along the three coordinate axes by examining the effect that it has on each vector in the basis. It leaves $|1\rangle$ unchanged, rotates $|2\rangle$ into $|3\rangle$, and $|3\rangle$ into $-|2\rangle$ so we have

$$R\left(\frac{\pi}{2}\mathbf{i}\right)|1\rangle = |1\rangle \tag{2}$$

$$R\left(\frac{\pi}{2}\mathbf{i}\right)|2\rangle = |3\rangle \tag{3}$$

$$R\left(\frac{\pi}{2}\mathbf{i}\right)|3\rangle = -|2\rangle \tag{4}$$

We can work out the matrix elements by applying 1 to these three transformation equations:

$$R\left(\frac{\pi}{2}\mathbf{i}\right) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{bmatrix} \tag{5}$$

As another example, suppose we have the matrix (also in the same basis)

$$\mathbf{\Omega} = \begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix} \tag{6}$$

This has the effects

$$\Omega|1\rangle = |2\rangle \quad (7)$$
$$\Omega|2\rangle = |3\rangle \quad (8)$$
$$\Omega|3\rangle = |1\rangle \quad (9)$$

Thus Ω cyclically permutes the three basis vectors, which is equivalent to a rotation by $\frac{2\pi}{3}$ about the line $x = y = z$.

PINGBACKS

Pingback: Unitary matrices - some examples

HERMITIAN OPERATORS - A FEW EXAMPLES

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References: Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Exercise 1.6.2.

Post date: 5 Nov 2016

Here are a few more results about hermitian operators.

Suppose we are given two hermitian operators Ω and Λ. We'll look at some combinations of these operators.

The operator $\Omega\Lambda$ has the hermitian conjugate

$$(\Omega\Lambda)^\dagger = \Lambda^\dagger\Omega^\dagger = \Lambda\Omega \tag{1}$$

Thus the product operator $\Omega\Lambda$ is hermitian only if Λ and Ω commute.

The operator $\Omega\Lambda + \lambda\Omega$ for some complex scalar λ has the hermitian conjugate

$$\begin{aligned}(\Omega\Lambda + \lambda\Omega)^\dagger &= \Lambda^\dagger\Omega^\dagger + \lambda^*\Omega^\dagger &(2)\\ &= \Lambda\Omega + \lambda^*\Omega &(3)\end{aligned}$$

This operator is therefore hermitian only if Λ and Ω commute and λ is real.

The commutator has the hermitian conjugate

$$\begin{aligned}[\Omega,\Lambda]^\dagger &= (\Omega\Lambda - \Lambda\Omega)^\dagger &(4)\\ &= \Lambda\Omega - \Omega\Lambda &(5)\\ &= [\Lambda,\Omega] &(6)\\ &= -[\Omega,\Lambda] &(7)\end{aligned}$$

Thus the commutator is anti-hermitian (the hermitian conjugate is the negative of the original operator).

Finally, what happens if we multiply the commutator by i?

$$
\begin{aligned}
\left(i\left[\Omega,\Lambda\right]\right)^{\dagger} &= -i\left(\Omega\Lambda-\Lambda\Omega\right)^{\dagger} && (8)\\
&= -i\left(\Lambda\Omega-\Omega\Lambda\right) && (9)\\
&= -i\left[\Lambda,\Omega\right] && (10)\\
&= i\left[\Omega,\Lambda\right] && (11)
\end{aligned}
$$

Thus the operator $i\left[\Omega,\Lambda\right]$ is hermitian.

UNITARY MATRICES - SOME EXAMPLES

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References: Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Exercises 1.6.3 - 1.6.6.

Post date: 5 Nov 2016

Here are a few more results about unitary operators.

Shankar defines a unitary operator U as one where

$$UU^\dagger = I \tag{1}$$

From this we can derive the other condition by which they can be defined, namely that a unitary operator preserves the norm of a vector:

$$|Uv| = |v| \tag{2}$$

This follows, for if we define the effect of U by

$$\left|v_1'\right\rangle = U\left|v_1\right\rangle \tag{3}$$

then

$$\begin{aligned} \left\langle v_1' \middle| v_1' \right\rangle &= \left\langle Uv_1 \middle| Uv_1 \right\rangle && (4)\\ &= \left\langle v_1 \middle| U^\dagger U v_1 \right\rangle && (5)\\ &= \left\langle v_1 \middle| v_1 \right\rangle && (6) \end{aligned}$$

Thus $|v_1'|^2 = |v_1|^2$.

Theorem 1. *The product of two unitary operators U_1 and U_2 is unitary.*

Proof. Using Shankar's definition 1, we have

$$\begin{aligned} \left(U_1U_2\right)^\dagger U_1U_2 &= U_2^\dagger U_1^\dagger U_1U_2 && (7)\\ &= U_2^\dagger I U_2 && (8)\\ &= U_2^\dagger U_2 && (9)\\ &= I && (10) \end{aligned}$$

□

Theorem 2. *The determinant of a unitary matrix U is a complex number with unit modulus.*

Proof. The determinant of a hermitian conjugate is the complex conjugate of the determinant of the original matrix, since $\det U = \det U^T$ (where the superscript T denotes the transpose) for any matrix, and the hermitian conjugate is the complex conjugate transpose. Therefore

$$\det\left(UU^\dagger\right) = [\det U]\,[\det U]^* = \det I = 1 \tag{11}$$

Therefore $|\det U|^2 = 1$ as required. □

Example 3. The rotation matrix $R\left(\frac{\pi}{2}\mathbf{i}\right)$ is unitary. We have

$$R\left(\frac{\pi}{2}\mathbf{i}\right) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{bmatrix} \tag{12}$$

By direct calculation

$$RR^\dagger = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{bmatrix} \tag{13}$$

$$= \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} = I \tag{14}$$

Example 4. Consider the matrix

$$U = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & i \\ i & 1 \end{bmatrix} \tag{15}$$

By calculating

$$UU^\dagger = \frac{1}{2} \begin{bmatrix} 1 & i \\ i & 1 \end{bmatrix} \begin{bmatrix} 1 & -i \\ -i & 1 \end{bmatrix} \tag{16}$$

$$= \frac{1}{2} \begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix} = I \tag{17}$$

Thus U is unitary, but because $U \neq U^\dagger$ it is not hermitian. Its determinant is

$$\det U = \left(\frac{1}{\sqrt{2}}\right)^2 \left(1 - i^2\right) = 1 \tag{18}$$

This is of the required form $e^{i\theta}$ with $\theta = 0$.

Example 5. Consider the matrix

$$U = \frac{1}{2}\begin{bmatrix} 1+i & 1-i \\ 1-i & 1+i \end{bmatrix} \tag{19}$$

$$UU^\dagger = \frac{1}{4}\begin{bmatrix} 1+i & 1-i \\ 1-i & 1+i \end{bmatrix}\begin{bmatrix} 1-i & 1+i \\ 1+i & 1-i \end{bmatrix} \tag{20}$$

$$= \frac{1}{4}\begin{bmatrix} 4 & 0 \\ 0 & 4 \end{bmatrix} = I \tag{21}$$

Thus U is unitary, but because $U \neq U^\dagger$ it is not hermitian. Its determinant is

$$\det U = \left(\frac{1}{2}\right)^2 \left[(1+i)^2 - (1-i)^2\right] \tag{22}$$

$$= i \tag{23}$$

This is of the required form $e^{i\theta}$ with $\theta = \frac{\pi}{2}$.

PINGBACKS

Pingback: Spectral theorem for normal operators
Pingback: Time-dependent propagators

UNITARY OPERATORS: ACTIVE AND PASSIVE TRANSFORMATIONS OF AN OPERATOR

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

References: Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Exercises 1.7.1 - 1.7.2.

Post date: 10 Nov 2016

A unitary operator transforms one orthonormal basis to another. Therefore if we have an operator Ω with matrix elements $\Omega_{ij}\left(\{f\}\right) = \langle f_i \left|\Omega\right| f_j\rangle$ in one orthonormal basis $(f_1, \ldots, f_n)$, we can transform the basis to another orthonormal basis $(e_1, \ldots, e_n)$ by a unitary transformation U so that

$$|e_i\rangle = U\,|f_i\rangle \tag{1}$$

This results in a transformation of the operator Ω's matrix elements:

$$\begin{aligned}\Omega_{ij}\left(\{e\}\right) &= \langle e_i \left|\Omega\right| e_j\rangle &(2)\\ &= \langle U f_i \left|\Omega\right| U f_j\rangle &(3)\\ &= \left\langle f_i \left| U^\dagger \Omega U \right| f_j \right\rangle &(4)\end{aligned}$$

Thus we can view the transformation as either a transformation of the basis vectors $e_i = U f_i$, known as an *active transformation*, or as a transformation of the operator according to $\Omega \rightarrow U^\dagger \Omega U$, known as a *passive transformation*. The matrix elements of $U^\dagger \Omega U$ in the original basis $\{f\}$ are equal to the matrix elements of the original operator Ω in the new basis $\{e\}$.

We've already seen a few results about the trace and determinant of products of matrices. We'll list these here for reference:

- $\mathrm{Tr}\left(\Omega\Lambda\right) = \mathrm{Tr}\left(\Lambda\Omega\right)$. That is, even if the operators don't commute, the trace of a product of operators doesn't depend on the order of the operators in the product.
- The trace of a product of 3 or more operators is invariant under cyclic permutation. $\mathrm{Tr}\left(\Omega\Lambda\theta\right) = \mathrm{Tr}\left(\Lambda\theta\Omega\right) = \mathrm{Tr}\left(\theta\Omega\Lambda\right)$. This follows directly from the previous result. For example, we can define $A \equiv \Lambda\theta$ so that $\mathrm{Tr}\left(\Omega\Lambda\theta\right) = \mathrm{Tr}\left(\Omega A\right) = \mathrm{Tr}\left(A\Omega\right) = \mathrm{Tr}\left(\Lambda\theta\Omega\right)$.
- The determinant of a unitary matrix is a complex number with modulus 1.

We can use these to prove a couple of further results about unitary transformations.

The trace of an operator is invariant under a unitary transformation:

$$\mathrm{Tr}\left(U^\dagger \Omega U\right) = \mathrm{Tr}\left(U U^\dagger \Omega\right) = \mathrm{Tr}\Omega \tag{5}$$

since $UU^\dagger = I$.

Finally, the determinant of an operator is also invariant under a unitary transformation. Since the determinant of a product is the product of the determinants,

$$\det\left(U^\dagger \Omega U\right) = \det U^\dagger \det\Omega \det U \tag{6}$$

$$= e^{-i\alpha} \det\Omega e^{i\alpha} \tag{7}$$

$$= \det\Omega \tag{8}$$

In the second line we used the fact that $\det U$ is a complex number with unit modulus, and the fact that $\det U^\dagger = (\det U)^*$.

PINGBACKS

Pingback: Hermitian matrices - example with 4 matrices

Pingback: Linear chain of oscillators - External force, unitary operator

EIGENVALUES AND EIGENVECTORS - EXAMPLES

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

References: Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Exercises 1.8.1 - 1.8.4.

Post date: 10 Nov 2016

Here are a few examples of calculating eigenvalues and eigenvectors.

Example 1. Find the eigenvalues and normalized eigenvectors of

$$\Omega = \begin{bmatrix} 1 & 3 & 1 \\ 0 & 2 & 0 \\ 0 & 1 & 4 \end{bmatrix} \tag{1}$$

The eigenvalues are solutions of $\det(\Omega - \lambda I) = 0$ which gives, calculating the determinant down the first column:

$$\begin{aligned} (1-\lambda)(2-\lambda)(4-\lambda) &= 0 && (2) \\ \lambda &= 1, 2, 4 && (3) \end{aligned}$$

The eigenvectors v_i satisfy $(\Omega - \lambda_i I) v_i = 0 v_i$ for each eigenvalue λ_i. We get, for $\lambda_1 = 1$:

$$\begin{bmatrix} 0 & 3 & 1 \\ 0 & 1 & 0 \\ 0 & 1 & 3 \end{bmatrix} \begin{bmatrix} a \\ b \\ c \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} \tag{4}$$

Solving, we find

$$\begin{aligned} b &= c = 0 && (5) \\ a &= \text{anything} && (6) \end{aligned}$$

Thus a normalized eigenvector is

$$v_1 = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \tag{7}$$

For $\lambda_2 = 2$, we have

$$\begin{bmatrix} -1 & 3 & 1 \\ 0 & 0 & 0 \\ 0 & 1 & 2 \end{bmatrix} \begin{bmatrix} a \\ b \\ c \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} \tag{8}$$

Solving:

$$\begin{aligned} b &= -2c && (9)\\ a &= 3b+c && (10)\\ &= -5c && (11) \end{aligned}$$

Choosing $c = 1$ and normalizing, we have

$$v_2 = \frac{1}{\sqrt{30}} \begin{bmatrix} -5 \\ -2 \\ 1 \end{bmatrix} \tag{12}$$

Finally, for $\lambda_3 = 4$ we have

$$\begin{bmatrix} -3 & 3 & 1 \\ 0 & -2 & 0 \\ 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} a \\ b \\ c \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} \tag{13}$$

Solving:

$$\begin{aligned} b &= 0 && (14)\\ 3a &= 3b+c && (15)\\ &= c && (16) \end{aligned}$$

Choosing $a = 1$ and normalizing:

$$v_3 = \frac{1}{\sqrt{10}} \begin{bmatrix} 1 \\ 0 \\ 3 \end{bmatrix} \tag{17}$$

The matrix Ω is not Hermitian since $\Omega^\dagger \neq \Omega$, and we can see by inspection that the eigenvectors are not orthogonal.

Example 2. Now we have

$$\Omega = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix} \tag{18}$$

It is hermitian since $\Omega^\dagger = \Omega^T = \Omega$. The eigenvalues are found from

$$(-\lambda)^3 + \lambda = 0 \tag{19}$$
$$\lambda = 0, -1, 1 \tag{20}$$

Solving for the eigenvectors in the same way as in the last example, we get, for $\lambda_i = 0, -1, 1$ in that order:

$$v_1 = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} \tag{21}$$
$$v_2 = \frac{1}{\sqrt{2}} \begin{bmatrix} -1 \\ 0 \\ 1 \end{bmatrix} \tag{22}$$
$$v_3 = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix} \tag{23}$$

The eigenvectors are orthogonal, as required for a hermitian matrix. We can diagonalize Ω by means of a unitary transformation U, where the columns of U are the eigenvectors of Ω. We have

$$U = \begin{bmatrix} 0 & -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ 1 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix} \tag{24}$$
$$U^\dagger = \begin{bmatrix} 0 & 1 & 0 \\ -\frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \end{bmatrix} \tag{25}$$

We can verify by direct matrix multiplication that

$$U^\dagger \Omega U = \begin{bmatrix} 0 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \tag{26}$$

Note that the order of eigenvalues in the diagonal is determined by the order in which we place the columns in U.

Example 3. We now have the hermitian matrix

$$\Omega = \frac{1}{2} \begin{bmatrix} 2 & 0 & 0 \\ 0 & 3 & -1 \\ 0 & -1 & 3 \end{bmatrix} \tag{27}$$

The eigenvectors follow from

$$(1-\lambda)\left[\left(\frac{3}{2}-\lambda\right)^2-\frac{1}{4}\right] = 0 \tag{28}$$

$$\lambda = 1,1,2 \tag{29}$$

Thus the eigenvalue $\lambda = 1$ is degenerate. We can find the eigenvector corresponding to $\lambda_3 = 2$ in the usual way and get

$$v_3 = \frac{1}{\sqrt{2}}\begin{bmatrix} 0 \\ -1 \\ 1 \end{bmatrix} \tag{30}$$

The other two eigenvectors span a 2-d subspace that must be orthogonal to v_3 (since Ω is hermitian; in the more general case, the orthogonality is not guaranteed). We can therefore find two vectors v_1, v_2 in the subspace by requiring $\langle v_1, v_3\rangle = \langle v_2, v_3\rangle = 0$. That is, if

$$v_{1,2} = \begin{bmatrix} a \\ b \\ c \end{bmatrix} \tag{31}$$

we must have

$$a = \text{anything} \tag{32}$$

$$b = c \tag{33}$$

These two equations can be satisfied by a variety of v_1 and v_2, but if we want $\langle v_1, v_2\rangle = 0$ as well, we can choose $a = 1$ and $b = c = 1$, then normalize, to get

$$v_1 = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \tag{34}$$

$$v_2 = \frac{1}{\sqrt{2}}\begin{bmatrix} 0 \\ 1 \\ 1 \end{bmatrix} \tag{35}$$

The 2-d subspace spanned by v_1 and v_2 is therefore

$$v = av_1 + bv_2 = \begin{bmatrix} a \\ b \\ b \end{bmatrix} \tag{36}$$

Thus any normalized eigenvector of $\lambda = 1$ has the form

$$e = \frac{1}{\sqrt{a^2 + 2b^2}} \begin{bmatrix} a \\ b \\ b \end{bmatrix} \tag{37}$$

Example 4. Now let's look at a non-hermitian matrix:

$$\Omega = \begin{bmatrix} 4 & 1 \\ -1 & 2 \end{bmatrix} \tag{38}$$

The eigenvalues are found from

$$\begin{aligned} (4-\lambda)(2-\lambda)+1 &= 0 && (39) \\ (\lambda-3)^2 &= 0 && (40) \\ \lambda &= 3,3 && (41) \end{aligned}$$

Thus there is one degenerate eigenvalue. To find the eigenvector(s), we solve $(\Omega - \lambda I)\, v = 0$ as usual:

$$\begin{bmatrix} 1 & 1 \\ -1 & -1 \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = 0 \tag{42}$$

This gives only one condition, namely $a = -b$. Thus there is only one normalized eigenvector:

$$v = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -1 \end{bmatrix} \tag{43}$$

EIGENVALUES AND EIGENVECTORS OF THE 2-D ROTATION OPERATOR

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

References: Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Exercise 1.8.5.

Post date: 11 Nov 2016

The 2-d rotation operator in matrix form relative to the basis of unit vectors along the x and y axes is

$$\Omega = \begin{bmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{bmatrix} \tag{1}$$

In a real vector space, this matrix has no eigenvectors, since no vector in the xy plane is left unaltered (unless θ is a multiple of 2π). However, in a complex vector space, it does have a couple of eigenvectors, as we can see by direct calculation. The eigenvectors are solutions of

$$\begin{aligned} (\cos\theta - \lambda)^2 + \sin^2\theta &= 0 && (2) \\ \lambda &= \cos\theta \pm i\sin\theta && (3) \\ &= e^{\pm i\theta} && (4) \end{aligned}$$

The eigenvectors are found from $(\Omega - \lambda I)\, v = 0$ so we get

$$\begin{aligned} \begin{bmatrix} \mp i\sin\theta & \sin\theta \\ -\sin\theta & \mp i\sin\theta \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} &= \begin{bmatrix} 0 \\ 0 \end{bmatrix} && (5) \\ \begin{bmatrix} \mp i & 1 \\ -1 & \mp i \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} &= \begin{bmatrix} 0 \\ 0 \end{bmatrix} && (6) \\ a &= \mp ib && (7) \end{aligned}$$

The two normalized eigenvectors are therefore

$$\begin{aligned} v_1 &= \frac{1}{\sqrt{2}} \begin{bmatrix} -i \\ 1 \end{bmatrix} && (8) \\ v_2 &= \frac{1}{\sqrt{2}} \begin{bmatrix} i \\ 1 \end{bmatrix} && (9) \end{aligned}$$

They are orthogonal, since $\langle v_1, v_2 \rangle = 0$.

We can form a matrix U out of the eigenvectors of Ω:

$$U = \frac{1}{\sqrt{2}} \begin{bmatrix} -i & i \\ 1 & 1 \end{bmatrix} \tag{10}$$

$$U^\dagger = \frac{1}{\sqrt{2}} \begin{bmatrix} i & 1 \\ -i & 1 \end{bmatrix} \tag{11}$$

U is unitary, as we can verify by calculating $UU^\dagger = I$.

By direct calculation, we find that

$$U^\dagger \Omega U = \begin{bmatrix} e^{i\theta} & 0 \\ 0 & e^{-i\theta} \end{bmatrix} \tag{12}$$

[A word of caution to anyone using Maple to do matrix calculations. The Adjoint operation in Maple's LinearAlgebra package does NOT correspond to the adjoint (that is, the hermitian conjugate) as used in physics. To calculate the hermitian conjugate, use the Dagger operation in Maple's Physics package.]

DETERMINANT AND TRACE OF NORMAL OPERATORS

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References: Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Exercises 1.8.6 - 1.8.7.

Post date: 11 Nov 2016

The spectral theorem for states that any normal operator Ω in a complex vector space is unitarily diagonalizable, that is

$$D_M = U^\dagger \Omega U \tag{1}$$

where U is a unitary operator and D_M is a diagonal matrix, whose diagonal elements are the eigenvalues ω_i of Ω. We can use this to derive a couple of relations about the trace and determinant of normal operators. Remember that hermitian and unitary operators are both normal.

Since the determinant is invariant under a unitary transformation, we have

$$\begin{aligned} \det D_M &= \det\left(U^\dagger \Omega U\right) && (2)\\ &= \det U^\dagger \det\Omega \det U && (3)\\ &= e^{-i\alpha} \times \det\Omega \times e^{i\alpha} && (4)\\ &= \det\Omega && (5) \end{aligned}$$

where we've used the facts that the determinant of a product is the product of the determinants, and the determinant of a unitary matrix is a complex number $e^{i\alpha}$ with unit modulus. Since the determinant of a diagonal matrix is the product of its diagonal elements, we see that for a normal matrix, its determinant is the product of its eigenvalues:

$$\det\Omega = \prod_i \omega_i \tag{6}$$

The trace of a product is equal to the trace of a cyclic permutation of that product, so we have

$$\begin{aligned} \mathrm{Tr}D_M &= \mathrm{Tr}\left(U^\dagger \Omega U\right) && (7)\\ &= \mathrm{Tr}\left(UU^\dagger \Omega\right) && (8)\\ &= \mathrm{Tr}\Omega && (9) \end{aligned}$$

Therefore, the trace of a normal operator is the sum of its eigenvalues:

$$\mathrm{Tr}\Omega = \sum_i \omega_i \tag{10}$$

We can use these two results as an alternative way to calculate the eigenvalues of a normal matrix. For example, suppose

$$\Omega = \begin{bmatrix} 1 & 2 \\ 2 & 1 \end{bmatrix} \tag{11}$$

We have

$$\begin{aligned} \det\Omega &= -3 = \omega_1\omega_2 && (12)\\ \mathrm{Tr}\Omega &= 2 = \omega_1 + \omega_2 && (13) \end{aligned}$$

Solving these two equations gives

$$\begin{aligned} -3 &= (2-\omega_2)\,\omega_2 && (14)\\ \omega &= -1, 3 && (15) \end{aligned}$$

We can also calculate them using the old determinant formula $\det(\Omega - \omega I) = 0$:

$$\begin{aligned} (1-\omega)^2 - 4 &= 0 && (16)\\ \omega &= -1, 3 && (17) \end{aligned}$$

PINGBACKS

Pingback: Hermitian matrices - example with 4 matrices

HERMITIAN MATRICES - EXAMPLE WITH 4 MATRICES

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References: Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Exercise 1.8.8.

Post date: 11 Nov 2016

Suppose we have four hermitian matrices M^i for $i = 1, 2, 3, 4$ that obey the relation

$$M^i M^j + M^j M^i = 2\delta^{ij} I \tag{1}$$

We can find the possible eigenvalues as follows. Suppose we choose an orthonormal basis (such a basis always exists for a hermitian matrix) $\{e\}$in which M^i is diagonal for one particular value of i. That is, for a basis vector $|e_k\rangle$ in this basis, we have $M^i |e_k\rangle = \omega_k^i |e_k\rangle$, where ω_k^i is the kth eigenvalue of M^i.

Then with $i = j$ above, we have

$$\begin{aligned} 2\left(M^i\right)^2 &= 2I & (2)\\ \left(M^i\right)^2 &= I & (3) \end{aligned}$$

Operating on a vector e from this basis, we get

$$\begin{aligned} \left(M^i\right)^2 |e_k\rangle &= |e_k\rangle & (4)\\ &= \left(\omega_k^i\right)^2 |e_k\rangle & (5) \end{aligned}$$

Therefore, the possible values of ω_k^i are ± 1. We didn't choose any particular value for i, so this is true of all four matrices.

Now, for $i \neq j$ we have

$$M^i M^j = -M^j M^i \tag{6}$$

We can find the trace of M^j as follows. Assuming $i \neq j$

$$\begin{aligned}
\mathrm{Tr}M^j &= \mathrm{Tr}\left(M^i M^i M^j\right) && (7)\\
&= -\mathrm{Tr}\left(M^i M^j M^i\right) && (8)\\
&= -\mathrm{Tr}\left(M^i M^i M^j\right) && (9)\\
&= -\mathrm{Tr}M^j && (10)
\end{aligned}$$

In line 1 we used 3, in line 2 we used 6 and in line 3 we used the cyclic property of the trace. Thus $\mathrm{Tr}M^j = -\mathrm{Tr}M^j = 0$.

Since each M^j has zero trace, the trace is the sum of the eigenvalues and the possible eigenvalues are ± 1, the eigenvalue $+1$ must occur the same number of times as -1, meaning that each M^j must have an even number of eigenvalues, so the matrices must be even-dimensional.

PINGBACKS

Pingback: Dirac equation: derivation

ANGULAR MOMENTUM AS AN EIGENVECTOR PROBLEM

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To leave a comment or report an error, please use the auxiliary blog.

References: Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Exercise 1.8.9.

Post date: 12 Nov 2016

The angular momentum in classical mechanics of a collection of point masses m_a located at positions $\mathbf{r}_a$ and moving with a common angular velocity $\boldsymbol{\omega}$ about a common axis is given by

$$\mathbf{L} = \sum_a m_a \left(\mathbf{r}_a \times \mathbf{v}_a\right) \tag{1}$$

where $\mathbf{v}_a = \boldsymbol{\omega} \times \mathbf{r}_a$ is the linear velocity of m_a. We can use the vector identity

$$\mathbf{A} \times (\mathbf{B} \times \mathbf{C}) = \mathbf{B}\left(\mathbf{A} \cdot \mathbf{C}\right) - \mathbf{C}\left(\mathbf{A} \cdot \mathbf{B}\right)$$

to write

$$\begin{aligned} \mathbf{r}_a \times \mathbf{v}_a &= \mathbf{r}_a \times (\boldsymbol{\omega} \times \mathbf{r}_a) && (2)\\ &= r_a^2 \boldsymbol{\omega} - \mathbf{r}_a \left(\mathbf{r}_a \cdot \boldsymbol{\omega}\right) && (3) \end{aligned}$$

In terms of components, this is

$$\begin{aligned} \left[\mathbf{r}_a \times \mathbf{v}_a\right]_i &= r_a^2 \omega_i - \left(r_a\right)_i \sum_j \left(r_a\right)_j \omega_j && (4)\\ &= \sum_j \left[r_a^2 \omega_j \delta_{ij} - \left(r_a\right)_i \left(r_a\right)_j \omega_j\right] && (5)\\ &= \sum_j \left[r_a^2 \delta_{ij} - \left(r_a\right)_i \left(r_a\right)_j\right] \omega_j && (6) \end{aligned}$$

We can therefore write the angular momentum as

$$\begin{aligned} \mathbf{L}_i &= \sum_j \sum_a m_a \left[r_a^2 \delta_{ij} - \left(r_a\right)_i \left(r_a\right)_j\right] \omega_j && (7)\\ &\equiv \sum_j M_{ij} \omega_j && (8) \end{aligned}$$

where the matrix M is

$$M_{ij} \equiv \sum_a m_a \left[r_a^2 \delta_{ij} - (r_a)_i (r_a)_j \right] \tag{9}$$

From the definition, we see that M is real and symmetric (interchanging i and j shows that $M_{ij} = M_{ji}$), so M is hermitian.

In Dirac's notation, we have the matrix equation

$$|L\rangle = M |\omega\rangle \tag{10}$$

From this equation, we can see that $\mathbf{L}$ and $\boldsymbol{\omega}$ are parallel only if $\boldsymbol{\omega}$ is an eigenvector of M. If the eigenvalues of M are non-degenerate, there are therefore three directions for $\boldsymbol{\omega}$ such that $\mathbf{L}$ and $\boldsymbol{\omega}$ are parallel, and these directions can be found by solving for the eigenvectors of M.

If some of the eigenvalues are degenerate, then there is a range of directions over which $\mathbf{L}$ and $\boldsymbol{\omega}$ can be parallel. In the case of a sphere, all 3 eigenvalues of M must be the same, as all directions are axes of symmetry of the sphere.

As an example, suppose we have only one mass $m = 1$ with position

$$\mathbf{r} = [1, 1, 0] \tag{11}$$

We can work out M by substituting into 9:

$$M = \begin{bmatrix} 1 & -1 & 0 \\ -1 & 1 & 0 \\ 0 & 0 & 2 \end{bmatrix} \tag{12}$$

The eigenvalues are 0, 2 and 2 with corresponding eigenvectors

$$|\lambda = 0\rangle = \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix} \tag{13}$$

$$|\lambda = 2\rangle = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}, \begin{bmatrix} -1 \\ 1 \\ 0 \end{bmatrix} \tag{14}$$

Thus if $\boldsymbol{\omega}$ is a linear combination of the two eigenvectors for $\lambda = 2$, it will be parallel to $\mathbf{L}$. If $\boldsymbol{\omega}$ is parallel to $\begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix}$, $\mathbf{L} = 0$, as in this case $\boldsymbol{\omega}$ is parallel to $\mathbf{r}$ so $\boldsymbol{\omega} \times \mathbf{r} = 0$, and the mass is located on the axis of rotation so has no angular momentum.

SIMULTANEOUS DIAGONALIZATION OF HERMITIAN MATRICES

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To leave a comment or report an error, please use the auxiliary blog.

References: Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Exercise 1.8.10.

Post date: 13 Nov 2016

The spectral theorem guarantees that any normal operator can be unitarily diagonalized. For commuting hermitian operators we can go one step further and show that a set of such operators can be simultaneously diagonalized with a single unitary transformation. The proof is a bit lengthy and is spelled out in full both in Zwiebach's notes (chapter 6) and in Shankar's book (chapter 1, theorem 13) so I won't reproduce it in full here. To summarize the main points:

We can start by considering two operators Ω and Λ and assume that at least one of them, say Ω, is nondegenerate, that is, for each eigenvalue there is only one eigenvector (up to multiplication by a scalar). Then for one eigenvalue ω_i of Ω we have

$$\Omega \left|\omega_i\right\rangle = \omega_i \left|\omega_i\right\rangle \tag{1}$$

We also have

$$\Lambda\Omega \left|\omega_i\right\rangle = \omega_i\Lambda \left|\omega_i\right\rangle \tag{2}$$

so that, provided $[\Lambda, \Omega] = 0$, $\Lambda \left|\omega_i\right\rangle$ is also an eigenvector of Ω for eigenvalue ω_i. However, since Ω is nondegenerate, $\Lambda \left|\omega_i\right\rangle$ must be a multiple of $\left|\omega_i\right\rangle$ so that, we have

$$\Lambda \left|\omega_i\right\rangle = \lambda_i \left|\omega_i\right\rangle \tag{3}$$

so that $\left|\omega_i\right\rangle$ is an eigenvector of Λ for eigenvalue λ_i. Therefore a unitary transformation that diagonalizes Ω will also diagonalize Λ. Note that in this case we didn't need to assume that Λ is nondegenerate.

If both Ω and Λ are degenerate, things are a bit more complicated, but the basic idea is this. Suppose we find a basis that diagonalizes Ω and arrange the basis vectors within the unitary matrix U in an order that groups all equal eigenvalues together, so that all the eigenvectors corresponding to eigenvalue ω_1 occur first, followed by all the eigenvectors corresponding to eigenvalue ω_2 and so on, up to eigenvalue ω_m where $m < n$ is the number

of distinct eigenvalues (which is less than the dimension n of the matrix Ω because Ω is degenerate).

Each subset of eigenvectors corresponding to a single eigenvalue forms a subspace, and we can show that the other matrix Λ, operating on a vector from that subspace transforms the vector to another vector that also lies within the same subspace. Now, any linearly independent selection of basis vectors within the subspace will still diagonalize Ω for that eigenvalue, so we can select such a set of basis vectors within that subspace that also diagonalizes Λ within that subspace. The process can be repeated for each eigenvalue of Ω resulting in a set of basis vectors that diagonalizes both matrices.

Obviously, I've left out the technical details of just how this is done, but you can refer to either Zwiebach's notes or Shankar's book for the details.

As an example, consider the two matrices

$$\Omega = \begin{bmatrix} 1 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 1 \end{bmatrix} \tag{4}$$

$$\Lambda = \begin{bmatrix} 2 & 1 & 1 \\ 1 & 0 & -1 \\ 1 & -1 & 2 \end{bmatrix} \tag{5}$$

We can verify that they commute:

$$\Omega\Lambda = \Lambda\Omega = \begin{bmatrix} 3 & 0 & 3 \\ 0 & 0 & 0 \\ 3 & 0 & 3 \end{bmatrix} \tag{6}$$

We can find the eigenvalues and eigenvectors of Ω and Λ in the usual way. For Ω we have

$$\det(\Omega - \omega I) = 0 \tag{7}$$

$$(1-\omega)\left[(-\omega(1-\omega))\right] + \omega = 0 \tag{8}$$

$$\omega\left(2\omega - \omega^2\right) = 0 \tag{9}$$

$$\omega = 0, 0, 2 \tag{10}$$

Solving the eigenvector equation, we get, for $\omega = 0$

$$(\Omega - \omega I)\begin{bmatrix} a \\ b \\ c \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} \tag{11}$$

$$\begin{bmatrix} 1 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 1 \end{bmatrix}\begin{bmatrix} a \\ b \\ c \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} \tag{12}$$

$$a = -c \tag{13}$$

$$b = \text{anything} \tag{14}$$

Thus 2 orthonormal eigenvectors are

$$|0_1\rangle = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ 0 \\ -1 \end{bmatrix} \tag{15}$$

$$|0_2\rangle = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} \tag{16}$$

For $\omega = 2$:

$$\begin{bmatrix} -1 & 0 & 1 \\ 0 & -2 & 0 \\ 1 & 0 & -1 \end{bmatrix}\begin{bmatrix} a \\ b \\ c \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} \tag{17}$$

$$a = c \tag{18}$$

$$b = 0 \tag{19}$$

$$|2\rangle = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix} \tag{20}$$

For Λ, we can go through the same procedure to find

$$\det(\Lambda - \lambda I) = 0 \tag{21}$$

$$-\lambda(2-\lambda)^2 + \lambda - 2 + \lambda - 2 - 2 + \lambda = 0 \tag{22}$$

$$(\lambda - 2)[\lambda(2-\lambda) + 3] = 0 \tag{23}$$

$$\lambda = -1, 2, 3 \tag{24}$$

We could calculate the eigenvectors from scratch, but from the simultaneous diagonalization theorem, we know that the eigenvector $|2\rangle$ from Ω must be an eigenvector of Λ, and we find by direct calculation that

$$\Lambda\,|2\rangle = 3\,|2\rangle \tag{25}$$

so $|2\rangle$ is the eigenvector for $\lambda = 3$.

For the other two eigenvalues of Λ, we know the eigenvectors must be linear combinations of $|0_1\rangle$ and $|0_2\rangle$ from Ω. Such a combination must have form

$$a\,|0_1\rangle + b\,|0_2\rangle = \begin{bmatrix} a \\ b \\ -a \end{bmatrix} \tag{26}$$

so we must have

$$\Lambda \begin{bmatrix} a \\ b \\ -a \end{bmatrix} = \begin{bmatrix} a+b \\ 2a \\ -a-b \end{bmatrix} = \lambda \begin{bmatrix} a \\ b \\ -a \end{bmatrix} \tag{27}$$

for $\lambda = -1, 2$. For $\lambda = 2$, we have

$$a = b \tag{28}$$

$$|\lambda = 2\rangle = \frac{1}{\sqrt{3}} \begin{bmatrix} 1 \\ 1 \\ -1 \end{bmatrix} \tag{29}$$

For $\lambda = -1$:

$$b = -2a \tag{30}$$

$$|\lambda = -1\rangle = \frac{1}{\sqrt{6}} \begin{bmatrix} 1 \\ -2 \\ -1 \end{bmatrix} \tag{31}$$

The columns of the unitary transformation matrix are therefore given by 29, 31 and 20, so we have

$$U = \begin{bmatrix} \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{3}} & -\frac{2}{\sqrt{6}} & 0 \\ -\frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{6}} & \frac{1}{\sqrt{2}} \end{bmatrix} \tag{32}$$

$$U^\dagger = \begin{bmatrix} \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{3}} \\ \frac{1}{\sqrt{6}} & -\frac{2}{\sqrt{6}} & -\frac{1}{\sqrt{6}} \\ \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \end{bmatrix} \tag{33}$$

By matrix multiplication, we can verify that this transformation diagonalizes both Ω and Λ:

$$U^\dagger \Omega U = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 2 \end{bmatrix} \tag{34}$$

$$U^\dagger \Lambda U = \begin{bmatrix} 2 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 3 \end{bmatrix} \tag{35}$$

PINGBACKS

Pingback: Coupled masses on springs - properties of the propagator

Pingback: Adding two spin-1/2 systems - product and total-s bases

Pingback: Nonrelativistic field theory - number, creation and annihilation operators

COUPLED MASSES ON SPRINGS - A SOLUTION USING MATRIX DIAGONALIZATION

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

References: Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Exercise 1.8.11.

Post date: 14 Nov 2016

Here's a practical example of how changing the basis by diagonalizing a hermitian matrix can make a problem easier to solve. Suppose we have two identical masses m free to slide in one dimension on a frictionless horizontal surface. The two masses are connected to 3 springs, with the spring on the left attached to a solid support at one end and to mass #1 at the other, the middle spring connected between the two masses, and the spring on the right connected to mass #2 at one end and to a solid support at the other. The springs all have spring constant k. Define two coordinates x_1 and x_2 to be the positions of the two masses, with $x_i = 0$ corresponding to the location at which mass i is at rest in equilibrium.

Now suppose that the two masses are displaced from their respective equilibrium points, so that x_1 and x_2 are non-zero. The length of the spring to the left of mass 1 is changed (stretched or compressed, depending on the sign of x_1) by x_1, so exerts a force $F_1 = -kx_1$ on mass 1. The length of the spring in the middle is changed by $x_2 - x_1$, so it exerts a force $F_{12} = k(x_2 - x_1)$ on mass 1, and an equal and opposite force $F_{21} = -k(x_2 - x_1)$ on mass 2. Finally, the length of the spring on the right is changed by x_2 and exerts a force $F_2 = -kx_2$ on mass 2. By applying Newton's law $F = ma$, we get the set of equations of motion:

$$\ddot{x}_1 = -2\frac{k}{m}x_1 + \frac{k}{m}x_2 \tag{1}$$

$$\ddot{x}_2 = \frac{k}{m}x_1 - 2\frac{k}{m}x_2 \tag{2}$$

While it's possible to solve such a coupled system directly, we can see how an easier method can be found by using matrix algebra. The 2 equations above can be written as a matrix equation

$$|\ddot{x}(t)\rangle = \Omega\,|x(t)\rangle \tag{3}$$

If we use the basis in which the displacement of each mass is taken to be independent of the other, we have the two basis vectors

$$|1\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \tag{4}$$

$$|2\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \tag{5}$$

In this basis

$$|x(t)\rangle = x_1(t)|1\rangle + x_2(t)|2\rangle \tag{6}$$

Here, the x_is are just numbers; the vector nature of the equation is delegated to the basis vectors.

In this basis, Ω is the operator whose matrix form is

$$\Omega = \begin{bmatrix} -2\frac{k}{m} & \frac{k}{m} \\ \frac{k}{m} & -2\frac{k}{m} \end{bmatrix} \tag{7}$$

Since Ω is hermitian, it can be diagonalized by finding its eigenvalues and normalized eigenvectors, and forming a unitary operator U whose columns are these eigenvectors. The basis vectors are now these eigenvectors $|I\rangle$ and $|II\rangle$ (I'm sticking to Shankar's notation, even though it's a bit clumsy), and they are found from $|1\rangle$ and $|2\rangle$ by applying the unitary transformation, that is

$$|I\rangle = U|1\rangle \tag{8}$$

$$|II\rangle = U|2\rangle \tag{9}$$

These transformations can be inverted:

$$|1\rangle = U^\dagger|I\rangle \tag{10}$$

$$|2\rangle = U^\dagger|II\rangle \tag{11}$$

Thus we can insert this into 3 and use $UU^\dagger = I$ to get

$$U^\dagger|\ddot{x}(t)\rangle = U^\dagger\Omega U U^\dagger|x(t)\rangle \tag{12}$$

and $U^\dagger\Omega U$ is the diagonalized version of Ω.

Shankar goes through the details of the calculation, with the results

$$|I\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix} \tag{13}$$

$$|II\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -1 \end{bmatrix} \tag{14}$$

$$U = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \tag{15}$$

$$U^{\dagger}\Omega U = \begin{bmatrix} -\omega_1^2 & 0 \\ 0 & -\omega_2^2 \end{bmatrix} \tag{16}$$

where

$$\omega_1 = \sqrt{\frac{k}{m}} \tag{17}$$

$$\omega_2 = \sqrt{\frac{3k}{m}} \tag{18}$$

Using $|I\rangle$ and $|II\rangle$ as the basis, the differential equations become decoupled, and we have

$$\ddot{x}_i + \omega_i^2 x_i = 0 \tag{19}$$

for $i = I, II$.

Second order ODEs require two initial conditions to be fully solved, and here we're assuming that both masses start off at rest, so that $\dot{x}_i(t) = 0$ for $i = I, II$. In this case, the solutions are

$$x_i(t) = x_i(0)\cos\omega_i t \tag{20}$$

for $i = I, II$.

(A full, general solution would also have a $\sin\omega_i t$ term, but this disappears because we require $\dot{x}_i(t) = 0$.)

The vector solution in the diagonal basis is therefore

$$\begin{bmatrix} x_I(t) \\ x_{II}(t) \end{bmatrix} = |I\rangle\, x_I(0)\cos\omega_I t + |II\rangle\, x_{II}(0)\cos\omega_{II} t \tag{21}$$

We now need to figure out what the coefficients $x_I(0)$ and $x_{II}(0)$ are. Assuming we know the initial position of each mass in the original basis as $x_1(0)$ and $x_2(0)$, we can find $x_I(0)$ and $x_{II}(0)$ by projecting $x_1(0)$ and $x_2(0)$ onto the basis $|I\rangle$ and $|II\rangle$. That is, we have

$$\begin{bmatrix} x_I(0) \\ x_{II}(0) \end{bmatrix} = U \begin{bmatrix} x_1(0) \\ x_2(0) \end{bmatrix} \tag{22}$$

$$= \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} x_1(0) \\ x_2(0) \end{bmatrix} \tag{23}$$

$$= \frac{1}{\sqrt{2}} \begin{bmatrix} x_1(0)+x_2(0) \\ x_1(0)-x_2(0) \end{bmatrix} \tag{24}$$

We get

$$\begin{bmatrix} x_I(t) \\ x_{II}(t) \end{bmatrix} = \frac{x_1(0)+x_2(0)}{\sqrt{2}} |I\rangle \cos\omega_I t + \frac{x_1(0)-x_2(0)}{\sqrt{2}} |II\rangle \cos\omega_{II} t \tag{25}$$

$$\begin{bmatrix} x_1(t) \\ x_2(t) \end{bmatrix} = \frac{1}{2} \begin{bmatrix} [x_1(0)+x_2(0)]\cos\sqrt{\frac{k}{m}}t + [x_1(0)-x_2(0)]\cos\sqrt{\frac{3k}{m}}t \\ [x_1(0)+x_2(0)]\cos\sqrt{\frac{k}{m}}t - [x_1(0)-x_2(0)]\cos\sqrt{\frac{3k}{m}}t \end{bmatrix} \tag{26}$$

where in the last line we substituted using 13 to write everything in terms of the original basis $|1\rangle$ and $|2\rangle$.

For the special case where the initial positions are given by $|1\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$, we have $x_1(0) = 1$ and $x_2(0) = 0$, so that

$$\begin{bmatrix} x_1(t) \\ x_2(t) \end{bmatrix} = \frac{1}{2} \begin{bmatrix} \cos\sqrt{\frac{k}{m}}t + \cos\sqrt{\frac{3k}{m}}t \\ \cos\sqrt{\frac{k}{m}}t - \cos\sqrt{\frac{3k}{m}}t \end{bmatrix} \tag{27}$$

Going back to 26, we can write the solution as a matrix equation

$$\begin{bmatrix} x_1(t) \\ x_2(t) \end{bmatrix} = \frac{1}{2} \begin{bmatrix} \cos\sqrt{\frac{k}{m}}t + \cos\sqrt{\frac{3k}{m}}t & \cos\sqrt{\frac{k}{m}}t - \cos\sqrt{\frac{3k}{m}}t \\ \cos\sqrt{\frac{k}{m}}t - \cos\sqrt{\frac{3k}{m}}t & \cos\sqrt{\frac{k}{m}}t + \cos\sqrt{\frac{3k}{m}}t \end{bmatrix} \begin{bmatrix} x_1(0) \\ x_2(0) \end{bmatrix} \tag{28}$$

The matrix with the cosines is independent of the initial state, so that once we know this matrix, we can work out the general solution as a function of time for any initial state. The matrix is known as the *propagator*. [Although Shankar uses the symbol $U(t)$ to refer to the propagator, it's *not* a unitary matrix. For example, its determinant is $\cos\left(\sqrt{\frac{k}{m}}t\right)\cos\left(\sqrt{\frac{3k}{m}}t\right) \neq 1$ for $t \neq 0$.]

PINGBACKS

Pingback: Lagrangians for harmonic oscillators
Pingback: Coupled masses on springs - properties of the propagator
Pingback: Vibrating string - normal mode analysis
Pingback: Linear chain of oscillators - Classical treatment, equations of motion

COUPLED MASSES ON SPRINGS - PROPERTIES OF THE PROPAGATOR

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

References: Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Exercise 1.8.12.

Post date: 15 Nov 2016

We'll continue our study of the system of two masses coupled by springs. The system is described by the matrix equation of motion:

$$|\ddot{x}(t)\rangle = \Omega |x(t)\rangle \tag{1}$$

where

$$|x(t)\rangle = x_1(t)|1\rangle + x_2(t)|2\rangle \tag{2}$$

in the basis

$$|1\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \tag{3}$$

$$|2\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \tag{4}$$

In this basis, Ω is the operator whose matrix form is

$$\Omega = \begin{bmatrix} -2\frac{k}{m} & \frac{k}{m} \\ \frac{k}{m} & -2\frac{k}{m} \end{bmatrix} \tag{5}$$

We found that the solution could be written as

$$\begin{bmatrix} x_1(t) \\ x_2(t) \end{bmatrix} = \frac{1}{2} \begin{bmatrix} \cos\sqrt{\frac{k}{m}}t + \cos\sqrt{\frac{3k}{m}}t & \cos\sqrt{\frac{k}{m}}t - \cos\sqrt{\frac{3k}{m}}t \\ \cos\sqrt{\frac{k}{m}}t - \cos\sqrt{\frac{3k}{m}}t & \cos\sqrt{\frac{k}{m}}t + \cos\sqrt{\frac{3k}{m}}t \end{bmatrix} \begin{bmatrix} x_1(0) \\ x_2(0) \end{bmatrix} \tag{6}$$

In compact form, we can write this as

$$|x(t)\rangle = U(t)|x(0)\rangle \tag{7}$$

where the propagator operator is defined as

$$U(t) \equiv \frac{1}{2}\begin{bmatrix} \cos\sqrt{\frac{k}{m}}t + \cos\sqrt{\frac{3k}{m}}t & \cos\sqrt{\frac{k}{m}}t - \cos\sqrt{\frac{3k}{m}}t \\ \cos\sqrt{\frac{k}{m}}t - \cos\sqrt{\frac{3k}{m}}t & \cos\sqrt{\frac{k}{m}}t + \cos\sqrt{\frac{3k}{m}}t \end{bmatrix} \tag{8}$$

From 1, we can operate on both sides of 7 with the operator $\frac{d^2}{dt^2} - \Omega$ to get

$$\left(\frac{d^2}{dt^2} - \Omega\right)|x(t)\rangle = \left(\frac{d^2}{dt^2} - \Omega\right)U(t)\,|x(0)\rangle = 0 \tag{9}$$

Since the initial positions $|x(0)\rangle$ are arbitrary and contains no time dependence, the matrix $U(t)$ satisfies the differential equation

$$\frac{d^2U(t)}{dt^2} = \Omega U(t) \tag{10}$$

By direct calculation (I used Maple, but you can do it by hand using the usual rules for matrix multiplication, although it's quite tedious), we can show that Ω and U commute and, since both Ω and U are hermitian, they are simultaneously diagonalizable. We already worked out the eigenvectors of Ω:

$$|I\rangle = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ 1 \end{bmatrix} \tag{11}$$

$$|II\rangle = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ -1 \end{bmatrix} \tag{12}$$

Since Ω is not degenerate, these must also be the eigenvectors of U, so the unitary matrix

$$D = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \tag{13}$$

can be used to diagonalize U according to

$$D^\dagger U D = \frac{1}{4}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}\begin{bmatrix} \cos\sqrt{\frac{k}{m}}t+\cos\sqrt{\frac{3k}{m}}t & \cos\sqrt{\frac{k}{m}}t-\cos\sqrt{\frac{3k}{m}}t \\ \cos\sqrt{\frac{k}{m}}t-\cos\sqrt{\frac{3k}{m}}t & \cos\sqrt{\frac{k}{m}}t+\cos\sqrt{\frac{3k}{m}}t \end{bmatrix}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \tag{14}$$

$$= \frac{1}{2}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}\begin{bmatrix} \cos\sqrt{\frac{k}{m}}t & \cos\sqrt{\frac{3k}{m}}t \\ \cos\sqrt{\frac{k}{m}}t & -\cos\sqrt{\frac{3k}{m}}t \end{bmatrix} \tag{15}$$

$$= \begin{bmatrix} \cos\sqrt{\frac{k}{m}}t & 0 \\ 0 & \cos\sqrt{\frac{3k}{m}}t \end{bmatrix} \tag{16}$$

This matches the diagonal form for U given as equation 1.8.43 in Shankar's book. The diagonal entries are the eigenvalues of $U(t)$.

PINGBACKS

Pingback: Postulates of quantum mechanics: Schrödinger equation and propagators

Pingback: Decoupling the two-particle Hamiltonian

FUNCTIONS OF HERMITIAN OPERATORS

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To leave a comment or report an error, please use the auxiliary blog.

References: Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Exercises 1.9.1 - 1.9.3.

Post date: 16 Nov 2016

One of the most common ways to define a function of an operator is to consider the case where the function can be expressed as a power series. That is, given an operator Ω, a function $f(\Omega)$ can be defined as

$$f(\Omega) = \sum_{n=0}^{\infty} a_n \Omega^n \tag{1}$$

where the coefficients a_n are, in general, complex scalars. This definition can still be difficult to deal with if Ω is not diagonalizable since, in that case, powers of Ω have no simple form, so it can be hard to tell if the series converges.

We can avoid this problem by restricting ourselves to hermitian operators, since such operators are always diagonalizable according to the spectral theorem and all eigenvalues of hermitian operators are real. Then powers of Ω are easy to calculate, since if the ith diagonal element of Ω is ω_i, the ith diagonal element of Ω^n is ω_i^n. The problem of finding $f(\Omega)$ is then reduced to examining whether the series converges for each diagonal element.

Example 1. Suppose we have the simplest such power series

$$f(\Omega) = \sum_{n=0}^{\infty} \Omega^n \tag{2}$$

If we look at this series in the eigenbasis (the basis of orthonormal eigenvectors that diagonalizes Ω), then we have

$$f(\Omega) = \begin{bmatrix} \sum_{n=0}^{\infty} \omega_1^n & & & \\ & \sum_{n=0}^{\infty} \omega_2^n & & \\ & & \ddots & \\ & & & \sum_{n=0}^{\infty} \omega_m^n \end{bmatrix} \tag{3}$$

Ω here is an $m \times m$ matrix with eigenvalues ω_i, $i = 1, \ldots, m$ (it's possible that some of the eigenvalues could be equal, if Ω is degenerate, but that doesn't affect the argument).

It's known that the geometric series

$$f(x) = \sum_{n=0}^{\infty} x^n = \frac{1}{1-x} \tag{4}$$

converges as shown, provided that $|x| < 1$. Thus we see that $f(\Omega)$ converges provided all its eigenvalues satisfy $|\omega_i| < 1$. The function is then

$$f(\Omega) = \begin{bmatrix} \frac{1}{1-\omega_1} & & & \\ & \frac{1}{1-\omega_2} & & \\ & & \ddots & \\ & & & \frac{1}{1-\omega_m} \end{bmatrix} \tag{5}$$

To see what operator it converges to, we consider the function

$$g(\Omega) = (I - \Omega)^{-1} \tag{6}$$

Still working in the eigenbasis where Ω is diagonal, the matrix $I - \Omega$ is also diagonal with diagonal elements $1 - \omega_i$. The inverse of a diagonal matrix is another diagonal matrix with diagonal elements equal to the reciprocal of the elements in the original matrix, so $(I - \Omega)^{-1}$ has diagonal elements $\frac{1}{1-\omega_i}$ so from 5 we see that

$$f(\Omega) = \sum_{n=0}^{\infty} \Omega^n = (I - \Omega)^{-1} \tag{7}$$

provided all the eigenvalues of Ω satisfy $|\omega_i| < 1$.

Example 2. If H is a hermitian operator, then e^{iH} is unitary. To see this, we again work in the eigenbasis of H. By expressing e^{iH} as a power series and using the same argument as in the previous example, we see that

$$U = e^{iH} = \begin{bmatrix} e^{i\omega_1} & & & \\ & e^{i\omega_2} & & \\ & & \ddots & \\ & & & e^{i\omega_m} \end{bmatrix} \tag{8}$$

The adjoint of e^{iH} is found by looking at the power series:

$$U^\dagger = \left(e^{iH}\right)^\dagger = \left[\sum_{n=0}^{\infty} \frac{(iH)^n}{n!}\right]^\dagger \tag{9}$$

$$= \sum_{n=0}^{\infty} \frac{\left(-iH^\dagger\right)^n}{n!} \tag{10}$$

$$= \sum_{n=0}^{\infty} \frac{(-iH)^n}{n!} \tag{11}$$

$$= e^{-iH} \tag{12}$$

where in the third line we used the hermitian property $H^\dagger = H$. Therefore

$$\left(e^{iH}\right)^\dagger = e^{-iH} = \begin{bmatrix} e^{-i\omega_1} & & & \\ & e^{-i\omega_2} & & \\ & & \ddots & \\ & & & e^{-i\omega_m} \end{bmatrix} \tag{13}$$

$$U^\dagger U = \left(e^{iH}\right)^\dagger e^{iH} = \begin{bmatrix} e^{-i\omega_1} & & & \\ & e^{-i\omega_2} & & \\ & & \ddots & \\ & & & e^{-i\omega_m} \end{bmatrix} \begin{bmatrix} e^{i\omega_1} & & & \\ & e^{i\omega_2} & & \\ & & \ddots & \\ & & & e^{i\omega_m} \end{bmatrix} \tag{14}$$

$$= I \tag{15}$$

Thus $\left(e^{iH}\right)^\dagger = \left(e^{iH}\right)^{-1}$ and e^{iH} is unitary.

From 8 we can find the determinant of e^{iH}:

$$\det U = \det e^{iH} = \exp\left[i\sum_{i=1}^{m} \omega_i\right] = \exp\left(i\mathrm{Tr}H\right) \tag{16}$$

since the trace of a hermitian matrix is the sum of its eigenvalues.

PINGBACKS

Pingback: Exponentials of operators - Baker-Campbell-Hausdorff formula

Pingback: Exponentials of operators - Hadamard's lemma

Pingback: Postulates of quantum mechanics: Schrödinger equation and propagators

Pingback: Time-dependent propagators

EXPONENTIALS OF OPERATORS - BAKER-CAMPBELL-HAUSDORFF FORMULA

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

References: Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 1.9.

Post date: 17 Nov 2016

Although the result in this post isn't covered in Shankar's book, it's a result that is frequently used in quantum theory, so it's worth including at this point.

We've seen how to define a function of an operator if that function can be expanded in a power series. A common operator function is the exponential:

$$f(\Omega) = e^{i\Omega} \tag{1}$$

If Ω is hermitian, the exponential $e^{i\Omega}$ is unitary. If we try to calculate the exponential of two operators such as e^{A+B}, the result isn't as simple as we might hope if A and B don't commute. To see the problem, we can write this out as a power series

$$\begin{aligned} e^{A+B} &= \sum_{n=0}^{\infty} \frac{(A+B)^n}{n!} && (2)\\ &= I + A + B + \frac{1}{2}(A+B)(A+B) + \ldots && (3)\\ &= I + A + B + \frac{1}{2}\left(A^2 + AB + BA + B^2\right) + \ldots && (4) \end{aligned}$$

The problem appears first in the fourth term in the series, since we can't condense the $AB + BA$ sum into $2AB$ if $[A, B] \neq 0$. In fact, the expansion of $e^A e^B$ can be written entirely in terms of the commutators of A and B with each other, nested to increasingly higher levels. This formula is known as the Baker-Campbell-Hausdorff formula. Up to the fourth order commutator, the BCH formula gives

$$e^A e^B = \exp\left[A + B + \frac{1}{2}[A, B] + \frac{1}{12}([A, [A, B]] + [B, [B, A]]) - \frac{1}{24}[B, [A, [A, B]]] + \ldots\right] \tag{5}$$

There is no known closed form expression for this result. However, an important special case that occurs frequently in quantum theory is the case where $[A, B] = cI$, where c is a complex scalar and I is the usual identity matrix. Since cI commutes with all operators, all terms from the third order upwards are zero, and we have

$$e^A e^B = e^{A+B+\frac{1}{2}[A,B]} \tag{6}$$

We can prove this result as follows. Start with the operator function

$$G(t) \equiv e^{t(A+B)} e^{-tA} \tag{7}$$

where t is a scalar parameter (not necessarily time!).
From its definition,

$$G(0) = I \tag{8}$$

The inverse is

$$G^{-1}(t) = e^{tA} e^{-t(A+B)} \tag{9}$$

and the derivative is

$$\frac{dG(t)}{dt} = (A+B)\, e^{t(A+B)} e^{-tA} - e^{t(A+B)} e^{-tA} A \tag{10}$$

Note that we have to keep the $(A+B)$ factor to the left of the A factor because $[A, B] \neq 0$. Now we multiply:

$$G^{-1} \frac{dG}{dt} = e^{tA} e^{-t(A+B)} \left[(A+B)\, e^{t(A+B)} e^{-tA} - e^{t(A+B)} e^{-tA} A \right] \tag{11}$$

$$= e^{tA} (A+B)\, e^{-tA} - A \tag{12}$$

$$= e^{tA} A e^{-tA} + e^{tA} B e^{-tA} - A \tag{13}$$

$$= e^{tA} B e^{-tA} \tag{14}$$

$$= B + t[A, B] \tag{15}$$

$$= B + ctI \tag{16}$$

We used Hadamard's lemma in the penultimate line, which in this case reduces to

$$e^{tA} B e^{-tA} = B + t[A, B] \tag{17}$$

because $[A, B] = cI$ so all higher order commutators are zero.

We end up with an expression in which A has disappeared. This gives the differential equation for G:

$$G^{-1}\frac{dG}{dt} = B + ctI \tag{18}$$

We try a solution of the form (this apparently appears from divine inspiration):

$$G(t) = e^{\alpha tB}e^{\beta ct^2} \tag{19}$$

From which we get

$$G^{-1} = e^{-\alpha tB}e^{-\beta ct^2} \tag{20}$$

$$\frac{dG}{dt} = (\alpha B + 2\beta ct)\, e^{\alpha tB}e^{\beta ct^2} \tag{21}$$

$$G^{-1}\frac{dG}{dt} = \alpha B + 2\beta ct \tag{22}$$

Comparing this to 18, we have

$$\alpha = 1 \tag{23}$$

$$\beta = \frac{1}{2} \tag{24}$$

$$G(t) = e^{tB}e^{\frac{1}{2}ct^2} \tag{25}$$

Setting this equal to the original definition of G in 7 and then taking $t = 1$ we have

$$e^{A+B}e^{-A} = e^{B}e^{c/2} \tag{26}$$

$$e^{A+B} = e^{B}e^{A}e^{\frac{1}{2}c} \tag{27}$$

$$= e^{B}e^{A}e^{\frac{1}{2}[A,B]} \tag{28}$$

If we swap A with B and use the fact that $A + B = B + A$, and also $[A, B] = -[B, A]$, we have

$$e^{A+B} = e^{A}e^{B}e^{-\frac{1}{2}[A,B]} \tag{29}$$

This is the restricted form of the BCH formula for the case where $[A, B]$ is a scalar.

PINGBACKS

Pingback: Time-dependent propagators
Pingback: Time reversal, antiunitary operators and Wigner's theorem
Pingback: Linear chain of oscillators - External force, unitary operator
Pingback: Linear chain of oscillators - External force, ground state

EXPONENTIALS OF OPERATORS - HADAMARD'S LEMMA

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

References: Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 1.9.

Post date: 17 Nov 2016

Although the result in this post isn't covered in Shankar's book, it's a result that is frequently used in quantum theory, so it's worth including at this point.

We've seen how to define a function of an operator if that function can be expanded in a power series. A common operator function is the exponential:

$$f(\Omega) = e^{i\Omega} \tag{1}$$

Here we'll look at a special function of two operators of the form

$$h(A,B) = e^{A}Be^{-A} \tag{2}$$

If $[A,B] = 0$, we can cancel the two exponentials and get the result $h(A,B) = B$. However, if $[A,B] \neq 0$ the two exponentials must remain separated by the middle B operator. To get a simpler form for this function, we'll consider the auxiliary function

$$f(t) = e^{tA}Be^{-tA} \tag{3}$$

where t is some parameter. We'll need the first 3 derivatives at $t = 0$:

$$f(0) = B \tag{4}$$

$$f'(t) = Ae^{tA}Be^{-tA} - e^{tA}Be^{-tA}A \tag{5}$$

$$= e^{tA}[A,B]e^{-tA} \tag{6}$$

$$f'(0) = [A,B] \tag{7}$$

$$f''(t) = Ae^{tA}[A,B]e^{-tA} - e^{tA}[A,B]e^{-tA}A \tag{8}$$

$$= e^{tA}[A,[A,B]]e^{-tA} \tag{9}$$

$$f''(0) = [A,[A,B]] \tag{10}$$

$$f'''(t) = e^{tA}[A,[A,[A,B]]]e^{-tA} \tag{11}$$

$$f'''(0) = [A,[A,[A,B]]] \tag{12}$$

We can now write a Taylor expansion of 3 around $t = 0$:

$$e^{tA}Be^{-tA} = f(0) + tf'(0) + \frac{t^2}{2}f''(0) + \frac{t^3}{6}f'''(0) + \dots \tag{13}$$

$$= B + [A,B]\,t + [A,[A,B]]\,\frac{t^2}{2!} + [A,[A,[A,B]]]\,\frac{t^3}{3!} + \dots \tag{14}$$

Taking $t = 1$ gives the required expansion

$$e^{A}Be^{-A} = B + [A,B] + \frac{1}{2!}[A,[A,B]] + \frac{1}{3!}[A,[A,[A,B]]] + \dots \tag{15}$$

This is known as *Hadamard's lemma*.
If we introduce the notation

$$\mathrm{ad}_A(B) \equiv [A,B] \tag{16}$$

$$\mathrm{ad}_A\mathrm{ad}_A(B) = [A,[A,B]] \tag{17}$$

and in general $(\mathrm{ad}_A)^n(B)$ is the nth order commutator of A with B, then we can write Hadamard's lemma as

$$e^{A}Be^{-A} = \sum_{n=0}^{\infty}\frac{1}{n!}(\mathrm{ad}_A)^n(B) \tag{18}$$

$$= \exp(\mathrm{ad}_A)(B) \tag{19}$$

PINGBACKS

Pingback: Exponentials of operators - Baker-Campbell-Hausdorff formula

Pingback: Finite transformations: correspondence between classical and quantum

NON-DENUMERABLE BASIS: POSITION AND MOMENTUM STATES

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To leave a comment or report an error, please use the auxiliary blog.

References: References: edX online course MIT 8.05 Section 5.6.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 1.10; Exercises 1.10.1 - 1.10.3.

Post date: 19 Nov 2016

Although we've looked at position and momentum operators in quantum mechanics before, it's worth another look at the ways that Zwiebach and Shankar introduce them.

First, we'll have a look at Shankar's treatment. He begins by considering a string fixed at each end, at positions $x = 0$ and $x = L$, then asks how we could convey the shape of the string to an observer who cannot see the string directly. We could note the position at some fixed finite number of points between 0 and L, but then the remote observer would have only a partial knowledge of the string's shape; the locations of those portions of the string between the points at which it was measured are still unknown, although the observer could probably get a reasonable picture by interpolating between these points.

We can increase the number of points at which the position is measured to get a better picture, but to convey the exact shape of the string, we need to measure its position at an infinite number of points. This is possible (in principle) but leads to a problem with the definition of the inner product. For two vectors defined on a finite vector space with an orthonormal basis, the inner product is given by the usual formula for the dot product:

$$\langle f \, | g \rangle = \sum_{i=1}^{n} f_i g_i \tag{1}$$

$$\langle f \, | f \rangle = \sum_{i=1}^{n} f_i^2 \tag{2}$$

where f_i and g_i are the components of f and g in the orthonormal basis. If we're taking f to be the displacement of a string and we try to increase the accuracy of the picture by increasing the number n of points at which measurements are taken, then the value of $\langle f \, | f \rangle$ continues to increase as n increases (provided that $f \neq 0$ everywhere). As $n \to \infty$ then $\langle f \, | f \rangle \to \infty$ as

well, even though the system we're measuring (a string of finite length with finite displacement) is certainly not infinite in any practical sense.

Shankar proposes getting around this problem by simply redefining the inner product for a *finite* vector space to be

$$\langle f|g\rangle = \sum_{i=1}^{n} f(x_i)\, g(x_i)\, \Delta \tag{3}$$

where $\Delta \equiv L/(n+1)$. That is, Δ now becomes the distance between adjacent points at which measurements are taken. If we let $n \to \infty$ this leads to the definition of the inner product as an integral

$$\langle f|g\rangle = \int_0^L f(x)\, g(x)\, dx \tag{4}$$

$$\langle f|f\rangle = \int_0^L f^2(x)\, dx \tag{5}$$

This looks familiar enough, if you've done any work with inner products in quantum mechanics, but there is a subtle point which Shankar overlooks. In going from 1 to 3, we have introduced a factor Δ which, in the string example at least, has the dimensions of length, so the physical interpretation of these two equations is different. The units of $\langle f|g\rangle$ appear to be different in the two cases. Now in quantum theory, inner products of the continuous type usually involve the wave function multiplied by its complex conjugate, with possibly another operator thrown in if we're trying to find the expectation value of some observable. The square modulus of the wave function, $|\Psi|^2$, is taken to be a probability density, so it has units of inverse length (in one dimension) or inverse volume (in three dimensions), which makes the integral work out properly.

Admittedly, when we're using f to represent the displacement of a string, it's not obvious what meaning the inner product of f with anything else would actually have, so maybe the point isn't worth worrying about. However, it does seem to be something that it would be worth Shankar including a comment about.

From this point, Shankar continues by saying that this infinite dimensional vector space is spanned by basis vectors $|x\rangle$, with one basis vector for each value of x. We require this basis to be orthogonal, which means that we must have, if $x \neq x'$

$$\langle x|x'\rangle = 0 \tag{6}$$

We then generalize the identity operator to be

$$I = \int |x\rangle \langle x| \, dx \tag{7}$$

which leads to

$$\langle x | f \rangle = \int \langle x | x' \rangle \langle x' | f \rangle \, dx' \tag{8}$$

The bra-ket $\langle x | f \rangle$ is the projection of the vector $|f\rangle$ onto the $|x\rangle$ basis vector, so it is just $f(x)$. This means

$$f(x) = \int \langle x | x' \rangle f(x') \, dx' \tag{9}$$

which leads to the definition of the Dirac delta function as the normalization of $\langle x | x' \rangle$:

$$\langle x | x' \rangle = \delta(x - x') \tag{10}$$

Shankar then describes some properties of the delta function and its derivative, most of which we've already covered. For example, we've seen these two results for the delta function:

$$\delta(ax) = \frac{\delta(x)}{|a|} \tag{11}$$

$$\frac{d\theta(x - x')}{dx} = \delta(x - x') \tag{12}$$

where θ is the step function

$$\theta(x - x') \equiv \begin{cases} 0 & x \leq x' \\ 1 & x > x' \end{cases} \tag{13}$$

One other result is that for a function $f(x)$ with zeroes at a number of points x_i, we have

$$\delta(f(x)) = \sum_i \frac{\delta(x_i - x)}{|df/dx_i|} \tag{14}$$

To see this, consider one of the x_i where $f(x_i) = 0$. Expanding in a Taylor series about this point, we have

$$f(x_i + (x - x_i)) = f(x_i) + (x - x_i) \frac{df}{dx_i} + \ldots \tag{15}$$

$$= 0 + (x - x_i) \frac{df}{dx_i} \tag{16}$$

From 11 we have

$$\delta\left(\left(x-x_i\right)\frac{df}{dx_i}\right)=\frac{\delta\left(x_i-x\right)}{\left|df/dx_i\right|} \tag{17}$$

The behaviour is the same at all points x_i and since $\delta\left(x_i-x\right)=0$ at all other $x_j\neq x_i$ where $f\left(x_j\right)=0$, we can just add the delta functions for each zero of f.

Turning now to Zwiebach's treatment, he begins with the basis states $|x\rangle$ and position operator $\hat{x}$ with the eigenvalue equation

$$\hat{x}\left|x\right\rangle=x\left|x\right\rangle \tag{18}$$

and simply *defines* the inner product between two position states to be

$$\left\langle x\left|y\right.\right\rangle=\delta\left(x-y\right) \tag{19}$$

With this definition, 9 follows immediately. We can therefore write a quantum state $|\psi\rangle$ as

$$\left|\psi\right\rangle=I\left|\psi\right\rangle=\int\left|x\right\rangle\left\langle x\left|\psi\right.\right\rangle dx=\int\left|x\right\rangle\psi\left(x\right)dx \tag{20}$$

That is, the vector $|\psi\rangle$ is the integral of its projections $\psi\left(x\right)$ onto the basis vectors $|x\rangle$.

The position operator $\hat{x}$ is hermitian as can be seen from

$$\begin{aligned}\left\langle x_1\left|\hat{x}^\dagger\right|x_2\right\rangle&=\left\langle x_2\left|\hat{x}\right|x_1\right\rangle^* &(21)\\ &=x_1\left\langle x_2\left|x_1\right.\right\rangle^* &(22)\\ &=x_1\delta\left(x_2-x_1\right)^* &(23)\\ &=x_1\delta\left(x_2-x_1\right) &(24)\\ &=x_2\delta\left(x_2-x_1\right) &(25)\\ &=\left\langle x_1\left|\hat{x}\right|x_2\right\rangle &(26)\end{aligned}$$

The fourth line follows because the delta function is real, and the fifth follows because $\delta\left(x_2-x_1\right)$ is non-zero only when $x_1=x_2$.

Zwiebach then introduces the momentum eigenstates $|p\rangle$ which are analogous to the position states $|x\rangle$, in that

$$\langle p' | p \rangle = \delta(p' - p) \tag{27}$$

$$I = \int dp \, |p\rangle \langle p| \tag{28}$$

$$\hat{p} |p\rangle = p |p\rangle \tag{29}$$

$$\tilde{\psi}(p) = \langle p | \psi \rangle \tag{30}$$

By the same calculation as for $|x\rangle$, we see that $\hat{p}$ is hermitian.

To get a relation between the $|x\rangle$ and $|p\rangle$ bases, we require that $\langle x | p \rangle$ is the wave function for a particle with momentum p in the x basis, which we've seen is

$$\psi(x) = \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar} \tag{31}$$

Zwiebach then shows that this is consistent with the equation

$$\langle x | \hat{p} | \psi \rangle = \frac{h}{i} \frac{d}{dx} \langle x | \psi \rangle = \frac{h}{i} \frac{d\psi(x)}{dx} \tag{32}$$

We can get a similar relation by switching x and p:

$$\langle p | \hat{x} | \psi \rangle = \int dx \, \langle p | x \rangle \langle x | \hat{x} | \psi \rangle \tag{33}$$

$$= \int dx \, \langle x | p \rangle^* \, x \, \langle x | \psi \rangle \tag{34}$$

From 31 we see

$$\langle x | p \rangle^* = \frac{1}{\sqrt{2\pi\hbar}} e^{-ipx/\hbar} \tag{35}$$

$$\langle x | p \rangle^* \, x = i\hbar \frac{d}{dp} \langle x | p \rangle^* \tag{36}$$

$$\int dx \, \langle x | p \rangle^* \, x \, \langle x | \psi \rangle = i\hbar \int dx \, \frac{d}{dp} \langle x | p \rangle^* \langle x | \psi \rangle \tag{37}$$

$$= i\hbar \frac{d}{dp} \int dx \, \langle x | p \rangle^* \langle x | \psi \rangle \tag{38}$$

$$= i\hbar \frac{d}{dp} \int dx \, \langle p | x \rangle \langle x | \psi \rangle \tag{39}$$

$$= i\hbar \frac{d\tilde{\psi}(p)}{dp} \tag{40}$$

In the fourth line, we took the $\frac{d}{dp}$ outside the integral since p occurs in only one term, and in the last line we used 7. Thus we have

$$\langle p\,|\hat{x}|\,\psi\rangle = i\hbar\frac{d\tilde{\psi}\,(p)}{dp} \tag{41}$$

PINGBACKS

Pingback: Differential operators - matrix elements and hermiticity
Pingback: Harmonic oscillator - eigenfunctions in momentum space

DIFFERENTIAL OPERATORS - MATRIX ELEMENTS AND HERMITICITY

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References: Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 1.10.

Post date: 20 Nov 2016

Here, we'll revisit the differential operator on a continuous vector space which we looked at earlier in its role as the momentum operator. This time around, we'll use the bra-ket notation and vector space results to analyze it, hopefully putting it on a slightly more mathematical foundation.

We define the differential operator D acting on a vector $|f\rangle$ in a continuous vector space as having the action

$$D|f\rangle = \left|\frac{df}{dx}\right\rangle \tag{1}$$

This notation means that D operating on $|f\rangle$ produces the vector (ket) $\left|\frac{df}{dx}\right\rangle$ corresponding to the function whose form in the $|x\rangle$ basis is $\frac{df(x)}{dx}$. That is, the projection of $\left|\frac{df}{dx}\right\rangle$ onto the basis vector $|x\rangle$ is

$$\frac{df(x)}{dx} = \left\langle x\left|\frac{df}{dx}\right.\right\rangle = \langle x|D|f\rangle \tag{2}$$

By a similar argument to that which we used to deduce the matrix element $\langle x|x'\rangle$, we can work out the matrix elements of D in the $|x\rangle$ basis. Inserting the unit operator, we have

$$\langle x|D|f\rangle = \int dx' \langle x|D|x'\rangle \langle x'|f\rangle \tag{3}$$

$$= \int dx' \langle x|D|x'\rangle f(x') \tag{4}$$

We need this to be equal to $\frac{df}{dx}$. To get this, we can introduce the derivative of the delta function, except this time the delta function is a function of $x - x'$ rather than just x on its own. To see the effect of this derivative, consider the integral

$$\int dx' \frac{d\delta\left(x-x'\right)}{dx} f\left(x'\right) = \frac{d}{dx}\int dx' \delta\left(x-x'\right) f\left(x'\right) = \frac{df\left(x\right)}{dx} \tag{5}$$

In the second step, we could take the derivative outside the integral since x is a constant with respect to the integration. Comparing this with 4 we see that

$$\left\langle x\left|D\right|x'\right\rangle \equiv D_{xx'} = \frac{d\delta\left(x-x'\right)}{dx} = \delta'\left(x-x'\right) \tag{6}$$

Here the prime in δ' means derivative with respect to x, not x'. [Note that this is *not* the same formula as that quoted in the earlier post, where we had $f\left(x\right)\delta'\left(x\right) = -f'\left(x\right)\delta\left(x\right)$ because in that formula it was the same variable x that was involved in the derivative of the delta function and in the integral.]

The operator D is not hermitian as it stands. Since the delta function is real, we have, looking at $D^{\dagger}_{xx'} = D^{*}_{x'x}$ in bra-ket notation, we see that

$$D^{\dagger}_{x'x} = \left\langle x'\left|D^{*}\right|x\right\rangle = \delta'\left(x'-x\right) = -\delta'\left(x-x'\right) \neq D_{xx'} \tag{7}$$

Thus D is anti-hermitian. It is easy to fix this and create a hermitian operator by multiplying by an imaginary number, such as $-i$ (this choice is, of course, to make the new operator consistent with the momentum operator). Calling this new operator $K \equiv -iD$ we have

$$K^{\dagger}_{x'x} = \left\langle x'\left|K^{*}\right|x\right\rangle = i\delta'\left(x'-x\right) = -i\delta'\left(x-x'\right) = K_{xx'} \tag{8}$$

A curious fact about K (and thus about the momentum operator as well) is that it is not automatically hermitian even with this correction. We've seen that it satisfies the hermiticity property with respect to its matrix elements in the position basis, but to be fully hermitian, it must satisfy

$$\left\langle g\left|K\right|f\right\rangle = \left\langle f\left|K\right|g\right\rangle^{*} \tag{9}$$

for any two vectors $\left|f\right\rangle$ and $\left|g\right\rangle$. Suppose we are interested in x over some range $[a,b]$. Then by inserting a couple of identity operators, we have

$$\langle g\,|K|\,f\rangle = \int_a^b \int_a^b \langle g\,|x\rangle \langle x\,|K|\,x'\rangle \langle x'\,|f\,\rangle\, dx\, dx' \tag{10}$$

$$= -i \int_a^b g^*(x) \frac{df}{dx} dx \tag{11}$$

$$= -i\, g^*(x)\, f(x)\big|_a^b + i \int_a^b f(x) \frac{dg^*}{dx} dx \tag{12}$$

$$= -i\, g^*(x)\, f(x)\big|_a^b + \langle f\,|K|\,g\rangle^* \tag{13}$$

The result is hermitian only if the first term in the last line is zero, which happens only for certain choices of f and g. If the limits are infinite, so we're integrating over all space, and the system is bounded so that both f and g go to zero at infinity, then we're OK, and K is hermitian. Another option is if g and f are periodic and the range of integration is equal to an integral multiple of the period, then $g^* f$ has the same value at each end and the term becomes zero.

However, as we've seen, in quantum mechanics there are cases where we deal with functions such as e^{ikx} (for k real) that oscillate indefinitely, no matter how large x is (see the free particle, for example). There isn't any mathematically airtight way around such cases (as far as I know), but a hand-wavy way of defining a limit for such oscillating functions is to consider their average behaviour as $x \to \pm\infty$. The average defined by Shankar is given as

$$\lim_{x\to\infty} e^{ikx} e^{-ik'x} = \lim_{\substack{L\to\infty \\ \Delta\to\infty}} \frac{1}{\Delta} \int_L^{L+\Delta} e^{i(k-k')x} dx \tag{14}$$

This is interpreted as looking at the function very far out on the x axis (at position L), and then considering a very long interval Δ starting at point L. Since the integral of $e^{i(k-k')x}$ over one period is zero (it's just a combination of sine and cosine functions), the integral is always bounded between 0 and the area under half a cycle, as successive half-cycles cancel each other. Dividing by Δ, which is monotonically increasing, ensures that the limit is zero.

This isn't an ideal solution, but it's just one of many cases where an infinitely oscillating function is called upon to do seemingly impossible things. The theory seems to hang together fairly well in any case.

PINGBACKS

Pingback: Differential operator - eigenvalues and eigenstates
Pingback: radial function for small r

DIFFERENTIAL OPERATOR - EIGENVALUES AND EIGENSTATES

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References: Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 1.10.

Post date: 21 Nov 2016

Continuing with our study of differential operators, we'll look now at their eigenvalues and eigenstates. The operator we're studying is

$$K = -i\frac{d}{dx} \tag{1}$$

The eigenvalue equation is as usual:

$$K\left|k\right\rangle = k\left|k\right\rangle \tag{2}$$

where $|k\rangle$is an eigenstate and k (outside the ket) is a (possibly complex) scalar. To find $|k\rangle$, we form the matrix element with $\langle x|$ and insert the unit operator:

$$\left\langle x\right|K\left|k\right\rangle = k\left\langle x\right|\left.k\right\rangle \tag{3}$$

$$\left\langle x\right|K\left|k\right\rangle = \int\left\langle x\right|K\left|x'\right\rangle\left\langle x'\right|\left.k\right\rangle dx' \tag{4}$$

$$= -i\int\delta'\left(x-x'\right)\psi_k\left(x'\right)dx' \tag{5}$$

$$= -i\frac{d}{dx}\psi_k\left(x\right) \tag{6}$$

In the third line we used the matrix element

$$\left\langle x\right|K\left|x'\right\rangle = -i\delta'\left(x-x'\right) \tag{7}$$

Equating the RHS on the first and last lines gives the differential equation

$$-i\frac{d}{dx}\psi_k\left(x\right) = k\psi_k\left(x\right) \tag{8}$$

which has the solution

$$\psi_k\left(x\right) = Ae^{ikx} \tag{9}$$

where A is a constant of integration. In order for $\psi_k(x)$ to be bounded as $x \to \pm\infty$, k must be real, so we'll restrict our attention to that case. The usual choice for A is $1/\sqrt{2\pi}$ so that

$$\psi_k(x) = \frac{e^{ikx}}{\sqrt{2\pi}} \tag{10}$$

This leads to the normalization condition

$$\left\langle k \middle| k' \right\rangle = \int_{-\infty}^{\infty} \langle k | x \rangle \left\langle x \middle| k' \right\rangle dx \tag{11}$$

$$= \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-i(k-k')x} dx \tag{12}$$

$$= \delta\left(k - k'\right) \tag{13}$$

where in the last line we used the traditional formula for the delta function. Thus the $|k\rangle$ basis is orthogonal, and normalized the same way as the $|x\rangle$ basis.

To convert between the $|k\rangle$ and $|x\rangle$ bases, we can use the unit operator in the two bases. Thus for some vector (function) $|f\rangle$ we have

$$f(k) = \langle k | f \rangle = \int \langle k | x \rangle \langle x | f \rangle dx = \int \psi_k^*(x) f(x) dx = \frac{1}{\sqrt{2\pi}} \int e^{-ikx} f(x) \tag{14}$$

Thus $f(k)$ is the Fourier transform of $f(x)$. We can use the same procedure to go in the reverse direction:

$$f(x) = \langle x | f \rangle = \int \langle x | k \rangle \langle k | f \rangle dk = \int \psi_k(x) f(k) dk = \frac{1}{\sqrt{2\pi}} \int e^{ikx} f(k) \tag{15}$$

The effect of the position operator X on a vector $|f(x)\rangle$ can be found by inserting the unit operator:

$$\langle x | X | f \rangle = \int \left\langle x \middle| X \middle| x' \right\rangle \left\langle x' \middle| f \right\rangle dx' \tag{16}$$

$$= \int x' \left\langle x \middle| x' \right\rangle \left\langle x' \middle| f \right\rangle dx' \tag{17}$$

$$= \int x' \delta\left(x - x'\right) \left\langle x' \middle| f \right\rangle dx' \tag{18}$$

$$= x \langle x | f \rangle \tag{19}$$

Thus X just multiplies any function of x by x itself. A similar argument in the $|k\rangle$ basis shows that

$$\langle k\,|K|\,f\,(k)\rangle = k\,\langle k\,|f\,(k)\rangle \tag{20}$$

We can use similar calculations to find the matrix elements of K in the $|x\rangle$ basis and of X (the position operator) in the $|k\rangle$ basis. We get

$$\begin{aligned}
\left\langle k\,|X|\,k'\right\rangle &= \int\int \langle k\,|x\rangle \left\langle x\,|X|\,x'\right\rangle \left\langle x'\,\middle|\,k'\right\rangle dx\,dx' && (21)\\
&= \frac{1}{2\pi}\int\int e^{-ikx}x'\left\langle x\,\middle|\,x'\right\rangle e^{ik'x'}dx\,dx' && (22)\\
&= \frac{1}{2\pi}\int\int e^{-ikx}x'\delta\left(x-x'\right)e^{ik'x'}dx\,dx' && (23)\\
&= \frac{1}{2\pi}\int xe^{i(k'-k)x}dx && (24)\\
&= i\frac{d}{dk}\left[\frac{1}{2\pi}\int e^{i(k'-k)x}dx\right] && (25)\\
&= i\delta'\left(k-k'\right) && (26)
\end{aligned}$$

The action of X on an arbitrary vector $|g\rangle$ in the k basis can be found from this:

$$\begin{aligned}
\langle k\,|X|\,g\,(k)\rangle &= \int \left\langle k\,|X|\,k'\right\rangle \left\langle k'\,|g\right\rangle dk' && (27)\\
&= i\int \delta'\left(k-k'\right)g\left(k'\right)dk' && (28)\\
&= i\frac{dg\,(k)}{dk} && (29)\\
&= i\left\langle k\,\middle|\,\frac{dg\,(k)}{dk}\right\rangle && (30)
\end{aligned}$$

where in the third line we've used the property of $\delta'\,(k-k')$ mentioned here.

By a similar calculation, we can find the matrix elements of K in the $|x\rangle$ basis:

$$\left\langle x\left|K\right|x'\right\rangle = \int\int \left\langle x\left|k\right.\right\rangle \left\langle k\left|K\right|k'\right\rangle \left\langle k'\left|x'\right.\right\rangle dk\, dk' \tag{31}$$

$$= \frac{1}{2\pi}\int\int e^{ikx}k'\left\langle k\left|k'\right.\right\rangle e^{-ik'x'}dk\, dk' \tag{32}$$

$$= \frac{1}{2\pi}\int\int e^{ikx}k'\delta\left(k-k'\right)e^{-ik'x'}dk\, dk' \tag{33}$$

$$= \frac{1}{2\pi}\int xe^{i(x-x')k}dk \tag{34}$$

$$= -i\frac{d}{dx}\left[\frac{1}{2\pi}\int e^{i(x-x')k}dk\right] \tag{35}$$

$$= -i\delta'\left(x-x'\right) \tag{36}$$

Similarly, we have

$$\left\langle x\left|K\right|g\left(x\right)\right\rangle = \int \left\langle x\left|K\right|x'\right\rangle \left\langle x'\left|g\right.\right\rangle dx' \tag{37}$$

$$= -i\int \delta'\left(x-x'\right)g\left(x'\right)dx' \tag{38}$$

$$= -i\frac{dg\left(x\right)}{dx} \tag{39}$$

$$= -i\left\langle x\left|\frac{dg\left(x\right)}{dx}\right.\right\rangle \tag{40}$$

From 30 and 40 we can work out the familiar commutator. Just for variety, we'll do this in the $|k\rangle$ basis:

$$XK\left|f\left(k\right)\right\rangle = X\left[k\left|f\left(k\right)\right\rangle\right] \tag{41}$$

$$= i\frac{d}{dk}\left[k\left|f\left(k\right)\right\rangle\right] \tag{42}$$

$$= i\left[\left|f\left(k\right)\right\rangle + k\left|\frac{df}{dk}\right\rangle\right] \tag{43}$$

$$KX\left|f\left(k\right)\right\rangle = iK\left|\frac{df}{dk}\right\rangle \tag{44}$$

$$= ik\left|\frac{df}{dk}\right\rangle \tag{45}$$

Therefore

$$\left[X,K\right]\left|f\left(k\right)\right\rangle = i\left|f\left(k\right)\right\rangle \tag{46}$$

or, looking just at the operators

$$[X, K] = iI \tag{47}$$

PINGBACKS

Pingback: Vibrating string - normal mode analysis
Pingback: Postulates of quantum mechanics: states and measurements

VIBRATING STRING - NORMAL MODE ANALYSIS

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

References: Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 1.10. Exercise 1.10.4.

Post date: 22 Nov 2016

I'll run through Shakar's example 1.10.1 on a vibrating string, so we can see an application of the theory of infinite dimensional spaces. Suppose we have a string (for example, a violin string) that is anchored at $x = 0$ and $x = L$. If we pluck the string at $t = 0$, its future position is governed by the wave equation:

$$\frac{\partial^2 \psi}{\partial t^2} = \frac{\partial^2 \psi}{\partial x^2} \tag{1}$$

[For simplicity, we're taking the wave speed to be 1, which is why there's no constant in this equation.] We can write this as an operator equation using the $K = -i\frac{\partial}{\partial x}$ operator we introduced last time. Viewing the wave as a vector in the $|x\rangle$ basis, we then have

$$\left|\ddot{\psi}(t)\right\rangle = -K^2 \left|\psi(t)\right\rangle \tag{2}$$

The idea is now to look at the RHS of this equation and diagonalize the K^2 operator by finding its eigenvalues and eigenvectors. Working in the $|x\rangle$ basis, we can write the eigenvalue problem as

$$\left\langle x \left| K^2 \right| \psi \right\rangle = k^2 \left\langle x \middle| \psi \right\rangle \tag{3}$$

$$-\frac{d^2\psi(x)}{dx^2} = k^2 \psi(x) \tag{4}$$

This has the general solution

$$\psi(x) = A\cos kx + B\sin kx \tag{5}$$

where A and B are constants of integration, to be determined by the boundary conditions. Since the ends of the string are fixed at $\psi(0) = \psi(L) = 0$, we must have $A = 0$, and we then have

$$B\sin kL = 0 \tag{6}$$

In order to avoid a trivial solution where $\psi(x) = 0$ everywhere, we have $B \neq 0$, so

$$kL = m\pi \tag{7}$$

for $m = 1, 2, 3, \ldots$. We therefore have the discrete set of solutions

$$\psi_m(x) = B \sin \frac{m\pi x}{L} \tag{8}$$

We can choose $B = \sqrt{\frac{2}{L}}$ to normalize the solution so that

$$\int \psi_m(x)\, \psi_{m'}(x)\, dx = \delta_{mm'} \tag{9}$$

So far, this is the same as the solution to the infinite square well in quantum mechanics, but now we follow a different path, since we need to satisfy the wave equation 1, and not Schrödinger's equation, which is first order in time.

We now have two different orthonormal bases that can be used to represent the states of the string. The $|x\rangle$ basis is continuous, consisting of all real values of x in the interval $[0, L]$. The other basis is also infinite, but it is discrete, as it consists of the possible values of k as given by 7. Since k is determined by the integer m, we'll call this the $|m\rangle$ basis. In the $|x\rangle$ basis, the state $|m\rangle$ is given by 8:

$$\langle x | m \rangle = \sqrt{\frac{2}{L}} \sin \frac{m\pi x}{L} \tag{10}$$

The general solution as a function of time is an abstract vector $|\psi(t)\rangle$. We can project this onto the $|x\rangle$ basis, when we would get

$$\langle x | \psi(t) \rangle = \psi(x, t) \tag{11}$$

Or we can project it onto the $|m\rangle$ basis, which gives that component of $|\psi(t)\rangle$ that is composed of a wave with index m. In the $|m\rangle$ basis, the operator K^2 is diagonal, since

$$K^2 \psi_m(x) = -\sqrt{\frac{2}{L}} \frac{d^2}{dx^2} \sin \frac{m\pi x}{L} = \left(\frac{m\pi}{L}\right)^2 \sqrt{\frac{2}{L}} \sin \frac{m\pi x}{L} = \left(\frac{m\pi}{L}\right)^2 \psi_m(x) = k^2 \psi_m(x) \tag{12}$$

We can write the projection of $|\psi(t)\rangle$ onto the $|m\rangle$ basis as $\langle m | \psi(t) \rangle$. Going back to 2, we see that each component $\langle m | \psi(t) \rangle$ individually satisfies the differential equation

$$\frac{d^2}{dt^2} \langle m | \psi(t) \rangle = -\left(\frac{m\pi}{L}\right)^2 \langle m | \psi(t) \rangle \tag{13}$$

This is the same equation as 4, except now we're dealing with a time derivative instead of a space derivative. The solution is therefore of the same form:

$$\langle m|\psi(t)\rangle = C\cos kt + D\sin kt \tag{14}$$

To find C and D, we now use the initial conditions at $t=0$. We'll assume that the string is held in some fixed shape and then released at $t=0$, which means that we need to specify this initial shape as $\langle m|\psi(0)\rangle$, and that the initial velocity is zero. The latter condition means that

$$\frac{d}{dt}\langle m|\psi(0)\rangle = -kC\sin k0 + kD\cos k0 = 0 \tag{15}$$

which gives us $D=0$, so we have

$$\langle m|\psi(t)\rangle = \langle m|\psi(0)\rangle\cos kt = \langle m|\psi(0)\rangle\cos\frac{m\pi t}{L} \tag{16}$$

The general solution is therefore found by inserting the unit operator in the form $1=\sum_m |m\rangle\langle m|$:

$$|\psi(t)\rangle = \sum_m |m\rangle\langle m|\psi(t)\rangle \tag{17}$$

$$= \sum_m |m\rangle\cos\frac{m\pi t}{L}\langle m|\psi(0)\rangle \tag{18}$$

This can be written as a propagator $U(t)$ acting on the initial state:

$$|\psi(t)\rangle = U(t)|\psi(0)\rangle \tag{19}$$

$$U(t) \equiv \sum_m |m\rangle\langle m|\cos\frac{m\pi t}{L} \tag{20}$$

Just as with our earlier example of two masses coupled by springs, all the time dependence has been incorporated into the propagator, so all we need to do is specify the initial shape of the spring to get the general solution. This solution can be restored to the $|x\rangle$ basis by applying the bra $\langle x|$ to 18 and using 10:

$$\psi(x,t) = \langle x|\psi(t)\rangle \tag{21}$$

$$= \sum_m \langle x|m\rangle\cos\frac{m\pi t}{L}\langle m|\psi(0)\rangle \tag{22}$$

$$= \sqrt{\frac{2}{L}}\sum_m \sin\frac{m\pi x}{L}\cos\frac{m\pi t}{L}\langle m|\psi(0)\rangle \tag{23}$$

We still need to get rid of the final $\langle m|$ bra in the last term, which we can do by inserting a unit operator using the $|x\rangle$ basis:

$$\psi(x,t) = \sqrt{\frac{2}{L}} \sum_m \sin\frac{m\pi x}{L} \cos\frac{m\pi t}{L} \int_0^L \langle m|x'\rangle \langle x'|\psi(0)\rangle \, dx' \tag{24}$$

$$= \frac{2}{L} \sum_m \sin\frac{m\pi x}{L} \cos\frac{m\pi t}{L} \int_0^L \sin\frac{m\pi x'}{L} \psi(x',0) \, dx' \tag{25}$$

The last line follows from 10 because $\langle m|x'\rangle = \langle x'|m\rangle^*$ and $\langle m|x'\rangle$ is real. Thus to get the final solution, we need to do the integral in the last line, which depends on the initial shape of the string.

For example, suppose the string is held at its midpoint a distance h away from the x axis, and follows a straight line on either side of the midpoint. Then the initial state is given by

$$\psi(x,0) = \begin{cases} \frac{2xh}{L} & 0 \le x \le \frac{L}{2} \\ \frac{2h}{L}(L-x) & \frac{L}{2} \le x \le L \end{cases} \tag{26}$$

We then need to do the integral

$$\int_0^L \sin\frac{m\pi x}{L} \psi(x,0) \, dx = \frac{2h}{L} \left[\int_0^{L/2} x \sin\frac{m\pi x}{L} dx + \int_{L/2}^L (L-x) \sin\frac{m\pi x}{L} dx \right] \tag{27}$$

The integrals can be done by parts although it's a bit tedious, so I used Maple to get

$$\frac{hL}{\pi^2 m^2} \left[-\left(m\pi \cos\frac{\pi m}{2} - 2\sin\frac{\pi m}{2} \right) + \left(m\pi \cos\frac{\pi m}{2} + 2\sin\frac{\pi m}{2} \right) \right] = \frac{4hL}{\pi^2 m^2} \sin\frac{\pi m}{2} \tag{28}$$

Plugging this back into 25 we get the final answer:

$$\psi(x,t) = \frac{8h}{\pi^2} \sum_m \frac{1}{m^2} \sin\frac{m\pi x}{L} \cos\frac{m\pi t}{L} \sin\frac{\pi m}{2} \tag{29}$$

Each term in the sum is a normal mode, and we can see that the amplitude drops off as $1/m^2$, so higher frequencies are less prevalent in the overall motion of the string.

Notice that if we start the string off in a pure sine wave shape, this is the only mode that is ever present. That is, if, for some fixed integer n and amplitude of initial displacement h:

$$\psi(x,0) = h \sin\frac{n\pi x}{L} \tag{30}$$

then

$$\int_0^L \sin\frac{m\pi x}{L}\psi(x,0)\,dx = \frac{hL}{2}\delta_{mn} \tag{31}$$

Thus the only mode present is $m = n$, and the string's motion is

$$\psi(x,t) = h\sin\frac{n\pi x}{L}\cos\frac{n\pi t}{L} \tag{32}$$

DIRAC DELTA FUNCTION AS LIMIT OF A GAUSSIAN INTEGRAL

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Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 1.10.

Post date: 6 Feb 2017.

Yet another form of the Dirac delta function is as the limit of a Gaussian integral. We start with

$$g_\Delta\left(x-x'\right)=\frac{1}{\left(\pi\Delta^2\right)^{1/2}}e^{-(x-x')^2/\Delta^2} \tag{1}$$

If Δ^2 is real and positive, we have

$$\frac{1}{\left(\pi\Delta^2\right)^{1/2}}\int_{-\infty}^{\infty}e^{-(x-x')^2/\Delta^2}dx=1 \tag{2}$$

Thus the area under the curve is always 1, for any real value of Δ^2. Now as $\Delta^2\to 0$ the exponential becomes zero except when $x=x'$. The factor $1/\left(\pi\Delta^2\right)^{1/2}$ tends to infinity as $\Delta^2\to 0$, but the exponential always tends to zero faster than any power of Δ, so $g_\Delta\left(x-x'\right)$ tends to zero everywhere except at $x=x'$. Thus it satisfies the requirements of a delta function: it is zero everywhere except when $x-x'=0$ and has an integral of 1. Thus

$$\lim_{\Delta\to 0}g_\Delta\left(x-x'\right)=\delta\left(x-x'\right) \tag{3}$$

However, if we plug the integral into Maple without any restrictions on Δ^2, it informs us that the integral is still 1 even if Δ^2 is pure imaginary, provided that the imaginary number is positive, that is, we can write $\Delta^2=i\beta^2$ for real β. Thus it would appear that g_Δ still gives a delta function in the limit $\Delta^2\to 0$ even if Δ^2 is a positive imaginary number.

Shankar provides a rationale for this in his footnote to equation 1.10.19. In terms of β we can integrate some smooth function $f\left(x'\right)$ multiplied by g_Δ over a region that includes $x'=x$.

$$\frac{1}{\left(\pi i\beta^2\right)^{1/2}}\int_{-\infty}^{\infty}e^{i(x-x')^2/\beta^2}f\left(x'\right)dx \tag{4}$$

As $\beta^2 \to 0$, the exponent becomes a very large positive imaginary number everywhere except at $x = x'$, so the exponential oscillates very rapidly. Provided that $f(x')$ doesn't vary as rapidly, the integral will contain equal positive and negative contributions everywhere except at $x = x'$ so in the limit of $\beta^2 = 0$, only the point $x = x'$ contributes, which means we can pull $f(x)$ out of the integral and get

$$\lim_{\beta^2 \to 0} \frac{1}{\left(\pi i \beta^2\right)^{1/2}} \int_{-\infty}^{\infty} e^{i(x-x')^2/\beta^2} f\left(x'\right) dx = f(x) \tag{5}$$

Thus 3 is valid for all real Δ and for Δ^2 positive imaginary.

PINGBACKS

Pingback: Path integral formulation of quantum mechanics: free particle propagator

LAGRANGIANS FOR HARMONIC OSCILLATORS

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To leave a comment or report an error, please use the auxiliary blog.

References: Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 2.1; Exercises 2.1.1 - 2.1.2.

Post date: 24 Nov 2016

The Euler-Lagrange equations of motion, derived from the principle of least action are

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{q}_i} - \frac{\partial L}{\partial q_i} = 0 \tag{1}$$

where q_i and $\dot{q}_i$ are the generalized coordinates and velocities, respectively. Here are a couple of simple examples of how these equations can be used to derive equations of motion.

Example 1. The harmonic oscillator. We have a mass m sliding on a frictionless horizontal surface with a spring of spring constant k connected between one end of the mass and a fixed support. The horizontal displacement of the mass from its equilibrium position is given by x, with $x < 0$ when the mass moves to the left, compressing the spring, and $x > 0$ when it moves to the right, stretching the spring.

For systems where the potential energy $V(q_i)$ is independent of the velocities $\dot{q}_i$, the Lagrangian can be written as

$$L = T - V \tag{2}$$

where T is the kinetic energy. In the case of the mass

$$T = \frac{1}{2}m\dot{x}^2 \tag{3}$$

$$V = \frac{1}{2}kx^2 \tag{4}$$

$$L = \frac{1}{2}m\dot{x}^2 - \frac{1}{2}kx^2 \tag{5}$$

described earlier

The equation of motion is

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{q}_i} - \frac{\partial L}{\partial q_i} = m\ddot{x} + kx = 0 \tag{6}$$

$$m\ddot{x} = -kx \tag{7}$$

which is the familiar equation for the force on the mass equal to $-kx$.

Example 2. We can revisit the problem of two masses coupled by three springs, as described earlier. In this case, we have two coordinates x_1 and x_2. The total kinetic energy is

$$T = \frac{1}{2}m\left(\dot{x}_1^2 + \dot{x}_2^2\right) \tag{8}$$

The total potential energy is

$$V = \frac{1}{2}kx_1^2 + \frac{1}{2}k\left(x_2 - x_1\right)^2 + \frac{1}{2}kx_2^2 \tag{9}$$

$$= k\left(x_1^2 + x_2^2 - x_1x_2\right) \tag{10}$$

The Lagrangian and equations of motion are then

$$L = \frac{1}{2}m\left(\dot{x}_1^2 + \dot{x}_2^2\right) - k\left(x_1^2 + x_2^2 - x_1x_2\right) \tag{11}$$

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{x}_1} - \frac{\partial L}{\partial x_1} = m\ddot{x}_1 + 2kx_1 - kx_2 = 0 \tag{12}$$

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{x}_2} - \frac{\partial L}{\partial x_2} = m\ddot{x}_2 + 2kx_2 - kx_1 = 0 \tag{13}$$

This gives the same equations of motion we had earlier.

$$\ddot{x}_1 = -2\frac{k}{m}x_1 + \frac{k}{m}x_2 \tag{14}$$

$$\ddot{x}_2 = \frac{k}{m}x_1 - 2\frac{k}{m}x_2 \tag{15}$$

PINGBACKS

Pingback: Hamiltonians for harmonic oscillators

Pingback: Invariance of Euler-Lagrange and Hamilton's equations under canonical transforma

LAGRANGIAN FOR A SPHERICALLY SYMMETRIC POTENTIAL ENERGY FUNCTION

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To leave a comment or report an error, please use the auxiliary blog.

References: Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 2.1; Exercise 2.1.3.

Post date: 26 Nov 2016

We now consider a more general example of the Euler-Lagrange equations of motion

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{q}_i} - \frac{\partial L}{\partial q_i} = 0 \tag{1}$$

where q_i and $\dot{q}_i$ are the generalized coordinates and velocities, respectively. For systems where the potential energy $V(q_i)$ is independent of the velocities $\dot{q}_i$, the Lagrangian can be written as

$$L = T - V \tag{2}$$

where T is the kinetic energy.

Suppose we consider a system in three dimensions and use spherical coordinates to represent the position of a particle of mass m. We'll restrict ourselves to potential energy functions that depend only on the radial distance r from the origin, so that $V(r, \theta, \phi) = V(r)$. To write down the Lagrangian, we need an expression for the kinetic energy T.

An infinitesimal line element in spherical coordinates has a length ds given by

$$ds^2 = dr^2 + r^2\, d\theta^2 + r^2 \sin^2\theta\, d\phi^2 \tag{3}$$

The square of the velocity is then given by dividing this expression through by dt^2, and using a dot above a symbol to indicate the derivative with respect to time t. We have

$$v^2 = \left(\frac{ds}{dt}\right)^2 = \dot{r}^2 + r^2\dot{\theta}^2 + r^2\sin^2\theta\dot{\phi}^2 \tag{4}$$

The Lagrangian is then

$$L = T - V \tag{5}$$

$$= \frac{1}{2} m \left[\dot{r}^2 + r^2 \dot{\theta}^2 + r^2 \sin^2 \theta \dot{\phi}^2 \right] - V(r) \tag{6}$$

We now get three equations of motion by applying 1 to each coordinate in turn. For r:

$$\frac{d}{dt} \frac{\partial L}{\partial \dot{r}} = \frac{\partial L}{\partial r} \tag{7}$$

$$\ddot{r} = r\dot{\theta}^2 + r \sin^2 \theta \dot{\phi}^2 - \frac{1}{m} \frac{dV}{dr} \tag{8}$$

For θ:

$$\frac{d}{dt} \frac{\partial L}{\partial \dot{\theta}} = \frac{\partial L}{\partial \theta} \tag{9}$$

$$\frac{d}{dt} \left(m r^2 \dot{\theta} \right) = m r^2 \sin \theta \cos \theta \dot{\phi}^2 \tag{10}$$

$$2r\dot{r}\dot{\theta} + r^2 \ddot{\theta} = r^2 \sin \theta \cos \theta \dot{\phi}^2 \tag{11}$$

$$\ddot{\theta} = -\frac{2}{r} \dot{r} \dot{\theta} + \sin \theta \cos \theta \dot{\phi}^2 \tag{12}$$

For ϕ:

$$\frac{d}{dt} \frac{\partial L}{\partial \dot{\phi}} = \frac{\partial L}{\partial \phi} \tag{13}$$

$$\frac{d}{dt} \left(m r^2 \sin^2 \theta \, \dot{\phi} \right) = 0 \tag{14}$$

$$2r\dot{r} \sin^2 \theta \dot{\phi} + 2r^2 \sin \theta \cos \theta \dot{\theta} \dot{\phi} + r^2 \sin^2 \theta \ddot{\phi} = 0 \tag{15}$$

$$\ddot{\phi} = -\frac{2}{r} \dot{r} \dot{\phi} - 2 \cot \theta \dot{\theta} \dot{\phi} \tag{16}$$

Although the only equation in which the potential energy V has a direct effect is the one for r, these three equations constitute a system of non-linear coupled differential equations so in the general case, they can be difficult to solve.

One important special case is that of a path that lies in the plane $\theta = \frac{\pi}{2}$, such as the orbit of a planet around the sun. In that case $\dot{\theta} = 0$, $\sin \theta = 1$ and $\cos \theta = 0$, so the equations simplify to

$$\ddot{r} = r\dot{\phi}^2 - \frac{1}{m}\frac{dV}{dr} \tag{17}$$

$$\ddot{\theta} = 0 \tag{18}$$

$$\ddot{\phi} = -\frac{2}{r}\dot{r}\dot{\phi} \tag{19}$$

ELECTROMAGNETIC LAGRANGIAN

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References: Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 2.2.

Post date: 27 Nov 2016

The Euler-Lagrange equations are

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{q}_i} - \frac{\partial L}{\partial q_i} = 0 \tag{1}$$

where q_i and $\dot{q}_i$ are the generalized coordinates and velocities, respectively. For systems where the potential energy $V(q_i)$ is independent of the velocities $\dot{q}_i$, the Lagrangian can be written as

$$L = T - V \tag{2}$$

where T is the kinetic energy. However, there is one important area in classical physics where the potential *does* depend on velocity, and that is electromagnetism.

The relation between the electric scalar potential ϕ, the magnetic vector potential $\mathbf{A}$ and the electric and magnetic fields $\mathbf{E}$ and $\mathbf{B}$ is given by Maxwell's equations in terms of potentials:

$$\mathbf{E} = -\nabla\phi - \frac{1}{c}\frac{\partial \mathbf{A}}{\partial t} \tag{3}$$

$$\mathbf{B} = \nabla \times \mathbf{A} \tag{4}$$

[These are the forms used by Shankar, which are in Gaussian units. All my earlier posts on electromagnetism are taken from Griffiths's book, which uses the MKS system of units, so various constants will be different in the two systems.]

The force on a charge q due to electric and magnetic fields $\mathbf{E}$ and $\mathbf{B}$ is given by

$$\mathbf{F} = q\left(\mathbf{E} + \frac{\mathbf{v}}{c} \times \mathbf{B}\right) \tag{5}$$

Shankar merely states that the correct force can be derived from 1 if we use the Lagrangian

$$L = \frac{1}{2} m \mathbf{v} \cdot \mathbf{v} - q\phi + \frac{q}{c} \mathbf{v} \cdot \mathbf{A} \tag{6}$$

It appears from a bit of googling that this Lagrangian is obtained more or less by trial and error, rather than by some rigorous derivation, so it seems we just need to accept it "because it works". The velocity **v** in rectangular coordinates is

$$\mathbf{v} = [\dot{x}_1, \dot{x}_2, \dot{x}_3] \tag{7}$$

$$\mathbf{v} \cdot \mathbf{v} = \sum_{i=1}^{3} \dot{x}_i^2 \tag{8}$$

$$\mathbf{v} \cdot \mathbf{A} = \sum_{i=1}^{3} \dot{x}_i A_i \tag{9}$$

Both ϕ and **A** are functions of position, so depend on x_i.

Thus from 1, we have

$$\frac{d}{dt}\left(m\dot{x}_i + \frac{q}{c} A_i\right) = -q \frac{\partial \phi}{\partial x_i} + \frac{q}{c} \frac{\partial \left(\mathbf{v} \cdot \mathbf{A}\right)}{\partial x_i} \tag{10}$$

The three equations represented here can be combined into a single vector equation by noticing that $\frac{\partial}{\partial x_i}$ are the components of the gradient.

$$\frac{d}{dt}\left(m\mathbf{v} + \frac{q}{c}\mathbf{A}\right) = -q\nabla\phi + \frac{q}{c}\nabla\left(\mathbf{v} \cdot \mathbf{A}\right) \tag{11}$$

The LHS contains the total time derivative $\frac{d\mathbf{A}}{dt}$ which is composed of two contributions. First, **A** itself can be time varying, in the sense that if we stayed at the same location, the value of **A** at that location can vary in time. The second contribution comes from the motion of the charge so that, even if **A** is constant in time, the charge will perceive a change in **A** as it moves because **A** can vary over space. That is, the total derivative of the first component A_1 is

$$\frac{dA_1}{dt} = \frac{\partial A_1}{\partial t} + \sum_{i=1}^{3} \frac{\partial A_1}{\partial x_i} \frac{dx_i}{dt} \tag{12}$$

$$= \frac{\partial A_1}{\partial t} + \left(\mathbf{v} \cdot \nabla\right) A_1 \tag{13}$$

The derivative of **A** can thus be written as

$$\frac{d\mathbf{A}}{dt} = \frac{\partial \mathbf{A}}{\partial t} + \left(\mathbf{v} \cdot \nabla\right) \mathbf{A} \tag{14}$$

Plugging this into 11 and rearranging, we get

$$\frac{d}{dt}(m\mathbf{v}) = -q\nabla\phi - \frac{q}{c}\frac{\partial \mathbf{A}}{\partial t} + \frac{q}{c}\left[\nabla(\mathbf{v}\cdot\mathbf{A}) - (\mathbf{v}\cdot\nabla)\mathbf{A}\right] \tag{15}$$

$$\mathbf{F} = -q\nabla\phi - \frac{q}{c}\frac{\partial \mathbf{A}}{\partial t} + \frac{q}{c}(\mathbf{v}\times(\nabla\times\mathbf{A})) \tag{16}$$

$$\mathbf{F} = q\left(\mathbf{E} + \frac{1}{c}\mathbf{v}\times\mathbf{B}\right) \tag{17}$$

In the second line, we used a standard vector identity:

$$\mathbf{v}\times(\nabla\times\mathbf{A}) = \nabla(\mathbf{v}\cdot\mathbf{A}) - (\mathbf{v}\cdot\nabla)\mathbf{A} \tag{18}$$

Thus the Lagrangian 6 does indeed give the correct force law. The Lagrangian is not of the form $T-V$ because the term $q\phi - \frac{q}{c}\mathbf{v}\cdot\mathbf{A}$ isn't a potential energy. In electrostatics, $q\phi$ is indeed potential energy, but because the magnetic force always acts perpendicular to the velocity, it does no work, so we can't interpret $-\frac{q}{c}\mathbf{v}\cdot\mathbf{A}$ as some form of 'magnetic potential energy'. The work done when moving a charge through an electromagnetic field in general depends on the path taken, so is not conservative, and we can't write the force as the gradient of some potential.

PINGBACKS

Pingback: Hamiltonian for the electromagnetic force

Pingback: Path integral to Schrödinger equation for a vector potential

Pingback: Principle of least action - where does it come from?

Pingback: Noether's theorem - internal symmetry of complex scalar field

Pingback: Euler-Lagrange equations for a free particle in an electromagnetic field

LAGRANGIAN FOR THE TWO-BODY PROBLEM

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

References: Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 2.3; Exercise 2.3.1.

Post date: 28 Nov 2016

A fundamental problem in classical physics is the two-body problem, in which two masses interact via a potential $V(\mathbf{r}_1 - \mathbf{r}_2)$ that depends only on the relative positions of the two masses. In such a case, the Lagrangian can be decoupled so that the problem gets reduced to a one-body problem.

The Euler-Lagrange equations are

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{q}_i} - \frac{\partial L}{\partial q_i} = 0 \tag{1}$$

where q_i and $\dot{q}_i$ are the generalized coordinates and velocities, respectively. For systems where the potential energy $V(q_i)$ is independent of the velocities $\dot{q}_i$, the Lagrangian can be written as

$$L = T - V \tag{2}$$

where T is the kinetic energy. In terms of the absolute positions and velocities, we have

$$L = \frac{1}{2}m_1 |\dot{\mathbf{r}}_1|^2 + \frac{1}{2}m_2 |\dot{\mathbf{r}}_2|^2 - V(\mathbf{r}_1 - \mathbf{r}_2) \tag{3}$$

To decouple this equation, we define two new position vectors:

$$\mathbf{r} \equiv \mathbf{r}_1 - \mathbf{r}_2 \tag{4}$$

$$\mathbf{r}_{CM} \equiv \frac{m_1\mathbf{r}_1 + m_2\mathbf{r}_2}{m_1 + m_2} \tag{5}$$

Here $\mathbf{r}$ is the relative position, and $\mathbf{r}_{CM}$ is the position of the centre of mass.

We can invert these equations to get

$$\mathbf{r}_1 = \mathbf{r} + \mathbf{r}_2 \tag{6}$$

$$(m_1 + m_2)\,\mathbf{r}_{CM} = m_1\mathbf{r} + (m_1 + m_2)\,\mathbf{r}_2 \tag{7}$$

$$\mathbf{r}_2 = \mathbf{r}_{CM} - \frac{m_1}{m_1 + m_2}\mathbf{r} \tag{8}$$

$$\mathbf{r}_1 = \mathbf{r}_{CM} - \frac{m_2}{m_1 + m_2}\mathbf{r} \tag{9}$$

To decouple the Lagrangian, we insert these last two equations into 3.

$$m_1 |\dot{\mathbf{r}}_1|^2 = m_1 \left[\dot{\mathbf{r}}_{CM} - \frac{m_2}{m_1 + m_2}\dot{\mathbf{r}}\right] \cdot \left[\dot{\mathbf{r}}_{CM} - \frac{m_2}{m_1 + m_2}\dot{\mathbf{r}}\right] \tag{10}$$

$$= m_1 |\dot{\mathbf{r}}_{CM}|^2 - 2\frac{m_1 m_2}{m_1 + m_2}\dot{\mathbf{r}}_{CM} \cdot \dot{\mathbf{r}} + m_1 \left(\frac{m_2}{m_1 + m_2}\right)^2 |\dot{\mathbf{r}}|^2 \tag{11}$$

$$m_2 |\dot{\mathbf{r}}_2|^2 = m_2 \left[\dot{\mathbf{r}}_{CM} + \frac{m_1}{m_1 + m_2}\dot{\mathbf{r}}\right] \cdot \left[\dot{\mathbf{r}}_{CM} + \frac{m_1}{m_1 + m_2}\dot{\mathbf{r}}\right] \tag{12}$$

$$= m_2 |\dot{\mathbf{r}}_{CM}|^2 + 2\frac{m_1 m_2}{m_1 + m_2}\dot{\mathbf{r}}_{CM} \cdot \dot{\mathbf{r}} + m_2 \left(\frac{m_1}{m_1 + m_2}\right)^2 |\dot{\mathbf{r}}|^2 \tag{13}$$

$$\frac{1}{2}m_1 |\dot{\mathbf{r}}_1|^2 + \frac{1}{2}m_2 |\dot{\mathbf{r}}_2|^2 = \frac{1}{2}(m_1 + m_2) |\dot{\mathbf{r}}_{CM}|^2 + \frac{1}{2}\frac{m_1 m_2^2 + m_2 m_1^2}{(m_1 + m_2)^2} |\dot{\mathbf{r}}|^2 \tag{14}$$

$$= \frac{1}{2}(m_1 + m_2) |\dot{\mathbf{r}}_{CM}|^2 + \frac{1}{2}\frac{m_1 m_2}{m_1 + m_2} |\dot{\mathbf{r}}|^2 \tag{15}$$

The Lagrangian 3 thus becomes

$$L = \frac{1}{2}(m_1 + m_2) |\dot{\mathbf{r}}_{CM}|^2 + \frac{1}{2}\frac{m_1 m_2}{m_1 + m_2} |\dot{\mathbf{r}}|^2 - V(\mathbf{r}) \tag{16}$$

$$\equiv L_{CM} + L_r \tag{17}$$

with

$$L_{CM} \equiv \frac{1}{2}(m_1 + m_2) |\dot{\mathbf{r}}_{CM}|^2 \tag{18}$$

$$L_r \equiv \frac{1}{2}\frac{m_1 m_2}{m_1 + m_2} |\dot{\mathbf{r}}|^2 - V(\mathbf{r}) \tag{19}$$

Thus L decouples into two Lagrangians, one of which depends only on $\dot{\mathbf{r}}_{CM}$ and the other of which depends only on $\mathbf{r}$ and $\dot{\mathbf{r}}$. The absence of $\mathbf{r}_{CM}$ means that, from 1

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{r}_{i,CM}} = \frac{d}{dt}\frac{\partial L_{CM}}{\partial \dot{r}_{i,CM}} = \frac{m_1 + m_2}{2}\frac{d\dot{r}_{i,CM}}{dt} = 0 \tag{20}$$

$$\dot{r}_{i,CM} = \text{constant} \tag{21}$$

which is separately true for each component of $\dot{\mathbf{r}}_{CM}$, which shows that the velocity of the centre of mass is a constant, as we'd expect for an isolated two-body system with no external force.

From the other Lagrangian, we get

$$\frac{m_1 m_2}{m_1 + m_2}\ddot{\mathbf{r}} = -\nabla V(\mathbf{r}) \tag{22}$$

which is the equation of motion of a single particle of mass $\frac{m_1 m_2}{m_1+m_2}$, called the *reduced mass*. Viewed from the centre of mass frame, where $\dot{\mathbf{r}}_{CM} = 0$, $\mathbf{r}$ becomes the absolute position of the reduced mass. We can transform the result back to the 'absolute' frame by using 4.

PINGBACKS

Pingback: Hamiltonian for the two-body problem

HAMILTONIAN FORMALISM AND LEGENDRE TRANSFORMATIONS

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

References: Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 2.5; Exercise 2.5.1.

Post date: 29 Nov 2016

The Lagrangian formulation of classical mechanics is one of two principal formalisms used to obtain equations of motion for a system. The other method is the Hamiltonian formalism. The main difference between the two methods is that the Lagrangian treats the generalized coordinates q_i and their respective velocities $\dot{q}_i$ as the independent variables, while in the Hamiltonian formalism, the coordinates and their associated momenta are the independent variables. The momentum p_i corresponding to a coordinate q_i is defined by

$$p_i \equiv \frac{dL}{d\dot{q}_i} \tag{1}$$

The Lagrangian is replaced by a function $H(q,p)$ (where we're using unsubscripted variables q and p to represent the sets of coordinates and momenta) with the property that

$$\dot{q}_i = \frac{\partial H}{\partial p_i} \tag{2}$$

The method for transforming from the Lagrangian picture to the Hamiltonian picture is known as a *Legendre transformation* and works as follows. Suppose we start with a function $f(x_1, x_2, \ldots, x_n)$ (here, the x_i can be any independent variables; we're not considering coordinates explicitly yet) and we want to replace a subset $\{x_i, i = 1 \ldots, j\}$ with different variables u_i, where

$$u_i \equiv \frac{\partial f}{\partial x_i} \tag{3}$$

We now construct the function

$$g(u_1, \ldots, u_j, x_{j+1}, \ldots, x_n) \equiv \sum_{i=1}^{j} u_i x_i - f(x_1, \ldots, x_n) \tag{4}$$

We're assuming that all the x_i in the set $\{x_i, i = 1 \ldots, j\}$ can be written as functions of $\{u_1, \ldots, u_j, x_{j+1}, \ldots, x_n\}$. In other words, when written out in full, 4 contains only the variables $\{u_1, \ldots, u_j, x_{j+1}, \ldots, x_n\}$. We can now take the derivative:

$$\frac{\partial g}{\partial u_i} = x_i + \sum_{k=1}^{j} \left[u_k \frac{\partial x_k}{\partial u_i} - \frac{\partial f}{\partial x_k} \frac{\partial x_k}{\partial u_i} \right] \tag{5}$$

$$= x_i + \sum_{k=1}^{j} \left[u_k \frac{\partial x_k}{\partial u_i} - u_k \frac{\partial x_k}{\partial u_i} \right] \tag{6}$$

$$= x_i \tag{7}$$

where the second line follows from the definition 3.

To move from the Lagrangian formalism to the Hamiltonian formalism, the Lagrangian plays the role of f, the generalized velocities $\dot{q}_i$ are the variables $\{x_i, i = 1 \ldots, j\}$ to be replaced, and the Hamiltonian is the new function g. That is, we have

$$H(q, p) = \sum_{i=1}^{n} p_i \dot{q}_i - L(q, \dot{q}) \tag{8}$$

There are a total of n momenta p_i and n coordinates q_i, for a total of $2n$ independent coordinates. In 8, it is assumed that we can express all the velocities $\dot{q}_i$ as functions of q_i and p_i. With these definitions, we can see by following through the derivation of 7 that 2 is satisfied.

We can get another equation by considering the derivative

$$\frac{\partial H}{\partial q_i} = \sum_{j=1}^{n} p_j \frac{\partial \dot{q}_j}{\partial q_i} - \frac{\partial L}{\partial q_i} - \sum_{j=1}^{n} \frac{\partial L}{\partial \dot{q}_j} \frac{\partial \dot{q}_j}{\partial q_i} \tag{9}$$

$$= \sum_{j=1}^{n} \left[p_j \frac{\partial \dot{q}_j}{\partial q_i} - \frac{\partial L}{\partial \dot{q}_j} \frac{\partial \dot{q}_j}{\partial q_i} \right] - \frac{\partial L}{\partial q_i} \tag{10}$$

$$= \sum_{j=1}^{n} \left[p_j \frac{\partial \dot{q}_j}{\partial q_i} - p_j \frac{\partial \dot{q}_j}{\partial q_i} \right] - \frac{\partial L}{\partial q_i} \tag{11}$$

$$= -\frac{\partial L}{\partial q_i} \tag{12}$$

$$= -\frac{d}{dt} \frac{\partial L}{\partial \dot{q}_i} \tag{13}$$

$$= -\dot{p}_i \tag{14}$$

In the third line, we used 1, in the fifth line we used the Euler-Lagrange equation

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{q}_i} - \frac{\partial L}{\partial q_i} = 0 \tag{15}$$

and in the last line, we used 1 again. We thus get Hamilton's canonical equations:

$$\frac{\partial H}{\partial p_i} = \dot{q}_i \tag{16}$$

$$-\frac{\partial H}{\partial q_i} = \dot{p}_i \tag{17}$$

[As an aside at this point, I was (and still am) unsure exactly what the term 'canonical' means in this, or in almost any other, context. Google is not very helpful in this respect, as it appears that nobody else really knows where the term came from. According to Wikepedia, the term 'canonical' is used to describe equations in several areas of mathematics, physics and even computer science, but ultimately the term appears to originate in religion, as in 'canon law', which is a system of laws created by the Catholic church. Presumably the term in physics is used to describe some equation or principle which is widely applicable and general. Any other thoughts are welcome in the comments.]

In cases where the potential energy doesn't depend on velocity, the Lagrangian is $T - V$, where T is the kinetic energy. The Hamiltonian (as you've probably guessed) can be interpreted as the total energy of such a system, as we can see as follows.

Using rectangular coordinates, where each mass m_i has a kinetic energy $T_i = \frac{1}{2}m_i\dot{x}_i^2$ (this is true in one dimension; to extend to 3 dimensions, we write $T_i = \frac{1}{2}m_i\left(\dot{x}_i^2 + \dot{y}_i^2 + \dot{z}_i^2\right)$ and the same argument follows). Thus the momentum is

$$p_i = \frac{\partial L}{\partial \dot{x}_i} = \frac{\partial T}{\partial \dot{x}_i} = m_i\dot{x}_i \tag{18}$$

Thus the first term in 8 is

$$\sum_{i=1}^{n} p_i\dot{q}_i = \sum_{i=1}^{n} m_i\dot{x}_i^2 = 2T \tag{19}$$

and the Hamiltonian is

$$H = 2T - L = 2T - T + V = T + V \tag{20}$$

Now consider a more general kinetic energy defined as

$$T = \sum_i \sum_j T_{ij}(q)\,\dot{q}_i \dot{q}_j \tag{21}$$

That is, T is a matrix that depends on the positions of the various masses. We have

$$p_k = \frac{\partial L}{\partial \dot{q}_k} = \frac{\partial T}{\partial \dot{q}_k} \tag{22}$$

$$= \sum_i \sum_j T_{ij}(q)\,\frac{\partial \dot{q}_i}{\partial \dot{q}_k}\dot{q}_j + \sum_i \sum_j T_{ij}(q)\,\dot{q}_i \frac{\partial \dot{q}_j}{\partial \dot{q}_k} \tag{23}$$

$$= \sum_i \sum_j T_{ij}(q)\,\delta_{ik}\dot{q}_j + \sum_i \sum_j T_{ij}(q)\,\dot{q}_i \delta_{jk} \tag{24}$$

$$= \sum_j T_{kj}(q)\,\dot{q}_j + \sum_i T_{ik}(q)\,\dot{q}_i \tag{25}$$

$$= \sum_j \left(T_{kj} + T_{jk}\right)\dot{q}_j \tag{26}$$

The first term in 8 now becomes

$$\sum_k p_k \dot{q}_k = \sum_k \sum_j \left(T_{kj} + T_{jk}\right)\dot{q}_j \dot{q}_k \tag{27}$$

$$= 2T \tag{28}$$

where the last line follows because the RHS of the first line is symmetric under the exchange of j and k.

PINGBACKS

Pingback: Hamiltonians for harmonic oscillators

Pingback: Hamiltonian for the two-body problem

Pingback: Hamiltonian for the electromagnetic force

Pingback: Cyclic coordinates and Poisson brackets

Pingback: Conditions for a transformation to be canonical

Pingback: Invariance of Euler-Lagrange and Hamilton's equations under canonical transforma

Pingback: Hamilton's equations of motion under a regular canonical transformation

Pingback: Postulates of quantum mechanics: states and measurements

Pingback: The classical limit of quantum mechanics; Ehrenfest's theorem

HAMILTONIANS FOR HARMONIC OSCILLATORS

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

References: Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 2.5; Exercises 2.5.2 - 2.5.3.

Post date: 1 Dec 2016

Here are a couple of examples of equations of motion using the Hamiltonian formalism. First, we look at the simple harmonic oscillator, in which we have a mass m sliding on a frictionless horizontal surface. The mass is connected to a spring with constant k, with the other end of the spring connected to a fixed support.

The Hamiltonian is given by

$$H(q,p) = \sum_i p_i \dot{q}_i - L(q,\dot{q}) \tag{1}$$

where the velocities $\dot{q}_i$ are expressed in terms of the positions q_i and momenta p_i. In this case, we have, using the coordinate x as the displacement from equilibrium

$$L(x,\dot{x}) = \frac{1}{2}m\dot{x}^2 - \frac{1}{2}kx^2 \tag{2}$$

$$p = \frac{\partial L}{\partial \dot{x}} = m\dot{x} \tag{3}$$

$$\dot{x} = \frac{p}{m} \tag{4}$$

$$L(x,\dot{x}(x,p)) = \frac{p^2}{2m} - \frac{1}{2}kx^2 \tag{5}$$

$$H = \frac{p^2}{m} - \left(\frac{p^2}{2m} - \frac{1}{2}kx^2\right) \tag{6}$$

$$= \frac{p^2}{2m} + \frac{1}{2}kx^2 \tag{7}$$

We can now apply Hamilton's canonical equations:

$$\frac{\partial H}{\partial p} = \dot{x} \tag{8}$$

$$-\frac{\partial H}{\partial x} = \dot{p} \tag{9}$$

We get

$$\frac{\partial H}{\partial p} = \frac{p}{m} = \dot{x} \tag{10}$$

$$-\frac{\partial H}{\partial x} = -kx = \dot{p} \tag{11}$$

We thus get a pair of first order ODEs which can be solved in the usual way, given $x(0)$ and $p(0)$. The second order ODE that we got by using the Lagrangian method can be obtained by differentiating the first equation and plugging it into the second:

$$\ddot{x} = \frac{\dot{p}}{m} \tag{12}$$

$$= -\frac{k}{m}x \tag{13}$$

From 7 we see that, since in the absence of external force, the total energy $H = T + V = E$ is a constant,

$$\frac{p^2}{2m} + \frac{1}{2}kx^2 = E = \text{constant} \tag{14}$$

This can be written as the equation of an ellipse:

$$\frac{p^2}{b^2} + \frac{x^2}{a^2} = 1 \tag{15}$$

where

$$a^2 = \frac{2E}{k} \tag{16}$$

$$b^2 = 2mE \tag{17}$$

We can use the Hamiltonian formalism to get the equations of motion of the coupled harmonic oscillator. From our Lagrangian treatment, we had

$$L = \frac{1}{2}m\left(\dot{x}_1^2 + \dot{x}_2^2\right) - k\left(x_1^2 + x_2^2 - x_1x_2\right) \tag{18}$$

Converting to coordinates and momenta, we have

$$p_i = \frac{\partial L}{\partial \dot{x}_i} = m\dot{x}_i \tag{19}$$

$$\dot{x}_i = \frac{p_i}{m} \tag{20}$$

$$H = \sum_i p_i \dot{x}_i - L(x, \dot{x}) \tag{21}$$

$$= \frac{1}{m}\left(p_1^2 + p_2^2\right) - \left[\frac{1}{2m} m\left(p_1^2 + p_2^2\right) - k\left(x_1^2 + x_2^2 - x_1 x_2\right)\right] \tag{22}$$

$$= \frac{1}{2m}\left(p_1^2 + p_2^2\right) + k\left(x_1^2 + x_2^2 - x_1 x_2\right) \tag{23}$$

Applying the canonical equations gives

$$\frac{\partial H}{\partial p_i} = \frac{p_i}{m} = \dot{x}_i \tag{24}$$

$$-\frac{\partial H}{\partial x_1} = -2kx_1 + kx_2 = \dot{p}_1 \tag{25}$$

$$-\frac{\partial H}{\partial x_2} = -2kx_2 + kx_1 = \dot{p}_2 \tag{26}$$

Again, by taking the derivative of the first line and substituting into the last two lines, we get back the previous equations of motion:

$$\ddot{x}_1 = -2\frac{k}{m}x_1 + \frac{k}{m}x_2 \tag{27}$$

$$\ddot{x}_2 = \frac{k}{m}x_1 - 2\frac{k}{m}x_2 \tag{28}$$

HAMILTONIAN FOR THE TWO-BODY PROBLEM

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

References: Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 2.5; Exercise 2.5.4.

Post date: 1 Dec 2016

Here we derive the equations of motion of the two-body problem using the Hamiltonian formalism.

The Hamiltonian is given by

$$H(q,p) = \sum_i p_i \dot{q}_i - L(q,\dot{q}) \tag{1}$$

where the velocities $\dot{q}_i$ are expressed in terms of the positions q_i and momenta p_i. In this case, we start with the Lagrangian in terms of the centre of mass position $\mathbf{r}_{CM}$ and the relative position $\mathbf{r}$ of mass 2 to mass 1.

$$L = \frac{1}{2}(m_1+m_2)|\dot{\mathbf{r}}_{CM}|^2 + \frac{1}{2}\frac{m_1 m_2}{m_1+m_2}|\dot{\mathbf{r}}|^2 - V(\mathbf{r}) \tag{2}$$

$$= \frac{M}{2}|\dot{\mathbf{r}}_{CM}|^2 + \frac{\mu}{2}|\dot{\mathbf{r}}|^2 - V(\mathbf{r}) \tag{3}$$

where $M = m_1 + m_2$ is the total mass and $\mu = \frac{m_1 m_2}{m_1+m_2}$ is the reduced mass.

There are potentially 6 velocity components and 6 coordinate components in the Lagrangian, but the 3 components of $\mathbf{r}_{CM}$ do not appear, which simplifies things a bit. To convert to a Hamiltonian, we need the momenta

$$p_i = \frac{\partial L}{\partial \dot{q}_i} \tag{4}$$

The x component of momentum of the centre of mass is

$$p_{CM,x} = \frac{\partial L}{\partial \dot{r}_{CM,x}} = M\dot{r}_{CM,x} \tag{5}$$

The other two components of the centre of mass velocity, and of the relative velocity, have a similar form, and in general we can write

$$p_{CM,i} = M\dot{r}_{CM,i} \tag{6}$$

$$p_i = \mu \dot{r}_i \tag{7}$$

In vector notation, this becomes

$$\dot{\mathbf{r}}_{CM} = \frac{\mathbf{p}_{CM}}{M} \tag{8}$$

$$\dot{\mathbf{r}} = \frac{\mathbf{p}}{\mu} \tag{9}$$

$$|\dot{\mathbf{r}}_{CM}|^2 = \frac{|\mathbf{p}_{CM}|^2}{M^2} \tag{10}$$

$$|\dot{\mathbf{r}}|^2 = \frac{|\mathbf{p}|^2}{\mu^2} \tag{11}$$

The Lagrangian thus becomes

$$L = \frac{|\mathbf{p}_{CM}|^2}{2M} + \frac{|\mathbf{p}|^2}{2\mu} - V(\mathbf{r}) \tag{12}$$

The Hamiltonian is

$$H = \mathbf{p}\cdot\dot{\mathbf{r}} + \mathbf{p}_{CM}\cdot\dot{\mathbf{r}}_{CM} - L \tag{13}$$

$$= \frac{|\mathbf{p}|^2}{\mu} + \frac{|\mathbf{p}_{CM}|^2}{M} - \left[\frac{|\mathbf{p}_{CM}|^2}{2M} + \frac{|\mathbf{p}|^2}{2\mu} - V(\mathbf{r})\right] \tag{14}$$

$$= \frac{|\mathbf{p}_{CM}|^2}{2M} + \frac{|\mathbf{p}|^2}{2\mu} + V(\mathbf{r}) \tag{15}$$

Once we've got the Hamiltonian, we can apply Hamilton's canonical equations to get the equations of motion.

$$\frac{\partial H}{\partial p_i} = \dot{r}_i \tag{16}$$

$$-\frac{\partial H}{\partial r_i} = \dot{p}_i \tag{17}$$

Since $\mathbf{r}_{CM}$ does not appear in the Hamiltonian, we have

$$\dot{\mathbf{p}}_{CM} = 0 \tag{18}$$

$$\mathbf{p}_{CM} = \text{constant} \tag{19}$$

so the momentum of the centre of mass does not change, as expected. For $\mathbf{r}$, we have

$$\frac{\partial H}{\partial p_i} = \frac{p_i}{\mu} = \dot{r}_i \tag{20}$$

$$\frac{\partial H}{\partial r_i} = \frac{\partial V}{\partial r_i} = -\dot{p}_i \tag{21}$$

The first equation tells us nothing new, while the second is just Newton's law for a central force: $\dot{\mathbf{p}} = -\nabla V$.

PINGBACKS

Pingback: Canonical transformations: a few more examples

HAMILTONIAN FOR THE ELECTROMAGNETIC FORCE

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

References: Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 2.6.

Post date: 3 Dec 2016

Here we derive the equations of motion for the electromagnetic force using the Hamiltonian formalism.

The Hamiltonian is given by

$$H(q,p) = \sum_i p_i \dot{q}_i - L(q,\dot{q}) \tag{1}$$

where the velocities $\dot{q}_i$ are expressed in terms of the positions q_i and momenta p_i. The electromagnetic Lagrangian is

$$L = \frac{1}{2} m\mathbf{v}\cdot\mathbf{v} - q\phi + \frac{q}{c}\mathbf{v}\cdot\mathbf{A} \tag{2}$$

where ϕ is the electric potential and $\mathbf{A}$ is the magnetic potential, with $\mathbf{v}$ the velocity of the charge q with mass m. To convert to the Hamiltonian, we need the momentum, defined as

$$p_i = \frac{\partial L}{\partial \dot{q}_i}$$

In this case, the generalized velocity is given by

$$\dot{q}_i = v_i \tag{3}$$

so we have

$$p_i = mv_i + \frac{q}{c}A_i \tag{4}$$

or, in vector notation

$$\mathbf{p} = m\mathbf{v} + \frac{q}{c}\mathbf{A} \tag{5}$$

$$\mathbf{v} = \frac{\mathbf{p}}{m} - \frac{q}{mc}\mathbf{A} \tag{6}$$

The Lagrangian is therefore

$$L = \frac{|\mathbf{p} - q\mathbf{A}/c|^2}{2m} - q\phi + \frac{q}{c}\left(\frac{\mathbf{p}}{m} - \frac{q}{mc}\mathbf{A}\right)\cdot\mathbf{A} \tag{7}$$

The first sum in the Hamiltonian is

$$\sum_i p_i \dot{q}_i = \mathbf{p}\cdot\mathbf{v} = \mathbf{p}\cdot\left(\frac{\mathbf{p}}{m} - \frac{q}{mc}\mathbf{A}\right) \tag{8}$$

The Hamiltonian is then

$$H = \mathbf{p}\cdot\left(\frac{\mathbf{p}}{m} - \frac{q}{mc}\mathbf{A}\right) - \frac{|\mathbf{p} - q\mathbf{A}/c|^2}{2m} + q\phi - \frac{q}{c}\left(\frac{\mathbf{p}}{m} - \frac{q}{mc}\mathbf{A}\right)\cdot\mathbf{A} \tag{9}$$

$$= \left(\frac{\mathbf{p}}{m} - \frac{q}{mc}\mathbf{A}\right)\left(\mathbf{p} - \frac{q}{c}\mathbf{A}\right) - \frac{|\mathbf{p} - q\mathbf{A}/c|^2}{2m} + q\phi \tag{10}$$

$$= \frac{|\mathbf{p} - q\mathbf{A}/c|^2}{2m} + q\phi \tag{11}$$

PINGBACKS

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Pingback: Second-order correction to zeeman effect in hydrogen
Pingback: Klein-Gordon equation - interaction with electromagnetic field
Pingback: Klein-Gordon equation with scalar 1/r potential

CYCLIC COORDINATES AND POISSON BRACKETS

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

References: Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 2.7; Exercises 2.7.1 - 2.7.2.

Post date: 3 Dec 2016

Hamilton's canonical equations are:

$$\frac{\partial H}{\partial p_i} = \dot{q}_i \tag{1}$$

$$-\frac{\partial H}{\partial q_i} = \dot{p}_i \tag{2}$$

If a coordinate q_i is missing in the Hamiltonian (that is, H is indepedent of q_i), then

$$\dot{p}_i = -\frac{\partial H}{\partial q_i} = 0 \tag{3}$$

Thus the conjugate momentum p_i is conserved. Such a missing coordinate q_i is known as a *cyclic coordinate*. [I'm not sure of the origin of this term. Again Google doesn't provide a definitive answer.]

There is a general method for calculating the rate of change of some function $\omega(p, q)$ that depends on the momenta and coordinates, but not explicitly on the time (ω is allowed to depend implicitly on time since p and/or q can depend on time). The time derivative can then be written using the chain rule:

$$\frac{d\omega}{dt} = \sum_i \left(\frac{\partial \omega}{\partial q_i}\dot{q}_i + \frac{\partial \omega}{\partial p_i}\dot{p}_i \right) \tag{4}$$

$$= \sum_i \left(\frac{\partial \omega}{\partial q_i}\frac{\partial H}{\partial p_i} - \frac{\partial \omega}{\partial p_i}\frac{\partial H}{\partial q_i} \right) \tag{5}$$

$$\equiv \{\omega, H\} \tag{6}$$

where in the second line we used Hamilton's equations 1 and 2. The last line defines the *Poisson bracket* of the function ω with the Hamiltonian H. We can see that if $\{\omega, H\} = 0$, the function ω is conserved.

Since $\{H, H\} = 0$ automatically, the total energy (represented by the Hamiltonian) is conserved, provided there is no explicit time dependence.

Such a time dependence can arise if the system is subject to some external force, for example.

From the definition 5 we can derive a few fundamental properties of Poisson brackets. We'll consider a general Poisson bracket between two arbitrary functions $\omega(p,q)$ and $\lambda(p,q)$. Then

$$\{\omega,\lambda\} = \sum_i \left(\frac{\partial\omega}{\partial q_i}\frac{\partial\lambda}{\partial p_i} - \frac{\partial\omega}{\partial p_i}\frac{\partial\lambda}{\partial q_i} \right) \tag{7}$$

$$= -\sum_i \left(\frac{\partial\omega}{\partial p_i}\frac{\partial\lambda}{\partial q_i} - \frac{\partial\omega}{\partial q_i}\frac{\partial\lambda}{\partial p_i} \right) \tag{8}$$

$$= -\sum_i \left(\frac{\partial\lambda}{\partial q_i}\frac{\partial\omega}{\partial p_i} - \frac{\partial\lambda}{\partial p_i}\frac{\partial\omega}{\partial q_i} \right) \tag{9}$$

$$= -\{\lambda,\omega\} \tag{10}$$

A Poisson bracket is distributive, in the sense that

$$\{\omega,\lambda+\sigma\} = \sum_i \left(\frac{\partial\omega}{\partial q_i}\frac{\partial(\lambda+\sigma)}{\partial p_i} - \frac{\partial\omega}{\partial p_i}\frac{\partial(\lambda+\sigma)}{\partial q_i} \right) \tag{11}$$

$$= \sum_i \left(\frac{\partial\omega}{\partial q_i}\left[\frac{\partial\lambda}{\partial p_i}+\frac{\partial\sigma}{\partial p_i}\right] - \frac{\partial\omega}{\partial p_i}\left[\frac{\partial\lambda}{\partial q_i}+\frac{\partial\sigma}{\partial q_i}\right] \right) \tag{12}$$

$$= \sum_i \left(\frac{\partial\omega}{\partial q_i}\frac{\partial\lambda}{\partial p_i} - \frac{\partial\omega}{\partial p_i}\frac{\partial\lambda}{\partial q_i} \right) + \sum_i \left(\frac{\partial\omega}{\partial q_i}\frac{\partial\sigma}{\partial p_i} - \frac{\partial\omega}{\partial p_i}\frac{\partial\sigma}{\partial q_i} \right) \tag{13}$$

$$= \{\omega,\lambda\} + \{\omega,\sigma\} \tag{14}$$

One more identity is useful, which we can derive using the product rule:

$$\{\omega,\lambda\sigma\} = \sum_i \left(\frac{\partial\omega}{\partial q_i}\frac{\partial(\lambda\sigma)}{\partial p_i} - \frac{\partial\omega}{\partial p_i}\frac{\partial(\lambda\sigma)}{\partial q_i} \right) \tag{15}$$

$$= \sum_i \sigma \left(\frac{\partial\omega}{\partial q_i}\frac{\partial\lambda}{\partial p_i} - \frac{\partial\omega}{\partial p_i}\frac{\partial\lambda}{\partial q_i} \right) + \sum_i \lambda \left(\frac{\partial\omega}{\partial q_i}\frac{\partial\sigma}{\partial p_i} - \frac{\partial\omega}{\partial p_i}\frac{\partial\sigma}{\partial q_i} \right) \tag{16}$$

$$= \{\omega,\lambda\}\,\sigma + \{\omega,\sigma\}\,\lambda \tag{17}$$

The Poisson brackets involving the coordinates q_i and momenta p_i turn up frequently, so it's worth deriving them in detail. We have

$$\{q_i,q_j\} = \sum_k \left(\frac{\partial q_i}{\partial q_k}\frac{\partial q_j}{\partial p_k} - \frac{\partial q_i}{\partial p_k}\frac{\partial q_j}{\partial q_k} \right) = 0 \tag{18}$$

This follows because, in the Hamiltonian formalism, the q_is and p_is are independent variables, so $\frac{\partial q_j}{\partial p_k} = \frac{\partial p_j}{\partial q_k} = 0$ for all j and k. For the same reason, we have

$$\{p_i, p_j\} = \sum_k \left(\frac{\partial p_i}{\partial q_k}\frac{\partial p_j}{\partial p_k} - \frac{\partial p_i}{\partial p_k}\frac{\partial p_j}{\partial q_k} \right) = 0 \tag{19}$$

The mixed Poisson bracket is a different story, however:

$$\{q_i, p_j\} = \sum_k \left(\frac{\partial q_i}{\partial q_k}\frac{\partial p_j}{\partial p_k} - \frac{\partial q_i}{\partial p_k}\frac{\partial p_j}{\partial q_k} \right) \tag{20}$$

$$= \sum_k \delta_{ik}\delta_{jk} - 0 \tag{21}$$

$$= \delta_{ij} \tag{22}$$

Hamilton's equations 1 and 2 can be written using Poisson brackets by setting ω equal to q_i and p_i respectively in 6:

$$\dot{q}_i = \{q_i, H\} \tag{23}$$

$$\dot{p}_i = \{p_i, H\} \tag{24}$$

Example. In two dimensions, we have a Hamiltonian:

$$H = p_x^2 + p_y^2 + ax^2 + by^2 \tag{25}$$

If $a = b$, then in polar coordiantes, the only coordinate appearing in H is the radial distance from the origin $r = \sqrt{x^2 + y^2}$, which means that the polar angle θ is a cyclic coordinate. This means that the conjugate momentum p_θ must be conserved. That is,

$$\dot{p}_\theta = \{p_\theta, H\} = 0 \tag{26}$$

However, p_θ is the angular momentum ℓ_z, so this just says that angular momentum is conserved.

To see this explicitly, it's easier to convert to polar coordinates. From Hamilton's equations

$$\dot{x} = \frac{\partial H}{\partial p_x} = 2p_x \tag{27}$$

$$\dot{y} = 2p_y \tag{28}$$

$$p_x^2 + p_y^2 = \frac{1}{4}\left(\dot{x}^2 + \dot{y}^2\right) \tag{29}$$

$$= \frac{v^2}{4} \tag{30}$$

$$= \frac{1}{4}\left(\dot{r}^2 + r^2\dot{\theta}^2\right) \tag{31}$$

where in the fourth line, v is the linear velocity and in the fifth line we converted this to polar coordinates. Thus the Hamiltonian becomes, in the case where $a = b$:

$$H = \frac{1}{4}\left(\dot{r}^2 + r^2\dot{\theta}^2\right) + ar^2 \tag{32}$$

To find the conjugate momenta in polar coordinates, we can write out the Lagrangian. We use $p_x\dot{x} = \frac{\dot{x}^2}{2}$ and $p_y\dot{y} = \frac{\dot{y}^2}{2}$ and get

$$L = \sum_i p_i\dot{q}_i - H \tag{33}$$

$$= \frac{1}{2}\left(\dot{x}^2 + \dot{y}^2\right) - \frac{1}{4}\left(\dot{r}^2 + r^2\dot{\theta}^2\right) - ar^2 \tag{34}$$

$$= \frac{1}{4}\left(\dot{r}^2 + r^2\dot{\theta}^2\right) - ar^2 \tag{35}$$

The conjugate momenta are thus

$$p_\theta = \frac{\partial L}{\partial \dot{\theta}} = \frac{1}{2}r^2\dot{\theta} \tag{36}$$

$$p_r = \frac{\partial L}{\partial \dot{r}} = \frac{\dot{r}}{2} \tag{37}$$

From this we can see that p_θ is indeed angular momentum as it's proportional to the product of r and the tangential velocity $v_\theta = r\dot{\theta}$. ('Real' momentum and angular momentum must, of course, also contain a factor of a mass, but from the definition of the Hamiltonian above, we see that the mass has been incorporated into the momentum parameters.)

Plugging these back into 32 we get

$$H = p_r^2 + p_\theta^2 + ar^2 \tag{38}$$

We can now calculate the Poisson brackets easily:

$$\{p_\theta, H\} = \sum_i \left(\frac{\partial p_\theta}{\partial q_i}\frac{\partial H}{\partial p_i} - \frac{\partial p_\theta}{\partial p_i}\frac{\partial H}{\partial q_i} \right) \tag{39}$$

$$= 0 - \frac{\partial p_\theta}{\partial p_\theta}\frac{\partial H}{\partial \theta} = 0 \tag{40}$$

$$\{p_r, H\} = \sum_i \left(\frac{\partial p_r}{\partial q_i}\frac{\partial H}{\partial p_i} - \frac{\partial p_r}{\partial p_i}\frac{\partial H}{\partial q_i} \right) \tag{41}$$

$$= 0 - \frac{\partial p_r}{\partial p_r}\frac{\partial H}{\partial r} \tag{42}$$

$$= -2ar \tag{43}$$

Thus p_θ (the angular momentum) is conserved, while $p_r < 0$, so that the object is always being pulled in towards the origin.

PINGBACKS

Pingback: Conditions for a transformation to be canonical

Pingback: Poisson brackets are invariant under a canonical transformation

Pingback: Passive, regular and active transformations.

Pingback: The classical limit of quantum mechanics; Ehrenfest's theorem

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Pingback: Nonrelativistic field theory - Schrödinger equation

Pingback: Poisson brackets, commutators and Jacobi identity

CONDITIONS FOR A TRANSFORMATION TO BE CANONICAL

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To leave a comment or report an error, please use the auxiliary blog.

References: Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 2.7; Exercise 2.7.3.

Post date: 5 Dec 2016

We've seen that the Euler-Lagrange equations are invariant under canonical transformations, but in the Hamiltonian formalism where the system moves in a $2n$-dimensional phase space with n coordinates q and n momenta p, more general transformations are possible:

$$\overline{q}_i = \overline{q}_i(q,p) \tag{1}$$
$$\overline{p}_i = \overline{p}_i(q,p) \tag{2}$$

In order for such a transformation to be canonical, we require that the new variables $\overline{q}$ and $\overline{p}$ satisfy Hamilton's equations, that is

$$\frac{\partial H}{\partial \overline{p}_i} = \dot{\overline{q}}_i \tag{3}$$
$$-\frac{\partial H}{\partial \overline{q}_i} = \dot{\overline{p}}_i \tag{4}$$

In principle, then, we could check the Hamiltonian in the new coordinates to see if these equations are valid, but it would seem that whether or not a set of coordinates and momenta is canonical should be determinable from the variables themselves, and not depend on the specific Hamiltonian. Here we derive a set of conditions on the $\overline{q}$ and $\overline{p}$ that determine whether or not the transformation is canonical.

The time derivative of any function ω can be written as a Poisson bracket:

$$\dot{\omega} = \{\omega, H\} \tag{5}$$

For the transformed velocities, we have

$$\dot{\overline{q}}_j = \left\{\overline{q}_j, H\right\} \tag{6}$$
$$= \sum_i \left(\frac{\partial \overline{q}_j}{\partial q_i}\frac{\partial H}{\partial p_i} - \frac{\partial \overline{q}_j}{\partial p_i}\frac{\partial H}{\partial q_i} \right) \tag{7}$$

Here, H is written as a function $H(q,p)$ of the original variables. If we write it as a function of the transformed variables, we can find the two derivatives of H in 7 by using the chain rule:

$$\frac{\partial H(\overline{q},\overline{p})}{\partial p_i} = \sum_k \left(\frac{\partial H}{\partial \overline{q}_k}\frac{\partial \overline{q}_k}{\partial p_i} + \frac{\partial H}{\partial \overline{p}_k}\frac{\partial \overline{p}_k}{\partial p_i} \right) \tag{8}$$

$$\frac{\partial H(\overline{q},\overline{p})}{\partial q_i} = \sum_k \left(\frac{\partial H}{\partial \overline{q}_k}\frac{\partial \overline{q}_k}{\partial q_i} + \frac{\partial H}{\partial \overline{p}_k}\frac{\partial \overline{p}_k}{\partial q_i} \right) \tag{9}$$

Inserting these into 7 we get

$$\dot{\overline{q}}_j = \sum_i \sum_k \left[\frac{\partial \overline{q}_j}{\partial q_i} \left(\frac{\partial H}{\partial \overline{q}_k}\frac{\partial \overline{q}_k}{\partial p_i} + \frac{\partial H}{\partial \overline{p}_k}\frac{\partial \overline{p}_k}{\partial p_i} \right) - \frac{\partial \overline{q}_j}{\partial p_i} \left(\frac{\partial H}{\partial \overline{q}_k}\frac{\partial \overline{q}_k}{\partial q_i} + \frac{\partial H}{\partial \overline{p}_k}\frac{\partial \overline{p}_k}{\partial q_i} \right) \right] \tag{10}$$

$$= \sum_k \frac{\partial H}{\partial \overline{q}_k} \sum_i \left(\frac{\partial \overline{q}_j}{\partial q_i}\frac{\partial \overline{q}_k}{\partial p_i} - \frac{\partial \overline{q}_j}{\partial p_i}\frac{\partial \overline{q}_k}{\partial q_i} \right) + \sum_k \frac{\partial H}{\partial \overline{p}_k} \sum_i \left(\frac{\partial \overline{q}_j}{\partial q_i}\frac{\partial \overline{p}_k}{\partial p_i} - \frac{\partial \overline{q}_j}{\partial p_i}\frac{\partial \overline{p}_k}{\partial q_i} \right) \tag{11}$$

$$= \sum_k \frac{\partial H}{\partial \overline{q}_k} \left\{ \overline{q}_j, \overline{q}_k \right\} + \sum_k \frac{\partial H}{\partial \overline{p}_k} \left\{ \overline{q}_j, \overline{p}_k \right\} \tag{12}$$

In order for this result to satisfy 3, we must have

$$\left\{ \overline{q}_j, \overline{q}_k \right\} = 0 \tag{13}$$

$$\left\{ \overline{q}_j, \overline{p}_k \right\} = \delta_{jk} \tag{14}$$

We can repeat the calculation for $\dot{\overline{p}}_i$:

$$\dot{\overline{p}}_j = \left\{ \overline{p}_j, H \right\} \tag{15}$$

$$= \sum_i \left(\frac{\partial \overline{p}_j}{\partial q_i}\frac{\partial H}{\partial p_i} - \frac{\partial \overline{p}_j}{\partial p_i}\frac{\partial H}{\partial q_i} \right) \tag{16}$$

$$= \sum_i \sum_k \left[\frac{\partial \overline{p}_j}{\partial q_i} \left(\frac{\partial H}{\partial \overline{q}_k}\frac{\partial \overline{q}_k}{\partial p_i} + \frac{\partial H}{\partial \overline{p}_k}\frac{\partial \overline{p}_k}{\partial p_i} \right) - \frac{\partial \overline{p}_j}{\partial p_i} \left(\frac{\partial H}{\partial \overline{q}_k}\frac{\partial \overline{q}_k}{\partial q_i} + \frac{\partial H}{\partial \overline{p}_k}\frac{\partial \overline{p}_k}{\partial q_i} \right) \right] \tag{17}$$

$$= \sum_k \frac{\partial H}{\partial \overline{q}_k} \sum_i \left(\frac{\partial \overline{p}_j}{\partial q_i}\frac{\partial \overline{q}_k}{\partial p_i} - \frac{\partial \overline{p}_j}{\partial p_i}\frac{\partial \overline{q}_k}{\partial q_i} \right) + \sum_k \frac{\partial H}{\partial \overline{p}_k} \sum_i \left(\frac{\partial \overline{p}_j}{\partial q_i}\frac{\partial \overline{p}_k}{\partial p_i} - \frac{\partial \overline{p}_j}{\partial p_i}\frac{\partial \overline{p}_k}{\partial q_i} \right) \tag{18}$$

$$= \sum_k \frac{\partial H}{\partial \overline{q}_k} \left\{ \overline{p}_j, \overline{q}_k \right\} + \sum_k \frac{\partial H}{\partial \overline{p}_k} \left\{ \overline{p}_j, \overline{p}_k \right\} \tag{19}$$

Requiring this to satsify 4, we have

$$\left\{\overline{p}_j, \overline{p}_k\right\} = 0 \tag{20}$$

$$\left\{\overline{p}_j, \overline{q}_k\right\} = -\delta_{jk} \tag{21}$$

The last equation is equivalent to

$$\left\{\overline{q}_j, \overline{p}_k\right\} = \delta_{jk} \tag{22}$$

which agrees with 14. Thus in order for the transformation to be canonical, the conditions are

$$\left\{\overline{q}_j, \overline{q}_k\right\} = \left\{\overline{p}_j, \overline{p}_k\right\} = 0 \tag{23}$$

$$\left\{\overline{q}_j, \overline{p}_k\right\} = \delta_{jk} \tag{24}$$

Note that these Poisson brackets require calculating the derivatives of the new variables $\overline{q}$ and $\overline{p}$ with respect to the original ones q and p, but they *don't* involve any particular Hamiltonian. Thus it's possible to determine whether or not a transformation is canonical entirely from the transformation equations 1 and 2.

PINGBACKS

Pingback: Canonical transformations in 2-d: rotations and polar coordinates

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Pingback: Poisson brackets are invariant under a canonical transformation

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CANONICAL TRANSFORMATIONS IN 2-D: ROTATIONS AND POLAR COORDINATES

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To leave a comment or report an error, please use the auxiliary blog.

References: Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 2.7; Exercises 2.7.4 - 2.7.5.

Post date: 5 Dec 2016

Here are a couple of examples of canonical variable transformations.

Example 1. We rotate the 2-d rectangular coordinates through an angle θ, giving the transformations

$$\overline{x} = x\cos\theta - y\sin\theta \tag{1}$$
$$\overline{y} = x\sin\theta + y\cos\theta \tag{2}$$
$$\overline{p}_x = p_x\cos\theta - p_y\sin\theta \tag{3}$$
$$\overline{p}_y = p_x\sin\theta + p_y\cos\theta \tag{4}$$

To show this is a canonical transformation, we must evaluate the Poisson brackets. Here, $q_1 = x$ and $q_2 = y$. Remember that θ is a constant in these derivatives.

$$\{\overline{x},\overline{y}\} = \sum_i \left(\frac{\partial\overline{x}}{\partial q_i}\frac{\partial\overline{y}}{\partial p_i} - \frac{\partial\overline{x}}{\partial p_i}\frac{\partial\overline{y}}{\partial q_i}\right) \tag{5}$$
$$= 0 \tag{6}$$

since neither coordinate depends on any momentum. Similarly $\left\{\overline{p}_x,\overline{p}_y\right\} = 0$ since this Poisson bracket contains derivatives of $\overline{p}_i$ with respect to q_i and these are all zero. The remaining Poisson bracket are of the form $\left\{\overline{q}_i,\overline{p}_j\right\}$. There are four of these, but we'll work out only a couple. The other two have similar forms.

$$\{\overline{x},\overline{p}_x\} = \sum_i \left(\frac{\partial \overline{x}}{\partial q_i}\frac{\partial \overline{p}_x}{\partial p_i} - \frac{\partial \overline{x}}{\partial p_i}\frac{\partial \overline{p}_x}{\partial q_i} \right) \tag{7}$$

$$= \frac{\partial \overline{x}}{\partial x}\frac{\partial \overline{p}_x}{\partial p_x} + \frac{\partial \overline{x}}{\partial y}\frac{\partial \overline{p}_x}{\partial p_y} \tag{8}$$

$$= \cos^2\theta + \sin^2\theta \tag{9}$$

$$= 1 \tag{10}$$

$$\{\overline{x},\overline{p}_y\} = \sum_i \left(\frac{\partial \overline{x}}{\partial q_i}\frac{\partial \overline{p}_y}{\partial p_i} - \frac{\partial \overline{x}}{\partial p_i}\frac{\partial \overline{p}_y}{\partial q_i} \right) \tag{11}$$

$$= \frac{\partial \overline{x}}{\partial x}\frac{\partial \overline{p}_y}{\partial p_x} + \frac{\partial \overline{x}}{\partial y}\frac{\partial \overline{p}_y}{\partial p_y} \tag{12}$$

$$= \sin\theta\cos\theta - \sin\theta\cos\theta \tag{13}$$

$$= 0 \tag{14}$$

Similarly

$$\{\overline{y},\overline{p}_x\} = 0 \tag{15}$$

$$\{\overline{y},\overline{p}_y\} = 1 \tag{16}$$

Example 2. The transformation from 2-d rectangular to polar coordinates is given by

$$\rho = \sqrt{x^2+y^2} \tag{17}$$

$$\phi = \arctan\frac{y}{x} \tag{18}$$

$$p_\rho = \frac{xp_x + yp_y}{\sqrt{x^2+y^2}} \tag{19}$$

$$p_\phi = xp_y - yp_x \tag{20}$$

For the Poisson brackets we have

$$\{\rho,\phi\} = \sum_i \left(\frac{\partial \rho}{\partial q_i}\frac{\partial \phi}{\partial p_i} - \frac{\partial \rho}{\partial p_i}\frac{\partial \phi}{\partial q_i} \right) \tag{21}$$

$$= 0 \tag{22}$$

because, again, the coordinates don't depend on the momenta.

In this case, however, the new momenta do depend on the old coordinates, so we need to actually do some calculation.

$$\{p_\rho, p_\phi\} = \sum_i \left(\frac{\partial p_\rho}{\partial q_i}\frac{\partial p_\phi}{\partial p_i} - \frac{\partial p_\rho}{\partial p_i}\frac{\partial p_\phi}{\partial q_i} \right) \tag{23}$$

$$= \left(-\frac{x\left(xp_x + yp_y\right)}{\left(x^2+y^2\right)^{3/2}} + \frac{p_x}{\sqrt{x^2+y^2}} \right)(-y) - \frac{x}{\sqrt{x^2+y^2}}p_y +$$

$$\left(-\frac{y\left(xp_x + yp_y\right)}{\left(x^2+y^2\right)^{3/2}} + \frac{p_y}{\sqrt{x^2+y^2}} \right)x - \frac{y}{\sqrt{x^2+y^2}}\left(-p_x\right) \tag{24}$$

$$= -\frac{y^2\left(yp_x - xp_y\right)}{\left(x^2+y^2\right)^{3/2}} - \frac{x}{\sqrt{x^2+y^2}}p_y - \frac{x^2\left(yp_x - xp_y\right)}{\left(x^2+y^2\right)^{3/2}} + \frac{y}{\sqrt{x^2+y^2}}p_x \tag{25}$$

$$= -\frac{y^3p_x + x^3p_y}{\left(x^2+y^2\right)^{3/2}} + \frac{y^3p_x + x^3p_y}{\left(x^2+y^2\right)^{3/2}} \tag{26}$$

$$= 0 \tag{27}$$

Finally, we need to work out the mixed brackets.

$$\{\rho, p_\rho\} = \sum_i \left(\frac{\partial \rho}{\partial q_i}\frac{\partial p_\rho}{\partial p_i} - \frac{\partial \rho}{\partial p_i}\frac{\partial p_\rho}{\partial q_i} \right) \tag{28}$$

$$= \frac{x^2}{x^2+y^2} - 0 + \frac{y^2}{x^2+y^2} - 0 \tag{29}$$

$$= 1 \tag{30}$$

$$\{\rho, p_\phi\} = \sum_i \left(\frac{\partial \rho}{\partial q_i}\frac{\partial p_\phi}{\partial p_i} - \frac{\partial \rho}{\partial p_i}\frac{\partial p_\phi}{\partial q_i} \right) \tag{31}$$

$$= -\frac{xy}{\sqrt{x^2+y^2}} - 0 + \frac{xy}{\sqrt{x^2+y^2}} - 0 \tag{32}$$

$$= 0 \tag{33}$$

$$\{\phi, p_\rho\} = \sum_i \left(\frac{\partial \phi}{\partial q_i}\frac{\partial p_\rho}{\partial p_i} - \frac{\partial \phi}{\partial p_i}\frac{\partial p_\rho}{\partial q_i} \right) \tag{34}$$

$$= -\frac{y}{x\left(1+\frac{y^2}{x^2}\right)\sqrt{x^2+y^2}} - 0 + \frac{y}{x\left(1+\frac{y^2}{x^2}\right)\sqrt{x^2+y^2}} - 0 \tag{35}$$

$$= 0 \tag{36}$$

$$\{\phi, p_\phi\} = \sum_i \left(\frac{\partial \phi}{\partial q_i}\frac{\partial p_\phi}{\partial p_i} - \frac{\partial \phi}{\partial p_i}\frac{\partial p_\phi}{\partial q_i} \right) \tag{37}$$

$$= \frac{y^2}{x^2\left(1+\frac{y^2}{x^2}\right)} - 0 + \frac{1}{1+\frac{y^2}{x^2}} - 0 \tag{38}$$

$$= \frac{y^2}{x^2+y^2} + \frac{x^2}{x^2+y^2} \tag{39}$$

$$= 1 \tag{40}$$

Thus all the Poisson brackets are correct, so the transformation is canonical.

PINGBACKS

Pingback: Infinitesimal rotations in canonical and noncanonical transformations

CANONICAL TRANSFORMATIONS: A FEW MORE EXAMPLES

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References: Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 2.7; Exercises 02.07.06 - 02.07.07, 02.07.08(4).

Post date: 6 Dec 2016

Here are a few more examples of canonical variable transformations.

Example 1. First, we revisit the two-body problem, in which we simplified the problem by transforming from the coordinates $\mathbf{r}_1$ and $\mathbf{r}_2$ of the masses m_1 and m_2 to two new position vectors:

$$\begin{aligned} \mathbf{r} &\equiv \mathbf{r}_1 - \mathbf{r}_2 && (1) \\ \mathbf{r}_{CM} &\equiv \frac{m_1\mathbf{r}_1 + m_2\mathbf{r}_2}{M} && (2) \end{aligned}$$

Here $M \equiv m_1 + m_2$ is the total mass, $\mathbf{r}$ is the relative position, and $\mathbf{r}_{CM}$ is the position of the centre of mass. The conjugate momenta in the original system are

$$\mathbf{p}_i = m\dot{\mathbf{r}}_i \tag{3}$$

The conjugate momenta transform according to

$$\begin{aligned} \mathbf{p}_{CM} &= M\mathbf{r}_{CM} = \mathbf{p}_1 + \mathbf{p}_2 && (4) \\ \mathbf{p} &= \mu\dot{\mathbf{r}} && (5) \\ &= \frac{m_2\mathbf{p}_1 - m_1\mathbf{p}_2}{M} && (6) \end{aligned}$$

where $\mu = m_1m_2/M$ is the reduced mass.

To check that this is a canonical transformation, we need to calculate the Poisson brackets. To make things easier, note that the new coordinates depend only on the old coordinates (and not on the momenta), and conversely, the new momenta depend only on the old momenta (and not on the coordinates). Since the Poisson brackets $\left\{\overline{q}_i, \overline{q}_j\right\}$and $\left\{\overline{p}_i, \overline{p}_j\right\}$all involve taking derivatives of coordinates with respect to momenta (in the first case) or momenta with respect to coordinates (in the second case), all these brackets are zero. We need, therefore, to check only the mixed brackets between coordinates and momenta.

Because we're dealing with 3-d vector equations, there are 3 components to each vector and to be thorough, we need to calculate all possible brackets between all pairs of components. However, if we do the x component of each, it should be obvious that the y and z components behave in the same way.

First, consider

$$\{r_x, p_x\} = \sum_i \left(\frac{\partial r_x}{\partial q_i} \frac{\partial p_x}{\partial p_i} - \frac{\partial r_x}{\partial p_i} \frac{\partial p_x}{\partial q_i} \right) \tag{7}$$

In the RHS, the term q_i stands for all 6 components of the original position vectors, that is $q_i = \{r_{1x}, r_{1y}, \ldots, r_{2z}\}$ and the term p_i in the denominators refers to all 6 components of the original momentum vectors. The p_x in the numerators refers to the x component of $\mathbf{p}$ in 6. Hopefully this won't cause too much confusion.

The second term on the RHS is zero because it involves derivatives of coordinates with respect to momenta (and vice versa). In the first term, r_x depends only the x components of $\mathbf{r}_1$ and $\mathbf{r}_2$, and p_x depends only on the x components of $\mathbf{p}_1$and $\mathbf{p}_2$, so we have

$$\begin{aligned} \{r_x, p_x\} &= \frac{\partial r_x}{\partial r_{1x}} \frac{\partial p_x}{\partial p_{1x}} + \frac{\partial r_x}{\partial r_{2x}} \frac{\partial p_x}{\partial p_{2x}} && (8) \\ &= (1) \frac{m_2}{M} + (-1) \left(-\frac{m_1}{M} \right) && (9) \\ &= \frac{m_1 + m_2}{M} && (10) \\ &= 1 && (11) \end{aligned}$$

The same result is obtained for the y and z components. If we look at mixing two different components, we have, for example

$$\{r_x, p_y\} = \frac{\partial r_x}{\partial r_{1x}} \frac{\partial p_y}{\partial p_{1x}} + \frac{\partial r_x}{\partial r_{2x}} \frac{\partial p_y}{\partial p_{2x}} + \frac{\partial r_x}{\partial r_{1y}} \frac{\partial p_y}{\partial p_{1y}} + \frac{\partial r_x}{\partial r_{2y}} \frac{\partial p_y}{\partial p_{2y}} = 0 \tag{12}$$

This is zero because each term in the sum contains a derivative of an x component with respect to a y component (or vice versa), all of which are zero.

For the centre of mass components, we have

$$\{r_{CMx}, p_{CMx}\} = \frac{\partial r_{CMx}}{\partial r_{1x}}\frac{\partial p_{CMx}}{\partial p_{1x}} + \frac{\partial r_{CMx}}{\partial r_{2x}}\frac{\partial p_{CMx}}{\partial p_{2x}} \tag{13}$$

$$= \frac{m_1}{M}(1) + \frac{m_2}{M}(1) \tag{14}$$

$$= 1 \tag{15}$$

$$\{r_{CMx}, p_{CMy}\} = \frac{\partial r_{CMx}}{\partial r_{1x}}\frac{\partial p_{CMy}}{\partial p_{1x}} + \frac{\partial r_{CMx}}{\partial r_{2x}}\frac{\partial p_{CMy}}{\partial p_{2x}} + \frac{\partial r_{CMx}}{\partial r_{1y}}\frac{\partial p_{CMy}}{\partial p_{1y}} + \frac{\partial r_{CMx}}{\partial r_{2y}}\frac{\partial p_{CMy}}{\partial p_{2y}} \tag{16}$$

$$= 0 \tag{17}$$

where the last bracket is zero for the same reason as $\{r_x, p_y\}$: we're mixing x and y in the derivatives. Again, it should be obvious that the brackets for the other combinations of x, y and z components work out the same way. We can also verify that the Poisson brackets between relative and centre of mass coordinates are zero by the same method. That is

$$\{r_{CMi}, p_j\} = \{r_i, p_{CMj}\} = 0 \tag{18}$$

where i and j take on the values x, y and z.

Example 2. A bizarre transformation of variables in one dimension is given by

$$\overline{q} = \ln\frac{\sin p}{q} = \ln\sin p - \ln q \tag{19}$$

$$\overline{p} = q\cot p \tag{20}$$

To show this is canonical, we need calculate only $\{\overline{q}, \overline{p}\}$ (since the Poisson bracket of a function with itself is always zero, we have $\{\overline{q}, \overline{q}\} = \{\overline{p}, \overline{p}\} = 0$). We need one rather obscure derivative of a trig function.

$$\frac{d}{dp}\cot p = \frac{d}{dp}\left(\frac{\cos p}{\sin p}\right) \tag{21}$$

$$= \frac{-\sin^2 p - \cos^2 p}{\sin^2 p} \tag{22}$$

$$= -1 - \cot^2 p \tag{23}$$

We get

$$\{\overline{q},\overline{p}\} = \frac{\partial\overline{q}}{\partial q}\frac{\partial\overline{p}}{\partial p} - \frac{\partial\overline{q}}{\partial p}\frac{\partial\overline{p}}{\partial q} \tag{24}$$

$$= \left(-\frac{1}{q}\right)\left(q\left(-1-\cot^2 p\right)\right) - \frac{\cos p}{\sin p}\cot p \tag{25}$$

$$= 1+\cot^2 p - \cot^2 p \tag{26}$$

$$= 1 \tag{27}$$

Thus the transformation is canonical.

Example 3. Finally, we return to the point transformation, which is given in general by

$$\overline{q}_i = \overline{q}_i(q_1,\ldots,q_n) \tag{28}$$

$$\overline{p}_i = \sum_j \frac{\partial q_j}{\partial\overline{q}_i}p_j \tag{29}$$

In this case, the coordinate transformation to $\overline{q}$ is completely arbitrary, but the momentum transformation must follow the formula given. The derivatives $\frac{\partial q_i}{\partial\overline{q}_j}$ in the formula for $\overline{p}_i$ are taken at constant $\overline{q}$. As in the earlier examples, since the coordinate formulas depend only on the old coordinates, and the momentum formulas depend only on the old momenta, the Poisson brackets satisfy

$$\left\{\overline{q}_i,\overline{q}_j\right\} = \left\{\overline{p}_i,\overline{p}_j\right\} = 0 \tag{30}$$

For the mixed brackets, we have

$$\left\{\overline{q}_i,\overline{p}_j\right\} = \sum_k\left(\frac{\partial\overline{q}_i}{\partial q_k}\frac{\partial\overline{p}_j}{\partial p_k} - \frac{\partial\overline{q}_i}{\partial p_k}\frac{\partial\overline{p}_j}{\partial q_k}\right) \tag{31}$$

$$= \sum_k \frac{\partial\overline{q}_i}{\partial q_k}\frac{\partial q_k}{\partial\overline{q}_j} \tag{32}$$

$$= \frac{\partial\overline{q}_i}{\partial\overline{q}_j} \tag{33}$$

$$= \delta_{ij} \tag{34}$$

The second term in the first line is zero (mixed derivatives again). We used 29 to calculate the derivative $\frac{\partial\overline{p}_j}{\partial p_k}$ and get the second line and then notice that the sum is an expansion of the chain rule for the derivative in line 3. Since $\overline{q}_i$ and $\overline{q}_j$ are independent variables, the result is that given in the last line. Thus a point transformation is a canonical transformation.

INVARIANCE OF EULER-LAGRANGE AND HAMILTON'S EQUATIONS UNDER CANONICAL TRANSFORMATIONS

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

References: Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 2.7; Exercise 2.7.8 (1-3).

Post date: 4 Dec 2016

Here we'll investigate how the Euler-Lagrange equations and Hamilton's canonical equations are affected by a change in coordinates of the form

$$q_i \rightarrow \overline{q}_i\left(q_1, \ldots, q_n\right) \tag{1}$$

Note that the new coordinates $\overline{q}$ depend only on the old coordinates and not on the velocities $\dot{q}_i$. We also assume that the transformation is invertible, so it's possible to find the q_i as functions of the $\overline{q}_i$.

First, we need to show that the Euler-Lagrange equations are invariant under such a transformation. Starting with the inverse equations

$$q_i = q_i\left(\overline{q}\right) \tag{2}$$

(we're using unsubscripted variables to refer to the entire set, so that $\overline{q} = (\overline{q}_1, \ldots, \overline{q}_n)$), we have

$$\dot{q}_i = \sum_j \frac{\partial q_i}{\partial \overline{q}_j} \dot{\overline{q}}_j \tag{3}$$

Since the velocities $\dot{\overline{q}}_j$ are independent variables, this implies that, if we hold the coordinates $\overline{q}$ constant,

$$\left(\frac{\partial \dot{q}_i}{\partial \dot{\overline{q}}_j}\right)_{\overline{q}} = \frac{\partial q_i}{\partial \overline{q}_j} \tag{4}$$

since the derivative just picks out the one term containing $\dot{\overline{q}}_j$ in the sum 3. Now consider the Euler-Lagrange equations in the new coordinates. To do this, we write the Lagrangian in terms of the new coordinates and velocities, so that

$$L = L\left(\overline{q}, \dot{\overline{q}}\right) \tag{5}$$

Taking derivatives, we have

$$\frac{\partial L}{\partial \overline{q}_i} = \sum_j \left[\frac{\partial L}{\partial q_j} \frac{\partial q_j}{\partial \overline{q}_i} + \frac{\partial L}{\partial \dot{q}_j} \frac{\partial \dot{q}_j}{\partial \overline{q}_i} \right] \tag{6}$$

The second term on the RHS is zero since the velocities don't depend on the coordinates (and vice versa), so we're left with

$$\frac{\partial L}{\partial \overline{q}_i} = \sum_j \frac{\partial L}{\partial q_j} \frac{\partial q_j}{\partial \overline{q}_i} \tag{7}$$

Now for the other derivative

$$\frac{\partial L}{\partial \dot{\overline{q}}_i} = \sum_j \left[\frac{\partial L}{\partial q_j} \frac{\partial q_j}{\partial \dot{\overline{q}}_i} + \frac{\partial L}{\partial \dot{q}_j} \frac{\partial \dot{q}_j}{\partial \dot{\overline{q}}_i} \right] \tag{8}$$

The first term on the RHS is zero (same reason as in the previous equation), and we can apply 4 to the second term to get

$$\frac{\partial L}{\partial \dot{\overline{q}}_i} = \sum_j \frac{\partial L}{\partial \dot{q}_j} \frac{\partial q_j}{\partial \overline{q}_i} \tag{9}$$

We can now take the derivative with respect to time and apply the Euler-Lagrange equation (which we know to be valid for the q coordinates). We're also assuming that the coordinates have no explicit time dependence. Thus

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{\overline{q}}_i} \right) = \sum_j \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_j} \right) \frac{\partial q_j}{\partial \overline{q}_i} \tag{10}$$

$$= \sum_j \frac{\partial L}{\partial q_j} \frac{\partial q_j}{\partial \overline{q}_i} \tag{11}$$

Comparing this with 7 we see that

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{\overline{q}}_i} \right) = \frac{\partial L}{\partial \overline{q}_i} \tag{12}$$

That is, the Euler-Lagrange equations are valid for the $\overline{q}$ coordinates as well.

We can use the Lagrangian to see how the momenta p_i transform under the coordinate change. The definition of the canonical momentum is

$$p_i = \frac{\partial L}{\partial \dot{q}_i} \tag{13}$$

If we write the Lagrangian in terms of the $\overline{q}$ coordinates and velocities as in 5, then the momenta in the new coordinate system are

$$\overline{p}_i = \frac{\partial L\left(\overline{q}, \dot{\overline{q}}\right)}{\partial \dot{\overline{q}}_i} \tag{14}$$

At this point, it's worth noting that although $L\left(\overline{q}, \dot{\overline{q}}\right)$ and $L\left(q, \dot{q}\right)$ are different functions, they have the same value at each point in the configuration space. That is, if we choose some point that has the coordinates $\left(q, \dot{q}\right)$ in the q system and coordinates $\left(\overline{q}, \dot{\overline{q}}\right)$ in the $\overline{q}$ system, then, numerically at that one point, we must have $L\left(\overline{q}, \dot{\overline{q}}\right) = L\left(q, \dot{q}\right)$. Because of this, we can write

$$\overline{p}_i = \left(\frac{\partial L\left(\overline{q}, \dot{\overline{q}}\right)}{\partial \dot{\overline{q}}_i}\right)_{\overline{q}} = \left(\frac{\partial L\left(q, \dot{q}\right)}{\partial \dot{\overline{q}}_i}\right)_{\overline{q}} \tag{15}$$

That is, if we're keeping $\overline{q}$ constant, the derivative of L with respect to $\dot{\overline{q}}_i$ must be the same (numerically) no matter what coordinates we're using to write L. Therefore, we can use the latter form and then use the chain rule to write out the derivative:

$$\overline{p}_i = \left(\frac{\partial L\left(q, \dot{q}\right)}{\partial \dot{\overline{q}}_i}\right)_{\overline{q}} = \sum_j \left[\frac{\partial L}{\partial q_j}\frac{\partial q_j}{\partial \dot{\overline{q}}_i} + \frac{\partial L}{\partial \dot{q}_j}\frac{\partial \dot{q}_j}{\partial \dot{\overline{q}}_i}\right] \tag{16}$$

Because the coordinates q don't depend on the velocities $\dot{\overline{q}}$, the first term on the RHS is zero. We can use 4 in the second term, and we have

$$\begin{aligned} \overline{p}_i &= \sum_j \frac{\partial L}{\partial \dot{q}_j}\frac{\partial q_j}{\partial \overline{q}_i} & (17)\\ &= \sum_j \frac{\partial q_j}{\partial \overline{q}_i} p_j & (18) \end{aligned}$$

where we used the definition of $p_j = \partial L / \partial \dot{q}_j$ in the last line.

If we review the derivation of Hamilton's equations, we see that nowhere did we make any assumptions about the particular coordinate system that was being used in the Lagrangian. All that is required for Hamilton's equations to be valid is that the momenta are defined as in 14, and that the Euler-Lagrange equations are satisfied. Therefore, in any such system, Hamilton's equations are valid:

$$\begin{aligned} \frac{\partial H}{\partial \overline{p}_i} &= \dot{\overline{q}}_i & (19)\\ -\frac{\partial H}{\partial \overline{q}_i} &= \dot{\overline{p}}_i & (20) \end{aligned}$$

A transformation of the form 1 and 18, that is, that obeys

$$\overline{q}_i = \overline{q}_i(q_1, \ldots, q_n) \tag{21}$$

$$\overline{p}_i = \sum_j \frac{\partial q_j}{\partial \overline{q}_i} p_j \tag{22}$$

is called a *point transformation*.

In the $2n$-dimensional phase space of the Hamiltonian formalism, where q and p are the variables rather than the q and $\dot{q}$ used in the Lagrangian, we can envision a more general transformation in which

$$\overline{q}_i = \overline{q}_i(q, p) \tag{23}$$

$$\overline{p}_i = \overline{p}_i(q, p) \tag{24}$$

In such a general transformation, there's no guarantee that 18 is satisfied, so such transformations need not be point transformations (though they *could* be). There's also no guarantee that the momenta are related to the Lagrangian by 14, and thus Hamilton's equations may not be satisfied.

However, a set of coordinates $(\overline{q}, \overline{p})$ that *does* satisfy Hamilton's equations 19 and 20 is known as a *canonical transformation*.

PINGBACKS

Pingback: Conditions for a transformation to be canonical

Pingback: Canonical transformations: a few more examples

Pingback: Poisson brackets are invariant under a canonical transformation

Pingback: Passive, regular and active transformations.

POISSON BRACKETS ARE INVARIANT UNDER A CANONICAL TRANSFORMATION

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References: Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 2.7; Exercise 2.7.9.

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The Poisson bracket of two functions is defined as

$$\{\omega,\sigma\} = \sum_i \left(\frac{\partial\omega}{\partial q_i}\frac{\partial\sigma}{\partial p_i} - \frac{\partial\omega}{\partial p_i}\frac{\partial\sigma}{\partial q_i} \right) \tag{1}$$

Calculating the Poisson bracket requires knowing ω and σ as functions of the coordinates q_i and momenta p_i in the particular coordinate system we're using. However, we've seen that the Euler-Lagrange and Hamilton's equations are invariant under a canonical transformation and since the Poisson bracket is a fundamental quantity in classical mechanics, in particular because the time derivative of a function ω is the Poisson bracket $\{\omega, H\}$ with the Hamiltonian, it's natural to ask how the Poisson bracket of two functions transforms under a canonical transformation.

The simplest way of finding out (although not the most elegant) is to write the canonical transformation as

$$\bar{q}_i = \bar{q}_i(q,p) \tag{2}$$
$$\bar{p}_i = \bar{p}(q,p) \tag{3}$$

We can then write the Poisson bracket in the new coordinates as

$$\{\omega,\sigma\}_{\bar{q},\bar{p}} = \sum_j \left(\frac{\partial\omega}{\partial\bar{q}_j}\frac{\partial\sigma}{\partial\bar{p}_j} - \frac{\partial\omega}{\partial\bar{p}_j}\frac{\partial\sigma}{\partial\bar{q}_j} \right) \tag{4}$$

Assuming the transformation is invertible, we can use the chain rule to calculate the derivatives with respect to the barred coordinates. This gives the following (we've used the summation convention in which any index repeated twice in a product is summed; thus in the following, there are implied sums over i, j and k):

$$\{\omega,\sigma\}_{\bar{q},\bar{p}} = \left(\frac{\partial\omega}{\partial q_i}\frac{\partial q_i}{\partial \bar{q}_j} + \frac{\partial\omega}{\partial p_i}\frac{\partial p_i}{\partial \bar{q}_j}\right)\left(\frac{\partial\sigma}{\partial q_k}\frac{\partial q_k}{\partial \bar{p}_j} + \frac{\partial\sigma}{\partial p_k}\frac{\partial p_k}{\partial \bar{p}_j}\right) - \left(\frac{\partial\omega}{\partial q_i}\frac{\partial q_i}{\partial \bar{p}_j} + \frac{\partial\omega}{\partial p_i}\frac{\partial p_i}{\partial \bar{p}_j}\right)\left(\frac{\partial\sigma}{\partial q_k}\frac{\partial q_k}{\partial \bar{q}_j} + \frac{\partial\sigma}{\partial p_k}\frac{\partial p_k}{\partial \bar{q}_j}\right) \tag{5}$$

$$= \frac{\partial\omega}{\partial q_i}\frac{\partial\sigma}{\partial p_k}\left(\frac{\partial q_i}{\partial \bar{q}_j}\frac{\partial p_k}{\partial \bar{p}_j} - \frac{\partial q_i}{\partial \bar{p}_j}\frac{\partial p_k}{\partial \bar{q}_j}\right) + \frac{\partial\omega}{\partial p_i}\frac{\partial\sigma}{\partial q_k}\left(\frac{\partial p_i}{\partial \bar{q}_j}\frac{\partial q_k}{\partial \bar{p}_j} - \frac{\partial p_i}{\partial \bar{p}_j}\frac{\partial q_k}{\partial \bar{q}_j}\right) + \frac{\partial\omega}{\partial q_i}\frac{\partial\sigma}{\partial q_k}\left(\frac{\partial q_i}{\partial \bar{q}_j}\frac{\partial q_k}{\partial \bar{p}_j} - \frac{\partial q_i}{\partial \bar{p}_j}\frac{\partial q_k}{\partial \bar{q}_j}\right) + \frac{\partial\omega}{\partial p_i}\frac{\partial\sigma}{\partial p_k}\left(\frac{\partial p_i}{\partial \bar{q}_j}\frac{\partial p_k}{\partial \bar{p}_j} - \frac{\partial p_i}{\partial \bar{p}_j}\frac{\partial p_k}{\partial \bar{q}_j}\right) \tag{6}$$

$$= \frac{\partial\omega}{\partial q_i}\frac{\partial\sigma}{\partial p_k}\{q_i,p_k\} + \frac{\partial\omega}{\partial p_i}\frac{\partial\sigma}{\partial q_k}\{p_i,q_k\} + \frac{\partial\omega}{\partial q_i}\frac{\partial\sigma}{\partial q_k}\{q_i,q_k\} + \frac{\partial\omega}{\partial p_i}\frac{\partial\sigma}{\partial p_k}\{p_i,p_k\} \tag{7}$$

For a canonical transformation, the Poisson brackets in the last equation satisfy

$$\{q_i,p_k\} = -\{p_i,q_k\} = \delta_{ik} \tag{8}$$

$$\{q_i,q_k\} = \{p_i,p_k\} = 0 \tag{9}$$

[Actually, we had worked out these conditions for the barred coordinates in terms of the original coordinates, but since the transformation is invertible and both sets of coordinates are canonical, the Poisson brackets work either way.] Applying these conditions to the above, we find

$$\{\omega,\sigma\}_{\bar{q},\bar{p}} = \left(\frac{\partial\omega}{\partial q_i}\frac{\partial\sigma}{\partial p_k} - \frac{\partial\omega}{\partial p_i}\frac{\partial\sigma}{\partial p_k}\right)\delta_{ik} \tag{10}$$

$$= \frac{\partial\omega}{\partial q_i}\frac{\partial\sigma}{\partial p_i} - \frac{\partial\omega}{\partial p_i}\frac{\partial\sigma}{\partial p_i} \tag{11}$$

$$= \{\omega,\sigma\}_{q,p} \tag{12}$$

Thus the Poisson bracket is invariant under a canonical transformation.

PASSIVE, REGULAR AND ACTIVE TRANSFORMATIONS. INVARIANCE OF THE HAMILTONIAN AND GENERATORS OF TRANSFORMATIONS

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

References: Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Sections 2.7 & 2.8; Exercises 2.8.1 - 2.8.2.

Post date: 11 Dec 2016

The canonical transformations we've considered so far are of the form

$$\overline{q}_i = \overline{q}_i(q,p) \tag{1}$$
$$\overline{p}_i = \overline{p}_i(q,p) \tag{2}$$

The interpretation of these transformations is that we are using a new set of coordinates and momenta to describe the *same* point in phase space. For example, in 2-d we can describe the point one unit along the y axis by the coordinates $x = 0, y = 1$ if we use rectangular coordinates, or by $r = 1, \theta = \frac{\pi}{2}$ if we use polar coordinates. The numerical values of the coordinates are different in the two systems, but the geometric point being described is the same. Such a transformation is called a *passive transformation*. In a passive transformation, any function ω always has the same value at a given point in phase space no matter which coordinate system we're using, so we can say that

$$\omega(q,p) = \omega(\bar{q},\bar{p}) \tag{3}$$

where it is understood that (q,p) and $(\bar{q},\bar{p})$ both refer to the same point, but in different representations.

One characteristic of a passive transformation is that the ranges of the variables used to represent a point in phase space need not be the same in the two systems. For example, in 2-d rectangular coordinates, both x and y can range from $-\infty$ to $+\infty$, while in polar coordinates r ranges between 0 and $+\infty$ while the angle θ runs between 0 and 2π.

A special type of transformation is a *regular transformation*, in which the variables in the two systems have the same ranges. For example, if we translate a 2-d system by 1 unit along the x axis, the new coordinates are related to the old ones by

$$\bar{x} = x - 1 \tag{4}$$
$$\bar{y} = y \tag{5}$$

Both the original and barred systems have the same range ($-\infty$ to $+\infty$).

Although we can interpret a regular transformation as a passive transformation, we can also think of it in a different way. We can image that instead of just providing a different label for the same point that the transformed coordinate has actually shifted the system to a new location in phase space. In the above example, this would mean that we have physically moved the system by 1 unit along the x axis. This interpretation is known as an *active transformation*.

If a function ω is invariant under an active transformation, then it satisfies the condition

$$\omega(q,p) = \omega(\bar{q},\bar{p}) \tag{6}$$

Although mathematically this is the same as 3, physically it means something quite different, since now the points (q,p) and $(\bar{q},\bar{p})$ refer to *different* points in phase space, so we're saying that the function ω does not change when we move the physical system in the way specified by the active transformation.

We now restrict ourselves to talking about regular canonical transformations. Consider some dynamical variable (it could be momentum or angular momentum, for example) $g(q,p)$ and suppose we define the transformations

$$\bar{q}_i = q_i + \epsilon\frac{\partial g}{\partial p_i} \equiv q_i + \delta q_i \tag{7}$$
$$\bar{p}_i = p_i - \epsilon\frac{\partial g}{\partial q_i} \equiv p_i + \delta p_i \tag{8}$$

where ϵ is some infinitesimal quantity.

First, we need to show that, to first order in ϵ, this is a canonical transformation. The required conditions for this are

$$\left\{\overline{q}_i,\overline{q}_j\right\} = \left\{\overline{p}_i,\overline{p}_j\right\} = 0 \tag{9}$$
$$\left\{\overline{q}_i,\overline{p}_j\right\} = \delta_{ij} \tag{10}$$

Consider first (we'll use the summation convention, so the index k is summed in what follows):

$$\{\overline{q}_i, \overline{p}_j\} = \frac{\partial}{\partial q_k}\left(q_i + \epsilon\frac{\partial g}{\partial p_i}\right)\frac{\partial}{\partial p_k}\left(p_j - \epsilon\frac{\partial g}{\partial q_j}\right) - \frac{\partial}{\partial p_k}\left(q_i + \epsilon\frac{\partial g}{\partial p_i}\right)\frac{\partial}{\partial q_k}\left(p_j - \epsilon\frac{\partial g}{\partial q_j}\right) \tag{11}$$

$$= \left(\delta_{ik} + \epsilon\frac{\partial^2 g}{\partial p_i q_k}\right)\left(\delta_{jk} - \epsilon\frac{\partial^2 g}{\partial p_k q_j}\right) - \left(0 + \epsilon\frac{\partial^2 g}{\partial p_i p_k}\right)\left(0 - \epsilon\frac{\partial^2 g}{\partial q_j q_k}\right) \tag{12}$$

The zeroes in the last line follow from the fact that q_k and p_k are independent variables. We can now keep terms only up to first order in ϵ to get

$$\{\overline{q}_i, \overline{p}_j\} = \delta_{ik}\delta_{jk} + \epsilon\left(\frac{\partial^2 g}{\partial p_i q_k}\delta_{jk} - \frac{\partial^2 g}{\partial p_k q_j}\delta_{ik}\right) \tag{13}$$

$$= \delta_{ij} + \epsilon\left(\frac{\partial^2 g}{\partial p_i q_j} - \frac{\partial^2 g}{\partial p_i q_j}\right) \tag{14}$$

$$= \delta_{ij} \tag{15}$$

The other two brackets work out similarly:

$$\{\overline{q}_i, \overline{q}_j\} = \frac{\partial}{\partial q_k}\left(q_i + \epsilon\frac{\partial g}{\partial p_i}\right)\frac{\partial}{\partial p_k}\left(q_j + \epsilon\frac{\partial g}{\partial p_j}\right) - \frac{\partial}{\partial p_k}\left(q_i + \epsilon\frac{\partial g}{\partial p_i}\right)\frac{\partial}{\partial q_k}\left(q_j + \epsilon\frac{\partial g}{\partial p_j}\right) \tag{16}$$

$$= \left(\delta_{ik} + \epsilon\frac{\partial^2 g}{\partial p_i q_k}\right)\left(0 + \epsilon\frac{\partial^2 g}{\partial p_k p_j}\right) - \left(0 + \epsilon\frac{\partial^2 g}{\partial p_i p_k}\right)\left(\delta_{jk} + \epsilon\frac{\partial^2 g}{\partial p_j q_k}\right) \tag{17}$$

$$= \delta_{ik}\epsilon\frac{\partial^2 g}{\partial p_k p_j} - \delta_{jk}\epsilon\frac{\partial^2 g}{\partial p_i p_k} \tag{18}$$

$$= \epsilon\left(\frac{\partial^2 g}{\partial p_i p_j} - \frac{\partial^2 g}{\partial p_i p_j}\right) \tag{19}$$

$$= 0 \tag{20}$$

$$\begin{aligned}
\{\overline{p}_i, \overline{p}_j\} &= \frac{\partial}{\partial q_k}\left(p_i - \epsilon\frac{\partial g}{\partial q_i}\right)\frac{\partial}{\partial p_k}\left(p_j - \epsilon\frac{\partial g}{\partial q_j}\right) - \\
&\quad \frac{\partial}{\partial p_k}\left(p_i - \epsilon\frac{\partial g}{\partial q_i}\right)\frac{\partial}{\partial q_k}\left(p_j - \epsilon\frac{\partial g}{\partial q_j}\right) && (21)\\
&= \left(0 - \epsilon\frac{\partial^2 g}{\partial q_i q_k}\right)\left(\delta_{jk} - \epsilon\frac{\partial^2 g}{\partial p_k q_j}\right) - \\
&\quad \left(\delta_{ik} - \epsilon\frac{\partial^2 g}{\partial q_i p_k}\right)\left(0 - \epsilon\frac{\partial^2 g}{\partial q_j q_k}\right) && (22)\\
&= -\delta_{jk}\epsilon\frac{\partial^2 g}{\partial q_i q_k} + \delta_{ik}\epsilon\frac{\partial^2 g}{\partial q_k q_j} && (23)\\
&= -\epsilon\left(\frac{\partial^2 g}{\partial q_i q_j} - \frac{\partial^2 g}{\partial q_i q_j}\right) && (24)\\
&= 0 && (25)
\end{aligned}$$

Thus all the brackets check out, so the transformation is canonical.

The point of all this is that, if the Hamiltonian is invariant under the transformations 7 and 8 then the variable g is conserved (that is, doesn't change with time). g is called the *generator* of the transformation. We can verify this by using the chain rule to calculate the variation in H:

$$\begin{aligned}
\delta H &= \frac{\partial H}{\partial q_i}\delta q_i + \frac{\partial H}{\partial p_i}\delta p_i && (26)\\
&= \epsilon\left[\frac{\partial H}{\partial q_i}\frac{\partial g}{\partial p_i} - \frac{\partial H}{\partial p_i}\frac{\partial g}{\partial q_i}\right] && (27)\\
&= \epsilon\{H, g\} && (28)
\end{aligned}$$

Since H is invariant, we must have $\delta H = 0$, so

$$\{H, g\} = 0 \tag{29}$$

However, this is the condition for g to be conserved. QED.

Example. Suppose we have a two particle system moving in one dimension, with positions q_1, q_2 and momenta p_1, p_2. If we take

$$g = p_1 + p_2 \tag{30}$$

we get

$$\delta q_i = \epsilon \frac{\partial g}{\partial p_i} = \epsilon \tag{31}$$

$$\delta p_i = -\epsilon \frac{\partial g}{\partial q_i} = 0 \tag{32}$$

That is, each particle gets shifted by the same amount ϵ but the momentum of each particle remains unchanged. Thus the total momentum is the generator of infinitesimal translations. The physical interpretation of this is that, since the momentum of each particle is conserved, the total kinetic energy

$$T = \frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2} \tag{33}$$

remains unchanged. Since the total energy is invariant, the total potential energy of the system is unaffected by a translation, which means that there is no external force on the system.

PINGBACKS

Pingback: Infinitesimal rotations in canonical and noncanonical transformations

Pingback: Hamilton's equations of motion under a regular canonical transformation

Pingback: Correspondence between classical and quantum transformations

Pingback: Translational invariance in quantum mechanics

Pingback: Finite transformations: correspondence between classical and quantum

INFINITESIMAL ROTATIONS IN CANONICAL AND NONCANONICAL TRANSFORMATIONS

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

References: Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 2.8; Exercises 2.8.3 - 2.8.4.

Here are a couple of examples of transformations of variables and their consequences with regard to conservation laws.

First, we look at the 2-d harmonic oscillator where the Hamiltonian is

$$H = \frac{1}{2m}\left(p_x^2 + p_y^2\right) + \frac{1}{2}m\omega^2\left(x^2 + y^2\right) \tag{1}$$

If we rotate the system so that both the coordinates and momenta get rotated, then

$$\begin{aligned} \bar{x} &= x\cos\theta - y\sin\theta && (2)\\ \bar{y} &= x\sin\theta + y\cos\theta && (3)\\ \bar{p}_x &= p_x\cos\theta - p_y\sin\theta && (4)\\ \bar{p}_y &= p_x\sin\theta + p_y\cos\theta && (5) \end{aligned}$$

We can show by direct calculation that H is invariant under this transformation, and we can verify that this is a canonical transformation. Shankar shows in his equation 2.8.8 that the generator of this transformation is the angular momentum $\ell_z = xp_y - yp_x$.

However, if we rotate only the coordinates and not the momenta, we get the transformation:

$$\begin{aligned} \bar{x} &= x\cos\theta - y\sin\theta && (6)\\ \bar{y} &= x\sin\theta + y\cos\theta && (7)\\ \bar{p}_x &= p_x && (8)\\ \bar{p}_y &= p_y && (9) \end{aligned}$$

Again, we can show by direct calculation that

$$\bar{x}^2 + \bar{y}^2 = x^2 + y^2 \tag{10}$$

so H is also invariant under this transformation. However, this transformation is noncanonical, as we can see by calculating one of the Poisson brackets:

$$\{\bar{x},\bar{p}_x\} = \sum_i \left(\frac{\partial \overline{x}}{\partial q_i}\frac{\partial \bar{p}_x}{\partial p_i} - \frac{\partial \overline{x}}{\partial p_i}\frac{\partial \bar{p}_x}{\partial q_i} \right) \tag{11}$$

$$= \cos\theta \neq 1 \tag{12}$$

The other mixed brackets (with a coordinate and a momentum) are also not either 0 or 1 as would be required if the transformation were to be canonical.

In order for this transformation to give rise to a conservation law, we would need to find a generator g that satisfied, for an infinitesimal rotation ε:

$$\bar{q}_i = q_i + \varepsilon\frac{\partial g}{\partial p_i} \equiv q_i + \delta q_i \tag{13}$$

$$\bar{p}_i = p_i - \varepsilon\frac{\partial g}{\partial q_i} \equiv p_i + \delta p_i \tag{14}$$

For an infinitesimal rotation, the transformation 6 becomes

$$\bar{x} = x - \varepsilon y \tag{15}$$

$$\bar{y} = y + \varepsilon x \tag{16}$$

$$\bar{p}_x = p_x \tag{17}$$

$$\bar{p}_y = p_y \tag{18}$$

Therefore, the generator would have to satisfy

$$\frac{\partial g}{\partial p_x} = -y \tag{19}$$

$$\frac{\partial g}{\partial p_y} = x \tag{20}$$

$$\frac{\partial g}{\partial x} = 0 \tag{21}$$

$$\frac{\partial g}{\partial y} = 0 \tag{22}$$

The last two conditions state that g cannot depend on x or y, but integrating the first two conditions, we get

$$g = -yp_x + xp_y + f(x,y) \tag{23}$$

where f is a function that depends only on x and/or y. Thus there is no g that satisfies all four conditions, so there is no conservation law associated with a rotation of the coordinates only, even though the Hamiltonian is invariant under this transformation. Only canonical transformations that leave H invariant give rise to conservation laws.

As another example, suppose he have the one-dimensional system with

$$H = \frac{1}{2}\left(p^2 + x^2\right) \tag{24}$$

and perform a rotation in phase space, that is, in the $x-p$ plane:

$$\begin{aligned} \bar{x} &= x\cos\theta - p\sin\theta & (25)\\ \bar{p} &= x\sin\theta + p\cos\theta & (26) \end{aligned}$$

The Hamiltonian is invariant:

$$\begin{aligned} \bar{p}^2 + \bar{x}^2 &= x^2\sin^2\theta + 2xp\sin\theta\cos\theta + p^2\cos^2\theta + & (27)\\ & x^2\cos^2\theta - 2xp\sin\theta\cos\theta + p^2\sin^2\theta & (28)\\ &= x^2 + p^2 & (29) \end{aligned}$$

The transformation is canonical as we can verify by calculating the Poisson bracket

$$\begin{aligned} \{\bar{x},\bar{p}\} &= \frac{\partial\overline{x}}{\partial x}\frac{\partial\bar{p}}{\partial p} - \frac{\partial\overline{x}}{\partial p}\frac{\partial\bar{p}}{\partial x} & (30)\\ &= \cos^2\theta - \left(-\sin^2\theta\right) & (31)\\ &= 1 & (32) \end{aligned}$$

An infinitesimal rotation gives the transformation

$$\begin{aligned} \bar{x} &= x - \varepsilon p & (33)\\ \bar{p} &= p + \varepsilon x & (34) \end{aligned}$$

To find the generator, we need to solve 13 and 14:

$$\begin{aligned} \frac{\partial g}{\partial p} &= -p & (35)\\ \frac{\partial g}{\partial x} &= -x & (36) \end{aligned}$$

These can be integrated to give

$$g(x,p) = -\frac{1}{2}\left(p^2 + x^2\right) + C \tag{37}$$

where C is a constant of integration. Thus the quantity that is conserved is (apart from the minus sign, which we could eliminate by rotating through $-\theta$ instead of θ) is just the original Hamiltonian, or total energy.

PINGBACKS

Pingback: Hamilton's equations of motion under a regular canonical transformation

HAMILTON'S EQUATIONS OF MOTION UNDER A REGULAR CANONICAL TRANSFORMATION

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To leave a comment or report an error, please use the auxiliary blog.

References: Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 2.8; Exercise 2.8.5.

Post date: 13 Dec 2016

If the Hamiltonian is invariant under a regular canonical transformation and we can find a generator g such that an infinitesimal version of this transformation is given by

$$\bar{q}_i = q_i + \varepsilon \frac{\partial g}{\partial p_i} \equiv q_i + \delta q_i \tag{1}$$

$$\bar{p}_i = p_i - \varepsilon \frac{\partial g}{\partial q_i} \equiv p_i + \delta p_i \tag{2}$$

then g is conserved.

If we are dealing with a *finite* regular canonical transformation where we go from $(q,p) \rightarrow (\bar{q},\bar{p})$, and the Hamiltonian is invariant under this transformation, then it turns out that if a trajectory $(q(t), p(t))$ satisfies Hamilton's equations of motion:

$$\frac{\partial H}{\partial p_i} = \dot{q}_i \tag{3}$$

$$-\frac{\partial H}{\partial q_i} = \dot{p}_i \tag{4}$$

then the trajectory obtained by transforming every point in the original trajectory $(q(t), p(t))$ to the barred system $(\bar{q}(t), \bar{p}(t))$ is also a solution of Hamilton's equations in the sense that

$$\frac{\partial H}{\partial \bar{p}_i} = \dot{\bar{q}}_i \tag{5}$$

$$-\frac{\partial H}{\partial \bar{q}_i} = \dot{\bar{p}}_i \tag{6}$$

The proof of this is a bit subtle, but goes as follows. To begin, review the derivation of the conditions for a transformation to be canonical. This derivation applied to a passive transformation, in which the two sets

of parameters $(q,p) \rightarrow (\bar{q},\bar{p})$ refer to the same point in phase space. The transformation we're considering here is an active transformation, in which $(q,p) \rightarrow (\bar{q},\bar{p})$ actually moves the point in phase space. The original derivation (for passive transformations) relied on the fact that the numerical value of the Hamiltonian is the same in both coordinate systems, since both (q,p) and $(\bar{q},\bar{p})$ refer to the same point in phase space. However, for our active transformation, we're assuming that the Hamiltonian is invariant under the transformation, that is $H(\bar{q},\bar{p}) = H(q,p)$, where (q,p) and $(\bar{q},\bar{p})$ now refer to *different* points in phase space. Since the assumption that the Hamiltonian satisfies $H(\bar{q},\bar{p}) = H(q,p)$ was all that we used in the original derivation, the same derivation works both for passive transformations (always) and for active transformations (if the Hamiltonian is invariant under the active transformation). We therefore end up with the equations

$$\dot{\bar{q}}_j = \sum_k \frac{\partial H}{\partial \bar{q}_k} \left\{ \bar{q}_j, \bar{q}_k \right\} + \sum_k \frac{\partial H}{\partial \bar{p}_k} \left\{ \bar{q}_j, \bar{p}_k \right\} \tag{7}$$

$$\dot{\bar{p}}_j = \sum_k \frac{\partial H}{\partial \bar{q}_k} \left\{ \bar{p}_j, \bar{q}_k \right\} + \sum_k \frac{\partial H}{\partial \bar{p}_k} \left\{ \bar{p}_j, \bar{p}_k \right\} \tag{8}$$

Since the transformation is specified to be canonical, the conditions on the Poisson brackets apply here:

$$\left\{ \bar{q}_j, \bar{q}_k \right\} = \left\{ \bar{p}_j, \bar{p}_k \right\} = 0 \tag{9}$$

$$\left\{ \bar{q}_j, \bar{p}_k \right\} = \delta_{jk} \tag{10}$$

The result is that the transformed trajectory also satisfies Hamilton's equations 5 and 6.

We can now revisit the 2-d harmonic oscillator to show that a noncanonical transformation violates these results. The Hamiltonian is

$$H = \frac{1}{2m}\left(p_x^2 + p_y^2\right) + \frac{1}{2} m\omega^2 \left(x^2 + y^2\right) \tag{11}$$

and we consider the transformation where we rotate the coordinates but not the momenta. The transformation is

$$\bar{x} = x\cos\theta - y\sin\theta \tag{12}$$

$$\bar{y} = x\sin\theta + y\cos\theta \tag{13}$$

$$\bar{p}_x = p_x \tag{14}$$

$$\bar{p}_y = p_y \tag{15}$$

As we've seen, this is a noncanonical transformation. To see what happens, we'll consider the initial conditions

$$\begin{aligned} x(0) &= a && (16)\\ p_x(0) &= b && (17)\\ y(0) &= p_y(0) = 0 && (18) \end{aligned}$$

The mass is started off at a point on the x axis with a momentum only in the x direction. In this case, the mass behaves like a one-dimensional harmonic oscillator, moving along the x axis only. To be precise, we can work out Hamilton's equations of motion:

$$\begin{aligned} \dot{p}_x &= -\frac{\partial H}{\partial x} = -m\omega^2 x && (19)\\ \dot{x} &= \frac{\partial H}{\partial p_x} = \frac{p_x}{m} && (20) \end{aligned}$$

The equations for y and p_y are the same, with x replaced by y everywhere. We can solve these ODEs in the usual way, by differentiating the first one and substituting the second one into the first to get

$$\ddot{p}_x = -m\omega^2 \dot{x} = -\omega^2 p_x \quad (21)$$

This has the general solution

$$p_x(t) = A\cos\omega t + B\sin\omega t \quad (22)$$

We can do the same for x and get

$$x(t) = C\cos\omega t + D\sin\omega t \quad (23)$$

Applying the initial conditions, we get

$$\begin{aligned} p_x(0) &= A = b && (24)\\ x(0) &= C = a && (25) \end{aligned}$$

Plugging these into the equations of motion 19 and 20 and solving for B and D we get the final solution

$$\begin{aligned} p_x(t) &= b\cos\omega t - m\omega a\sin\omega t && (26)\\ x(t) &= a\cos\omega t + \frac{b}{m\omega}\sin\omega t && (27)\\ y(t) &= p_y(t) = 0 && (28) \end{aligned}$$

Now suppose we start off with $x(0) = 0$, $y(0) = a$, $p_x(0) = b$ and $p_y(0) = 0$. That is, we have rotated the coordinates through $\frac{\pi}{2}$, but not the momenta. We now begin with the mass on the y axis, but moving in the x direction, so as time progresses, it will have components of momentum in both the x and y directions. Although it's fairly obvious that this motion will not be simply the motion in the first case rotated through $\frac{\pi}{2}$, let's go through the equations. By the same technique as above, we can solve the equations to get

$$\begin{aligned} p_x(t) &= b\cos\omega t && (29)\\ p_y(t) &= -m\omega a\sin\omega t && (30)\\ x(t) &= \frac{b}{m\omega}\sin\omega t && (31)\\ y(t) &= a\cos\omega t && (32) \end{aligned}$$

If we look at the system at, say, $t = \frac{\pi}{2\omega}$, then $\cos\omega t = 0$ and $\sin\omega t = 1$. The mass that started off on the x axis will be at position $(x, y) = \left(\frac{b}{m\omega}, 0\right)$ and so will the mass that started off on the y axis. Since the two masses are in the same place, obviously one is not the rotated version of the other.

Another, probably easier, way to see this is that since the first mass moves only along the x axis, if the rotated version of the trajectory was also to be a solution, the rotated trajectory would have to lie entirely along the y axis, which is certainly not true for the mass that starts off on the y axis, but with a momentum $p_x \neq 0$.

In the general case, if the transformation is noncanonical, then the Poisson brackets in 7 and 8 don't satisfy the conditions 9 and 10, with the result that Hamilton's equations aren't satisfied in the $(\bar{q}, \bar{p})$ coordinates. (There may be a deeper, physical interpretation that I've missed, but from a mathematical point of view, that's what goes wrong.)

RELATION BETWEEN ACTION AND ENERGY

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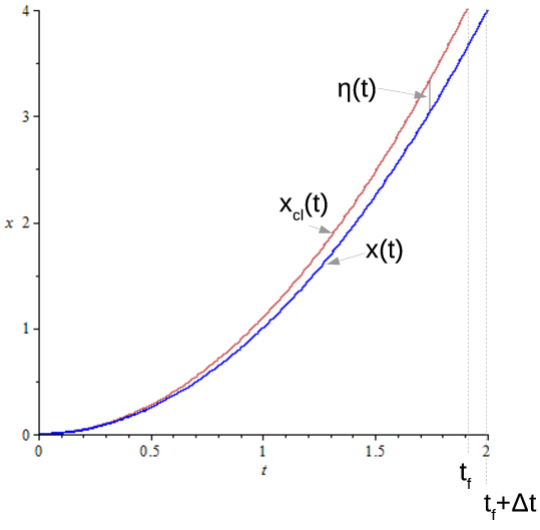
References: Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 2.8; Exercises 2.8.6 - 2.8.7.

Post date: 15 Dec 2016

Here we'll examine an interesting relation between the action S and the total energy of a system, as given by the Hamiltonian H. Suppose a single particle moving in one dimension follows a classical path given by $x_{cl}(t)$, and moves from an initial position at time t_i of $x_{cl}(t_i) = x_i$ to a final position at time t_f of $x_{cl}(t_f) = x_f$. The action S_{cl} of this classical path is given by the integral of the Lagrangian

$$S_{cl} = \int_{t_i}^{t_f} L(x, \dot{x})\, dt \tag{1}$$

What can we say about the rate of change of the action with respect to the final time t_f? That is, we want to calculate $\partial S_{cl}/\partial t_f$, where all other parameters $t_i, x_i$and x_f are held constant. The situation can be illustrated as shown:



Since the only thing that is changing is t_f, the particle starts at the same initial time (which we've taken to be $t_i = 0$ in the diagram) and moves to the same location x_f, but at a different time (in the diagram, later time).

This means that the particle must follow a different path, possibly over its entire trajectory. This path, which we'll call $x(t)$, is related to the original path $x_{cl}(t)$ by perturbing the original path by an amount $\eta(t)$:

$$x(t) = x_{cl}(t) + \eta(t) \tag{2}$$

In the diagram, the original path x_{cl} is shown in red and the perturbed path x in blue. The amount η is seen to be the vertical distance between these two curves at each time, and in the case of the paths shown in the diagram, $\eta(t) < 0$.

The difference in the action between the two paths is due to two contributions: first, there is the contribution due to the extra time, from t_f to $t_f + \Delta t$, that the particle takes to complete its path. Second, there is the difference in the two actions over the path from t_i to t_f. The first contribution is entirely new and, for an infinitesimal extra time Δt, it is given by

$$\delta S_1 = L\left(t_f\right)\Delta t \tag{3}$$

where $L\left(t_f\right)$ is the Lagrangian evaluated at time t_f. The other contribution can be obtained by varying the action over the path from $t_i = 0$ to t_f:

$$\delta S_2 = \int_0^{t_f} \delta L \, dt \tag{4}$$

Since L depends on x and $\dot{x}$, we have

$$\delta L = \frac{\partial L}{\partial x}\delta x + \frac{\partial L}{\partial \dot{x}}\delta \dot{x} \tag{5}$$

For infinitesimally different trajectories, we can see from the diagram above that $\delta x = \eta(t)$ at each point on the curve, so $\delta \dot{x} = \dot{\eta}(t)$, so we get

$$\delta S_2 = \int_0^{t_f} \left[\frac{\partial L}{\partial x}\eta(t) + \frac{\partial L}{\partial \dot{x}}\dot{\eta}(t)\right] dt \tag{6}$$

$$= \int_0^{t_f} \left[-\frac{d}{dt}\frac{\partial L}{\partial \dot{x}} + \frac{\partial L}{\partial x}\right]\eta(t)\, dt + \int_0^{t_f} \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{x}}\eta(t)\right) dt \tag{7}$$

$$= 0 + \left.\frac{\partial L}{\partial \dot{x}}\eta(t)\right|_{t_f} \tag{8}$$

In these equations, the derivatives of L are evaluated on the original curve x_{cl}. To verify the second line, use the product rule on the second integrand and cancel terms to get the first line. The second term in the last is evaluated at $t = t_f$ only since we're assuming that $\eta(0) = 0$.

The quantity in brackets in the first integral is zero, because of the Euler-Lagrange equations which are valid on the original curve x_{cl}:

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{x}} - \frac{\partial L}{\partial x} = 0 \tag{9}$$

Putting everything together, we get for the total variation in the action:

$$\begin{aligned} \delta S_{cl} &= \delta S_1 + \delta S_2 && (10)\\ &= \left[\frac{\partial L}{\partial \dot{x}}\eta(t) + L\Delta t\right]_{t_f} && (11)\end{aligned}$$

Looking at the diagram above, the slope of the blue curve $x\left(t_f\right)$ at the time t_f is given by

$$\dot{x}\left(t_f\right) = \frac{\left|\eta\left(t_f\right)\right|}{\Delta t} \tag{12}$$

From the definition 2 of η we see that $\eta\left(t_f\right) < 0$, so

$$\eta\left(t_f\right) = -\dot{x}\left(t_f\right)\Delta t \tag{13}$$

This gives the final equation for the variation of the action:

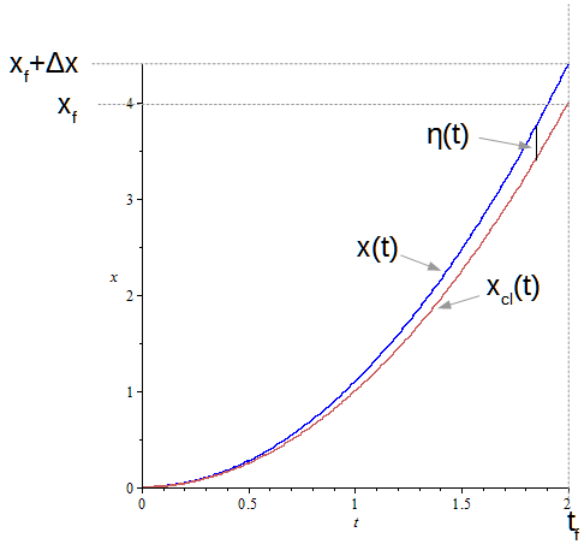
$$\begin{aligned} \delta S_{cl} &= \left[-\frac{\partial L}{\partial \dot{x}}\dot{x} + L\right]_{t_f}\Delta t && (14)\\ &= \left(-p\dot{x} + L\right)\Delta t && (15)\\ &= -H\Delta t && (16)\end{aligned}$$

where the second line follows from the definition of the canonical momentum $p = \partial L/\partial \dot{x}$.

The required derivative is

$$\boxed{\frac{\partial S_{cl}}{\partial t_f} = -H\left(t_f\right)} \tag{17}$$

Using a similar technique, we can work out $\partial S_{cl}/\partial x_f$. In this case, the situation is as shown in this diagram:



The two trajectories now take the same time, but in the modified trajectory, the particle moves a distance Δx further. Since both paths take the same time, there is no extra contribution $L\Delta t$. In this case $\eta(t) > 0$, since the new (blue) curve $x(t)$ is above the old (red) one $x_{cl}(t)$. The derivation is the same as above up to 8, and the total variation in the action is now

$$\delta S_{cl} = \frac{\partial L}{\partial \dot{x}} \eta(t) \Big|_{t_f} \tag{18}$$

At $t = t_f$, $\eta\left(t_f\right) = \Delta x$, so we get

$$\delta S_{cl} = \frac{\partial L}{\partial \dot{x}}\Big|_{t_f} \Delta x \tag{19}$$

$$\frac{\partial S_{cl}}{\partial x_f} = \frac{\partial L}{\partial \dot{x}}\Big|_{t_f} = p\left(t_f\right) \tag{20}$$

Example. We can verify 17 for the case of the one-dimensional harmonic oscillator. The general solution for the position is given by

$$x(t) = A\cos\omega t + B\sin\omega t \tag{21}$$

$$\dot{x}(t) = -A\omega\sin\omega t + B\omega\cos\omega t \tag{22}$$

The total energy is given by

$$E = \frac{1}{2}m\dot{x}^2 + \frac{1}{2}m\omega^2 x^2 \tag{23}$$
$$= \frac{m}{2}\left((-A\omega\sin\omega t + B\omega\cos\omega t)^2 + \omega^2\left(A\cos\omega t + B\sin\omega t\right)^2\right) \tag{24}$$
$$= \frac{m\omega^2}{2}\left(A^2 + B^2\right) \tag{25}$$

where we just multiplied out the second line, cancelled terms and used $\cos^2 x + \sin^2 x = 1$.

To get the action, we need the Lagrangian:

$$L = T - V \tag{26}$$
$$= \frac{1}{2}m\dot{x}^2 - \frac{1}{2}m\omega^2 x^2 \tag{27}$$
$$= \frac{m}{2}\left((-A\omega\sin\omega t + B\omega\cos\omega t)^2 - \omega^2\left(A\cos\omega t + B\sin\omega t\right)^2\right) \tag{28}$$
$$= \frac{m\omega^2}{2}\left[A^2\left(\sin^2\omega t - \cos^2\omega t\right) + B^2\left(\cos^2\omega t - \sin^2\omega t\right) - 4AB\sin\omega t\cos\omega t\right] \tag{29}$$
$$= \frac{m\omega^2}{2}\left(\left(B^2 - A^2\right)\cos 2\omega t - 2AB\sin 2\omega t\right) \tag{30}$$

The action for a trajectory from $t = 0$ to $t = T$ is then

$$S = \int_0^T L dt \tag{31}$$
$$= \frac{m\omega}{4}\left[\left(B^2 - A^2\right)\sin 2\omega t + 2AB\cos 2\omega t\right]_0^T \tag{32}$$
$$= \frac{m\omega}{4}\left[\left(B^2 - A^2\right)\sin 2\omega T + 2AB\left(\cos 2\omega T - 1\right)\right] \tag{33}$$
$$= \frac{m\omega}{2}\left[\left(B^2 - A^2\right)\sin\omega T\cos\omega T + AB\left(\cos^2\omega T - \sin^2\omega T - 1\right)\right] \tag{34}$$
$$= \frac{m\omega}{2}\left[\left(B^2 - A^2\right)\sin\omega T\cos\omega T - 2AB\sin^2\omega T\right] \tag{35}$$

To proceed further, we need to specify A and B, since these depend on the boundary conditions (that is, on where we require the mass to be at $t = 0$ and $t = T$). If we require $x(0) = x_1$ and $x(T) = x_2$, then

$$A = x_1 \tag{36}$$

$$x_1 \cos\omega T + B \sin\omega T = x_2 \tag{37}$$

$$B = \frac{x_2 - x_1 \cos\omega T}{\sin\omega T} \tag{38}$$

Plugging these into 25 gives the energy as

$$E = \frac{m\omega^2}{2}\left(x_1^2 + \left(\frac{x_2 - x_1\cos\omega T}{\sin\omega T}\right)^2\right) \tag{39}$$

$$= \frac{m\omega^2}{2\sin^2\omega T}\left(x_1^2 + x_2^2 - 2x_1x_2\cos\omega T\right) \tag{40}$$

Plugging A and B into 35, we get (using $c \equiv \cos\omega T$ and $s \equiv \sin\omega T$, so that $s^2 + c^2 = 1$):

$$S = \frac{m\omega}{2s}\left[(x_2 - x_1c)^2 c - x_1 s^2 c - 2x_1 s^2 (x_2 - x_1 c)\right] \tag{41}$$

$$= \frac{m\omega}{2s}\left[\left(x_2^2 - 2x_1x_2c + x_1^2c^2\right)c - x_1^2 s^2 c - 2x_1x_2s^2 + 2x_1s^2c\right] \tag{42}$$

$$= \frac{m\omega}{2s}\left[\left(x_1^2 + x_2^2\right)c - 2x_1x_2\right] \tag{43}$$

$$= \frac{m\omega}{2\sin\omega T}\left[\left(x_1^2 + x_2^2\right)\cos\omega T - 2x_1x_2\right] \tag{44}$$

Taking the derivative, we get

$$\frac{\partial S}{\partial T} = \frac{m\omega}{2s^2}\left[-\omega\left(x_1^2 + x_2^2\right)s^2 - \left(\left(x_1^2 + x_2^2\right)c - 2x_1x_2\right)\omega c\right] \tag{45}$$

$$= \frac{m\omega^2}{2s^2}\left[-\left(x_1^2 + x_2^2\right) + 2x_1x_2c\right] \tag{46}$$

$$= -\frac{m\omega^2}{2\sin^2\omega T}\left(x_1^2 + x_2^2 - 2x_1x_2\cos\omega T\right) \tag{47}$$

$$= -E \tag{48}$$

Thus the result is verified for the harmonic oscillator.

PINGBACKS

Pingback: Path integrals for special potentials; use of classical action

DENSITY MATRIX

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 4.2.

Post date: 22 Aug 2017

[If some equations are too small to read easily, use your browser's magnifying option (Ctrl + on Chrome, probably something similar on other browsers).]

The standard probabilistic interpretation of quantum mechanical wave functions is that if you have a collection of a large number of systems all prepared in the same state, then we can calculate expectation values for the various observable quantities such as energy, spin and so on. In practice, most systems consist of a collection of various states. We can treat the statistics of such systems using a density matrix.

Suppose we have an ensemble of N sysytems, where there are n_i systems in state $|i\rangle$, so that

$$\sum_i n_i = N \tag{1}$$

We're assuming that the collection of $|i\rangle$ states form an orthonormal basis.

The density matrix is defined as

$$\rho \equiv \sum_i p_i \left|i\right\rangle \left\langle i\right| \tag{2}$$

where p_i is the probability of a single system being state $|i\rangle$. We can calculate a few properties of ρ as follows.

First, the most important property is probably the ensemble average of some observable quantity represented by an operator Ω. Within a single state, the expectation value of Ω is

$$\langle \Omega \rangle = \left\langle i\right|\left|\Omega\right|\left|i\right\rangle \tag{3}$$

Thus over the ensemble of systems described above, the expectation value is

$$\left\langle \bar{\Omega} \right\rangle = \sum_i p_i \left\langle i\right|\left|\Omega\right|\left|i\right\rangle \tag{4}$$

The angle bracket plus overbar notation indicates that two averages are occurring - an average over each individual state, represented by 3, and an ensemble average over the whole collection of systems.

This ensemble average can be expressed in terms of the density matrix, as follows.

$$\begin{aligned}
\mathrm{Tr}\left(\Omega\rho\right) &= \sum_j \left\langle j\right|\left|\Omega\rho\right|\left. j\right\rangle && (5)\\
&= \sum_j\sum_i \left\langle j\right|\left|\Omega\right|\left. i\right\rangle p_i \left\langle i\right|\left. j\right\rangle && (6)\\
&= \sum_j\sum_i \left\langle j\right|\left|\Omega\right|\left. i\right\rangle p_i\delta_{ij} && (7)\\
&= \sum_i p_i \left\langle i\right|\left|\Omega\right|\left. i\right\rangle && (8)\\
&= \left\langle\bar{\Omega}\right\rangle && (9)
\end{aligned}$$

If we want the probability of obtaining a particular eigenvalue ω of the operator Ω, then we first project out the component of the ensemble along the eigenvector $|\omega\rangle$, which we do with the projection operator $\mathbb{P}_\omega$. Thus the probability of obtaining the value ω is

$$\overline{P\left(\omega\right)} = \mathrm{Tr}\left(\mathbb{P}_\omega\rho\right) \tag{10}$$

A few other properties can be derived.

(1) From 2, we have $\rho^\dagger = \left[\sum_i p_i \left|i\right\rangle\left\langle i\right|\right]^\dagger = \sum_i p_i^* \left|i\right\rangle\left\langle i\right| = \sum_i p_i \left|i\right\rangle\left\langle i\right| = \rho$, since p_i, being a probability, is a real number.
(2) $\mathrm{Tr}\rho = \sum_j\sum_i p_i \left\langle j\right|\left. i\right\rangle\left\langle i\right|\left. j\right\rangle = \sum_j\sum_i p_i\delta_{ji}\delta_{ij} = \sum_i p_i = 1$, since probabilities must add up to 1.
(3) For a pure ensemble, there is only one state, say $|i\rangle$, in the ensemble, so $\rho = \left|i\right\rangle\left\langle i\right|$ and in this case $\rho^2 = \left|i\right\rangle\left\langle i\right|\left. i\right\rangle\left\langle i\right| = \left|i\right\rangle\left\langle i\right| = \rho$.
(4) If the ensemble is uniformly distributed over k states, then $p_i = \frac{1}{k}$ for all states in the ensemble, and $\rho = \frac{1}{k}\sum_i \left|i\right\rangle\left\langle i\right| = \frac{1}{k}I$.
(5) $\mathrm{Tr}\rho^2 = \mathrm{Tr}\sum_j\sum_i p_j p_i \left|j\right\rangle\left\langle j\right|\left. i\right\rangle\left\langle i\right| = \mathrm{Tr}\sum_j\sum_i p_j p_i \left|j\right\rangle\delta_{ij}\left\langle i\right| = \mathrm{Tr}\sum_i p_i^2 \left|i\right\rangle\left\langle i\right| = \sum_k\sum_i p_i^2 \left\langle k\right|\left. i\right\rangle\left\langle i\right|\left. k\right\rangle = \sum_i p_i^2$. Since $0 \le p_i \le 1$ and squaring a number in this range either makes it smaller (if $0 < p_i < 1$) or leaves it unchanged (if $p_i = 0$ or $p_i = 1$), and since $\sum_i p_i = 1$, we must have $\sum_i p_i^2 \le 1$, with equality only for a pure ensemble.

PINGBACKS

Pingback: Ensemble of electrons in magnetic field
Pingback: Single-particle density matrix

Pingback: Thermal average of a harmonic oscillator

POSTULATES OF QUANTUM MECHANICS: STATES AND MEASUREMENTS

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

References: Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Sections 4.1 - 4.2; Exercise 4.2.1.

Post date: 19 Dec 2016

Although we've covered the basics of nonrelativistic quantum mechanics before, the approach taken by Shankar in his Chapter 4 provides a new way of looking at it, so it's worth a summary.

Quantum mechanics is based on four postulates, the first three of which describe the quantum state at a fixed instant in time, and the fourth which describes its time evolution via the Schrödinger equation. We'll summarize the first three postulates here, and compare each with its classical analogue.

First, in classical mechanics, the path of a particle is, in the Hamiltonian formalism, described by specifying its position $x(t)$ and momentum $p(t)$ as functions of time. Both the position and momentum are specified precisely at all times. In quantum mechanics, the state of a particle is specified by a vector (ket) $|\psi(t)\rangle$ in a Hilbert space.

Second, in classical mechanics, any dynamical variable ω is a function of the two phase-space coordinates x and p: $\omega = \omega(x,p)$. In quantum mechanics, the spatial coordinate x is replaced by the Hermitian operator X and the momentum p is replaced by the differential operator $P = \hbar K$ which we discussed earlier. The matrix elements of X and P in position space are

$$\langle x|X|x'\rangle = x\delta(x-x') \tag{1}$$

$$\langle x|P|x'\rangle = -i\hbar\delta'(x-x') \tag{2}$$

The classical dynamical variable $\omega(x,p)$ becomes a Hermitian operator $\Omega(X,P)$, where x and p in $\omega(x,p)$ are replaced by their corresponding operators X and P.

The third postulate states how measurements work in quantum mechanics. In classical mechanics, it is assumed that (in principle) any dynamical variable ω may be measured with arbitrary precision without changing the state of the particle. In quantum mechanics, if we wish to measure the value of a variable represented by the operator Ω, we must determine the eigenvalues ω_i and corresponding eigenvectors $|\omega_i\rangle$ of Ω, then express the state $|\psi\rangle$ as a linear combination of the $|\omega_i\rangle$. Then the best we can do is to state that

the particular eigenvalue ω_i will be measured with probability $|\langle\omega_i|\psi\rangle|^2$. After the measurement, the state $|\psi\rangle$ 'collapses' to become the state $|\omega_i\rangle$. The only possible outcomes of a measurement of Ω are its eigenvalues; no intermediate values are possible.

To illustrate these postulates, suppose we have the following three operators on a complex 3-d Hilbert space (essentially these are the spin-1 operators without the $\hbar$)

$$L_x = \frac{1}{\sqrt{2}} \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \tag{3}$$

$$L_y = \frac{1}{\sqrt{2}} \begin{bmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{bmatrix} \tag{4}$$

$$L_z = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix} \tag{5}$$

Since L_z is diagonal, its eigenvalues can be read off from the diagonal elements as $0, \pm 1$, so these are the possible values of L_z that could be obtained in a measurement. Also because L_z is diagonal, its eigenvectors are

$$|L_z = +1\rangle = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \tag{6}$$

$$|L_z = 0\rangle = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} \tag{7}$$

$$|L_z = -1\rangle = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \tag{8}$$

Suppose we start with the state $|L_z = +1\rangle$ in which $L_z = +1$, and we want to measure L_x in this state. To find the expectation values $\langle L_x\rangle$ and $\langle L_x^2\rangle$ in this state, we calculate

$$\langle L_x \rangle = \langle L_z = +1 \, | L_x | \, L_z = +1 \rangle \tag{9}$$

$$= \begin{bmatrix} 1 & 0 & 0 \end{bmatrix} \frac{1}{\sqrt{2}} \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \tag{10}$$

$$= \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} \tag{11}$$

$$= 0 \tag{12}$$

To get $\langle L_x^2 \rangle$ we first find the operator

$$L_x^2 = \frac{1}{2} \begin{bmatrix} 1 & 0 & 1 \\ 0 & 2 & 0 \\ 1 & 0 & 1 \end{bmatrix} \tag{13}$$

Now we have

$$\langle L_x^2 \rangle = \begin{bmatrix} 1 & 0 & 0 \end{bmatrix} \frac{1}{2} \begin{bmatrix} 1 & 0 & 1 \\ 0 & 2 & 0 \\ 1 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \tag{14}$$

$$= \frac{1}{2} \begin{bmatrix} 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix} \tag{15}$$

$$= \frac{1}{2} \tag{16}$$

The uncertainty, or variance, is

$$\Delta L_x = \sqrt{\langle L_x^2 \rangle - \langle L_x \rangle^2} = \frac{1}{\sqrt{2}} \tag{17}$$

To find the possible values of L_x and their probabilities, we need to find the eigenvalues and eigenvectors of L_x, which we can do in the L_z basis, since this basis is given by the three vectors in 6. The eigenvalues are found in the usual way from the determinant:

$$\begin{vmatrix} -\lambda & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & -\lambda & \frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} & -\lambda \end{vmatrix} = -\lambda\left(\lambda^2 - \frac{1}{2}\right) - \frac{1}{\sqrt{2}}\left(\frac{-\lambda}{\sqrt{2}}\right) \tag{18}$$

$$= -\lambda^3 + \lambda = 0 \tag{19}$$

$$\lambda = 0, \pm 1 \tag{20}$$

The eigenvectors can be found in the usual way, by solving

$$(L_x - \lambda I)\,|L_x = \lambda\rangle = 0 \tag{21}$$

where the ket takes on the three possible values of λ successively. We let

$$|L_x = \lambda\rangle = \begin{bmatrix} a \\ b \\ c \end{bmatrix} \tag{22}$$

For $\lambda = +1$ we have

$$-a + \frac{b}{\sqrt{2}} = 0 \tag{23}$$

$$\frac{1}{\sqrt{2}}\left(a - \sqrt{2}b + c\right) = 0 \tag{24}$$

$$\frac{b}{\sqrt{2}} - c = 0 \tag{25}$$

Only two of these three equations are independent, so we can set $a = 1$ and solve for b and c to get

$$a = 1 \tag{26}$$

$$b = \sqrt{2} \tag{27}$$

$$c = 1 \tag{28}$$

Normalizing the eigenvector gives

$$|L_x = +1\rangle = \frac{1}{2}\begin{bmatrix} 1 \\ \sqrt{2} \\ 1 \end{bmatrix} \tag{29}$$

The other two eigenvectors can be found the same way, with the result

$$|L_x = 0\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 0 \\ -1 \end{bmatrix} \tag{30}$$

$$|L_x = -1\rangle = \frac{1}{2} \begin{bmatrix} 1 \\ -\sqrt{2} \\ 1 \end{bmatrix} \tag{31}$$

Note that these eigenvectors are orthonormal.

Now that we have the eigenvectors of L_x we can answer the following question. If we start with the state $|L_z = -1\rangle$ and measure L_x, what are the possible outcomes and the probability of each?

First, we need to express $|L_z = -1\rangle$ in terms of the eigenvectors of L_x which we can do by solving three simultaneous linear equations, and we find

$$|L_z = -1\rangle = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} = \frac{1}{2}\left(|L_x = +1\rangle + |L_x = -1\rangle\right) - \frac{1}{\sqrt{2}}|L_x = 0\rangle \tag{32}$$

(You can verify this by direct substitution.) Thus all 3 possible values of L_x can result from a measurement, and the probability of each is

$$P(L_x = +1) = |\langle L_x = +1 | L_z = -1 \rangle|^2 \tag{33}$$

$$= \left(\frac{1}{2} \begin{bmatrix} 1 & \sqrt{2} & 1 \end{bmatrix} \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \right)^2 \tag{34}$$

$$= \frac{1}{4} \tag{35}$$

$$P(L_x = 0) = |\langle L_x = 0 | L_z = -1 \rangle|^2 \tag{36}$$

$$= \left(\frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 0 & -1 \end{bmatrix} \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \right)^2 \tag{37}$$

$$= \frac{1}{2} \tag{38}$$

$$P(L_x = -1) = |\langle L_x = -1 | L_z = -1 \rangle|^2 \tag{39}$$

$$= \left(\frac{1}{2} \begin{bmatrix} 1 & -\sqrt{2} & 1 \end{bmatrix} \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \right)^2 \tag{40}$$

$$= \frac{1}{4} \tag{41}$$

Now suppose we start with the state, written in the L_z basis:

$$|\psi\rangle = \begin{bmatrix} \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{\sqrt{2}} \end{bmatrix} \tag{42}$$

We take a measurement of L_z^2 and obtain $+1$. The operator L_z^2 is given by squaring 5:

$$L_z^2 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \tag{43}$$

This has a degenerate eigenvalue $\lambda = +1$, so the most we can say about the state $|\psi\rangle$ after the measurement is that it is projected onto the subspace $a \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} + b \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}$. That is, the state after the measurement is given by

$$|\psi\rangle_{after} = \mathbb{P}_{L_z=\pm 1}\,|\psi\rangle_{before} \tag{44}$$

$$= \left[|L_z=+1\rangle\langle L_z=+1| + |L_z=-1\rangle\langle L_z=-1|\right]\begin{bmatrix} \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{\sqrt{2}} \end{bmatrix} \tag{45}$$

$$= \left(\begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}\begin{bmatrix} 1 & 0 & 0 \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}\begin{bmatrix} 0 & 0 & 1 \end{bmatrix}\right)\begin{bmatrix} \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{\sqrt{2}} \end{bmatrix} \tag{46}$$

$$= \begin{bmatrix} \frac{1}{2} \\ 0 \\ \frac{1}{\sqrt{2}} \end{bmatrix} \tag{47}$$

We can normalize this state to get

$$|\psi\rangle_{after} = \frac{2}{\sqrt{3}}\begin{bmatrix} \frac{1}{2} \\ 0 \\ \frac{1}{\sqrt{2}} \end{bmatrix} \tag{48}$$

Thus if we measure L_z immediately after the measurement of L_z^2 above, we get $L_z = +1$ with probability $\frac{1}{3}$ and $L_z = -1$ with probability $\frac{2}{3}$.

Finally, suppose we have a state $|\psi\rangle$ with the probabilities of measurements of L_z given as $P(L_z = 1) = \frac{1}{4}$, $P(L_z = 0) = \frac{1}{2}$ and $P(L_z = -1) = \frac{1}{4}$. Since these probabilities are given by $|\langle L_z = \lambda\,|\psi\rangle|^2$ for each of the three possible values of λ, and the vectors $|L_z = \lambda\rangle$ are orthonormal, the most general form for $|\psi\rangle$ is

$$|\psi\rangle = \frac{e^{i\delta_1}}{2}|L_z = 1\rangle + \frac{e^{i\delta_2}}{\sqrt{2}}|L_z = 0\rangle + \frac{e^{i\delta_3}}{2}|L_z = -1\rangle \tag{49}$$

where the δ_i are real numbers. For example

$$|\langle L_z = 1\,|\psi\rangle|^2 = \left|\frac{e^{i\delta_1}}{2}\right|^2 = \frac{1}{4} \tag{50}$$

While the presence of a phase factor in a solitary state doesn't affect the physics of that state, if we have a sum of states, each with its own (different) phase factor, we can't ignore these phase factors. For example, if we measure L_x in this state and want the probability that $L_x = 0$, we have, using 30

$$P(L_x = 0) = |\langle L_x = 0 | \psi \rangle|^2 \tag{51}$$

$$= \left| \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 0 & -1 \end{bmatrix} \left(\frac{e^{i\delta_1}}{2} |L_z = 1\rangle + \frac{e^{i\delta_2}}{\sqrt{2}} |L_z = 0\rangle + \frac{e^{i\delta_3}}{2} |L_z = -1\rangle \right) \right|^2 \tag{52}$$

$$= \left| \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 0 & -1 \end{bmatrix} \left(\frac{e^{i\delta_1}}{2} \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} + \frac{e^{i\delta_2}}{\sqrt{2}} \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} + \frac{e^{i\delta_3}}{2} \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \right) \right|^2 \tag{53}$$

$$= \frac{1}{8} \left| e^{i\delta_1} - e^{i\delta_3} \right|^2 \tag{54}$$

$$= \frac{1}{8} \left| 1 - e^{i(\delta_3 - \delta_1)} \right|^2 \tag{55}$$

The last line will have a different result for different values of the phase factors δ_1 and δ_3, so they can't be ignored.

PINGBACKS

Pingback: Postulates of quantum mechanics: momentum

Pingback: Postulates of quantum mechanics: Schrödinger equation and propagators

Pingback: Poisson brackets to commutators: classical to quantum

POSTULATES OF QUANTUM MECHANICS: MOMENTUM

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

References: Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Sections 4.1 - 4.2; Exercises 4.2.2 - 4.2.3.

Post date: 25 Dec 2016

One of the postulates of quantum mechanics is that the momentum operator P in position space is given by

$$\left\langle x\left|P\right|x'\right\rangle = -i\hbar\delta'\left(x-x'\right) \tag{1}$$

By using the properties of the derivative of the delta function, we can find the eigenfunctions of P. We have

$$\begin{aligned}
\left\langle x\left|P\right|\psi\right\rangle &= \int\left\langle x\left|P\right|x'\right\rangle\left\langle x'\left|\psi\right.\right\rangle dx' && (2)\\
&= -i\hbar\int\delta'\left(x-x'\right)\left\langle x'\left|\psi\right.\right\rangle dx' && (3)\\
&= -i\hbar\frac{d}{dx}\left\langle x\left|\psi\right.\right\rangle && (4)\\
&= -i\hbar\frac{d\psi\left(x\right)}{dx} && (5)
\end{aligned}$$

The eigenvector of P is $\left|p\right\rangle$ and has the property that

$$P\left|p\right\rangle = p\left|p\right\rangle \tag{6}$$

If we project this onto position space and use 5 we get

$$\begin{aligned}
\left\langle x\left|P\right|\psi\right\rangle &= p\left\langle x\left|p\right.\right\rangle && (7)\\
-i\hbar\frac{d\psi_{p}\left(x\right)}{dx} &= p\psi_{p}\left(x\right) && (8)
\end{aligned}$$

where

$$\psi_{p}\left(x\right)\equiv\left\langle x\left|p\right.\right\rangle \tag{9}$$

Solving this differential equation and normalizing so that $\left\langle p'\left|p\right.\right\rangle = \delta\left(p-p'\right)$ we get

$$\psi_p(x) = \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar} \tag{10}$$

For an arbitrary wave function $|\psi\rangle$, if we know its position-space form, we can find its momentum-space version as follows:

$$\begin{aligned}
\langle p|\psi\rangle &= \int \langle p|x\rangle \langle x|\psi\rangle \, dx && (11)\\
&= \int \psi_p^*(x) \langle x|\psi\rangle \, dx && (12)\\
&= \frac{1}{\sqrt{2\pi\hbar}} \int e^{-ipx/\hbar} \psi(x) \, dx && (13)
\end{aligned}$$

This has an interesting consequence if the position-space function $\psi(x)$ is real. The probability density for finding a particle in a state with momentum p is $|\langle p|\psi\rangle|^2$, which we can write as

$$\begin{aligned}
|\langle p|\psi\rangle|^2 &= \langle p|\psi\rangle^* \langle p|\psi\rangle && (14)\\
&= \frac{1}{2\pi\hbar} \int\int e^{ip(x-x')/\hbar} \psi(x) \psi\left(x'\right) dx \, dx' && (15)\\
&= \frac{1}{2\pi\hbar} \int\int e^{-ip(x'-x)/\hbar} \psi(x) \psi\left(x'\right) dx \, dx' && (16)\\
&= \frac{1}{2\pi\hbar} \int\int e^{-ip(x-x')/\hbar} \psi\left(x'\right) \psi(x) dx \, dx' && (17)\\
&= |\langle -p|\psi\rangle|^2 && (18)
\end{aligned}$$

In the fourth line, since x and x' are dummy integration variables, both of which are integrated over the same range, we can simply swap them without changing anything. Note that the derivation relies on $\psi(x)$ being real, since if it were complex we would have

$$\begin{aligned}
|\langle p|\psi\rangle|^2 &= \langle p|\psi\rangle^* \langle p|\psi\rangle && (19)\\
&= \frac{1}{2\pi\hbar} \int\int e^{ip(x-x')/\hbar} \psi(x) \psi^*\left(x'\right) dx \, dx' && (20)\\
&= \frac{1}{2\pi\hbar} \int\int e^{-ip(x'-x)/\hbar} \psi(x) \psi^*\left(x'\right) dx \, dx' && (21)\\
&= \frac{1}{2\pi\hbar} \int\int e^{-ip(x-x')/\hbar} \psi\left(x'\right) \psi^*(x) dx \, dx' && (22)\\
&\neq |\langle -p|\psi\rangle|^2 && (23)
\end{aligned}$$

since

$$|\langle -p|\psi\rangle|^2 = \frac{1}{2\pi\hbar}\int\int e^{-ip(x-x')/\hbar}\psi(x)\,\psi^*\left(x'\right)dx\,dx' \tag{24}$$

That is, for $|\langle -p|\psi\rangle|^2$ the position x' that is the argument of the $\psi^*(x')$ factor appears as the positive term ipx' in the exponential, but in 22 the argument of the complex conjugate wave function is x, which appears as the negative term $-ipx$ in the exponential.

Thus for any real wave function, the probability of the particle having momentum $+p$ is equal to the probability of it having $-p$, so for such wave functions, the mean momentum is always $\langle P\rangle = 0$.

As another example, suppose we have a wave function $\psi(x)$ with a mean momentum $\bar{p}$, so that

$$\langle\psi|P|\psi\rangle = \bar{p} \tag{25}$$

If we now multiply ψ by $e^{ip_0x/\hbar}$ where p_0 is a constant momentum, we can calculate the new mean momentum using 5:

$$\begin{aligned}
\langle P\rangle &= \left\langle e^{ip_0x/\hbar}\psi\,|P|\,e^{ip_0x/\hbar}\psi\right\rangle && (26)\\
&= -i\hbar\int e^{-ip_0x/\hbar}\psi^*(x)\frac{d}{dx}\left(e^{ip_0x/\hbar}\psi(x)\right)dx && (27)\\
&= -i\hbar\int e^{-ip_0x/\hbar}\psi^*\left[\frac{ip_0}{\hbar}e^{ip_0x/\hbar}\psi(x) + e^{ip_0x/\hbar}\frac{d}{dx}\psi(x)\right]dx && (28)\\
&= \int p_0\psi^*\psi dx - i\hbar\int\psi^*(x)\frac{d}{dx}\psi(x)\,dx && (29)\\
&= p_0 + \bar{p} && (30)
\end{aligned}$$

The first integral in the fourth line uses the fact that p_0 is constant and ψ is normalized so that

$$\int\psi^*\psi dx = 1 \tag{31}$$

PINGBACKS

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POSTULATES OF QUANTUM MECHANICS: SCHRÖDINGER EQUATION AND PROPAGATORS

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To leave a comment or report an error, please use the auxiliary blog.

References: Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 4.3.

Post date: 27 Dec 2016

The first three postulates of quantum mechanics concern the properties of a quantum state. The fourth postulate concerns how states evolve with time. The postulate simply states that in non-relativistic quantum mechanics, a state satisfies the Schrödinger equation:

$$i\hbar\frac{\partial}{\partial t}\left|\psi\right\rangle = H\left|\psi\right\rangle \tag{1}$$

where H is the Hamiltonian, which is obtained from the classical Hamiltonian by means of the other postulates of quantum mechanics, namely that we replace all references to the position x by the quantum position operator X with matrix elements (in the x basis) of

$$\left\langle x'\left|X\right|x\right\rangle = \delta\left(x-x'\right) \tag{2}$$

and all references to classical momentum p by the momentum operator P with matrix elements

$$\left\langle x'\left|P\right|x\right\rangle = -i\hbar\delta'\left(x-x'\right) \tag{3}$$

Although we've posted many articles based on Griffiths's book in which we solved the Schrödinger equation, the approach taken by Shankar is a bit different and, in some ways, a lot more elegant. We begin with a Hamiltonian that does not depend explicitly on time, and then by observing that, since the Schrödinger equation contains only the first derivative with respect to time, The time evolution of a state can be uniquely determined if we specify only the initial state $\left|\psi\left(0\right)\right\rangle$. [A differential equation that is second order in time, such as the wave equation, requires both the initial position and initial velocity to be specified.]

The solution of the Schrödinger equation is then found in analogy to the approach we used in solving the coupled masses problem earlier. We find the eigenvalues and eigenvectors of the Hamiltonian in some basis and use these to construct the propagator $U\left(t\right)$. We can then write the solution as

$$|\psi(t)\rangle = U(t)\,|\psi(0)\rangle \tag{4}$$

For the case of a time-independent Hamiltonian, we can actually construct $U(t)$ in terms of the eigenvectors of H. The eigenvalue equation is

$$H\,|E\rangle = E\,|E\rangle \tag{5}$$

where E is an eigenvalue of H and $|E\rangle$ is its corresponding eigenvector. Since the eigenvectors form a vector space, we can expand the wave function in terms of them in the usual way

$$\begin{aligned} |\psi(t)\rangle &= \sum |E\rangle\,\langle E\,|\psi(t)\,\rangle & (6)\\ &\equiv \sum a_E(t)\,|E\rangle & (7)\end{aligned}$$

The coefficient $a_E(t)$ is the component of $|\psi(t)\rangle$ along the $|E\rangle$ vector as a function of time. We can now apply the Schrödinger equation 1 to get (a dot over a symbol indicates a time derivative):

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle &= i\hbar\sum \dot{a}_E(t)\,|E\rangle & (8)\\ &= H\,|\psi(t)\rangle & (9)\\ &= \sum a_E(t)\,H\,|E\rangle & (10)\\ &= \sum a_E(t)\,E\,|E\rangle & (11)\end{aligned}$$

Since the eigenvectors $|E\rangle$ are linearly independent (as they form a basis for the vector space), each term in the sum in the first line must be equal to the corresponding term in the sum in the last line, so we have

$$i\hbar\dot{a}_E(t) = a_E(t)\,E \tag{12}$$

The solution is

$$\begin{aligned} a_E(t) &= a_E(0)\,e^{-iEt/\hbar} & (13)\\ &= e^{-iEt/\hbar}\,\langle E\,|\psi(0)\,\rangle & (14)\end{aligned}$$

The general solution 7 is therefore

$$|\psi(t)\rangle = \sum e^{-iEt/\hbar}\,|E\rangle\,\langle E\,|\psi(0)\,\rangle \tag{15}$$

from which we can read off the propagator:

$$U(t) = \sum e^{-iEt/\hbar}\,|E\rangle\,\langle E| \tag{16}$$

Thus if we can determine the eigenvalues and eigenvectors of H, we can write the propagator in terms of them and get the general solution. We can see from this that $U(t)$ is unitary:

$$U^\dagger U = \sum_{E'}\sum_{E} e^{-i(E-E')t/\hbar} |E\rangle \langle E|E'\rangle \langle E'| \tag{17}$$

$$= \sum_{E'}\sum_{E} e^{-i(E-E')t/\hbar} |E\rangle \delta_{EE'} \langle E'| \tag{18}$$

$$= \sum_{E} |E\rangle \langle E| \tag{19}$$

$$= 1 \tag{20}$$

This derivation uses the fact that the eigenvectors are orthonormal and form a complete set, so that $\langle E|E'\rangle = \delta_{EE'}$ and $\sum_E |E\rangle\langle E| = 1$. Since a unitary operator doesn't change the norm of a vector, we see from 4 that if $|\psi(0)\rangle$ is normalized, then so is $|\psi(t)\rangle$ for all times t. Further, the probability that the state will be measured to be in eigenstate $|E\rangle$ is constant over time, since this probability is given by

$$|a_E(t)|^2 = \left| e^{-iEt/\hbar} \langle E|\psi(0)\rangle \right|^2 = |\langle E|\psi(0)\rangle|^2 \tag{21}$$

This derivation assumed that the spectrum of H was discrete and non-degenerate. If the possible eigenvalues E are continuous, then the sum is replaced by an integral

$$U(t) = \int e^{-iEt/\hbar} |E\rangle\langle E| \, dE \tag{22}$$

If the spectrum is discrete and degenerate, then we need to find an orthonormal set of eigenvectors that spans each degenerate subspace, and sum over these sets. For example, if E_1 is degenerate, then we find a set of eigenvectors $|E_1, \alpha\rangle$ that spans the subspace for which E_1 is the eigenvalue. The index α runs from 1 up to the degree of degeneracy of E_1, and the propagator is then

$$U(t) = \sum_{\alpha}\sum_{E_i} e^{-iE_i t/\hbar} |E_i, \alpha\rangle\langle E_i, \alpha| \tag{23}$$

The sum over E_i runs over all the distinct eigenvalues, and the sum over α runs over the eigenvectors for each different E_i.

Another form of the propagator can be written directly in terms of the time-independent Hamiltonian as

$$U(t) = e^{-iHt/\hbar} \tag{24}$$

This relies on the concept of the function of an operator, so that $e^{-iHt/\hbar}$ is a matrix whose elements are power series of the exponent $-\frac{iHt}{\hbar}$. The power series must, of course, converge for this solution to be valid. Since H is Hermitian, $U(t)$ is unitary. We can verify that the solution using this form of $U(t)$ satisfies the Schrödinger equation:

$$|\psi(t)\rangle = U(t)|\psi(0)\rangle \tag{25}$$
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The derivative of $U(t)$ can be calculated from the derivatives of its matrix elements, which are all power series.

PINGBACKS

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POSTULATES OF QUANTUM MECHANICS: SCHRÖDINGER EQUATION AND PROPAGATORS

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To leave a comment or report an error, please use the auxiliary blog.

References: Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 4.3.

Post date: 27 Dec 2016

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TIME-DEPENDENT PROPAGATORS

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To leave a comment or report an error, please use the auxiliary blog.

References: Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 4.3.

Post date: 1 Jan 2017

The fourth postulate of non-relativistic quantum mechanics concerns how states evolve with time. The postulate simply states that in non-relativistic quantum mechanics, a state satisfies the Schrödinger equation:

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$$\left\langle x'\left|X\right|x\right\rangle = \delta\left(x-x'\right) \tag{2}$$

and all references to classical momentum p by the momentum operator P with matrix elements

$$\left\langle x'\left|P\right|x\right\rangle = -i\hbar\delta'\left(x-x'\right) \tag{3}$$

In our earlier examination of the Schrödinger equation, we assumed that the Hamiltonian is independent of time, which allowed us to obtain an explicit expression for the propagator

$$U\left(t\right) = e^{-iHt/\hbar} \tag{4}$$

The propagator is applied to the initial state $\left|\psi\left(0\right)\right\rangle$ to obtain the state at any future time t:

$$\left|\psi\left(t\right)\right\rangle = U\left(t\right)\left|\psi\left(0\right)\right\rangle \tag{5}$$

What happens if $H = H\left(t\right)$, that is, there is an explicit time dependence in the Hamiltonian? The approach taken by Shankar is a bit hand-wavy, but goes as follows. We divide the time interval $[0,t]$ into N small increments $\Delta = t/N$. To first order in Δ, we can integrate 1 by taking the first order term in a Taylor expansion:

$$|\psi(\Delta)\rangle = |\psi(0)\rangle + \Delta \frac{d}{dt}|\psi(t)\rangle\Big|_{t=0} + \mathcal{O}\left(\Delta^2\right) \tag{6}$$

$$= |\psi(0)\rangle + -\frac{i\Delta}{\hbar}H(0)|\psi(0)\rangle + \mathcal{O}\left(\Delta^2\right) \tag{7}$$

$$= \left(1 - \frac{i\Delta}{\hbar}H(0)\right)|\psi(0)\rangle + \mathcal{O}\left(\Delta^2\right) \tag{8}$$

So far, we've been fairly precise, but now the hand-waving starts. We note that the term multiplying $|\psi(0)\rangle$ consists of the first two terms in the expansion of $e^{-i\Delta H(0)/\hbar}$, so we state that to evolve from $t = 0$ to $t = \Delta$, we multiply the initial state $|\psi(0)\rangle$ by $e^{-i\Delta H(0)/\hbar}$. That is, we propose that

$$|\psi(\Delta)\rangle = e^{-i\Delta H(0)/\hbar}|\psi(0)\rangle \tag{9}$$

[The reason this is hand-waving is that there are many functions whose first order Taylor expansion matches $\left(1 - \frac{i\Delta}{\hbar}H(0)\right)$, so it seems arbitrary to choose the exponential. I imagine the motivation is that in the time-independent case, the result reduces to 4.]

In any case, if we accept this, then we can iterate the process to evolve to later times. To get to $t = 2\Delta$, we have

$$|\psi(2\Delta)\rangle = e^{-i\Delta H(\Delta)/\hbar}|\psi(\Delta)\rangle \tag{10}$$

$$= e^{-i\Delta H(\Delta)/\hbar}e^{-i\Delta H(0)/\hbar}|\psi(0)\rangle \tag{11}$$

The snag here is that we can't, in general, combine the two exponentials into a single exponential by adding the exponents. This is because $H(\Delta)$ and $H(0)$ will not, in general, commute, as the Baker-Campbell-Hausdorff formula tells us. For example, the time dependence of $H(t)$ might be such that at $t = 0$, $H(0)$ is a function of the position operator X only, while at $t = \Delta$, $H(\Delta)$ becomes a function of the momentum operator P only. Since X and P don't commute, $[H(0), H(\Delta)] \neq 0$, so $e^{-i\Delta H(\Delta)/\hbar}e^{-i\Delta H(0)/\hbar} \neq e^{-i\Delta[H(0)+H(\Delta)]/\hbar}$.

This means that the best we can usually do is to write

$$|\psi(t)\rangle = |\psi(N\Delta)\rangle \tag{12}$$

$$= \prod_{n=0}^{N-1} e^{-i\Delta H(n\Delta)/\hbar}|\psi(0)\rangle \tag{13}$$

The propagator then becomes, in the limit

$$U(t) = \lim_{N\to\infty} \prod_{n=0}^{N-1} e^{-i\Delta H(n\Delta)/\hbar} \tag{14}$$

This limit is known as a *time-ordered integral* and is written as

$$T\left\{\exp\left[-\frac{i}{\hbar}\int_0^t H\left(t'\right)dt'\right]\right\} \equiv \lim_{N\to\infty} \prod_{n=0}^{N-1} e^{-i\Delta H(n\Delta)/\hbar} \tag{15}$$

One final note about the propagators. Since each term in the product is the exponential of i times a Hermitian operator, each term is a unitary operator. Further, since the product of two unitary operators is still unitary, the propagator in the time-dependent case is a unitary operator.

We've defined a propagator as a unitary operator that carries a state from $t = 0$ to some later time t, but we can generalize the notation so that $U(t_2, t_1)$ is a propagator that carries a state from $t = t_1$ to $t = t_2$, that is

$$|\psi(t_2)\rangle = U(t_2, t_1)\,|\psi(t_1)\rangle \tag{16}$$

We can chain propagators together to get

$$\begin{aligned} |\psi(t_3)\rangle &= U(t_3, t_2)\,|\psi(t_2)\rangle && (17)\\ &= U(t_3, t_2)\,U(t_2, t_1)\,|\psi(t_1)\rangle && (18)\\ &= U(t_3, t_1)\,|\psi(t_1)\rangle && (19) \end{aligned}$$

Therefore

$$U(t_3, t_1) = U(t_3, t_2)\,U(t_2, t_1) \tag{20}$$

Since the Hermitian conjugate of a unitary operator is its inverse, we have

$$U^\dagger(t_2, t_1) = U^{-1}(t_2, t_1) \tag{21}$$

We can combine this with 20 to get

$$\begin{aligned} |\psi(t_1)\rangle &= I\,|\psi(t_1)\rangle && (22)\\ &= U^{-1}(t_2, t_1)\,U(t_2, t_1)\,|\psi(t_1)\rangle && (23)\\ &= U^\dagger(t_2, t_1)\,U(t_2, t_1)\,|\psi(t_1)\rangle && (24) \end{aligned}$$

Therefore

$$\begin{aligned} U^\dagger(t_2, t_1)\,U(t_2, t_1) &= U(t_1, t_1) = I && (25)\\ U^\dagger(t_2, t_1) &= U(t_1, t_2) && (26) \end{aligned}$$

That is, the Hermitian conjugate (or inverse) of a propagator carries a state 'backwards in time' to its starting point.

PINGBACKS

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Pingback: Time translation and conservation of energy

FREE PARTICLE REVISITED: SOLUTION IN TERMS OF A PROPAGATOR

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

References: Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 5.1, Exercise 5.1.1.

Post date: 3 Jan 2017

Having reviewed the background mathematics and postulates of quantum mechanics as set out by Shankar, we can now revisit some of the classic problems in non-relativistic quantum mechanics using Shankar's approach, as opposed to that of Griffiths that we've already studied.

The first problem we'll look it is that of the free particle. Following the fourth postulate, we write down the classical Hamiltonian for a free particle, which is

$$H = \frac{p^2}{2m} \tag{1}$$

where p is the momentum (we're working in one dimension) and m is the mass. To get the quantum version, we replace p by the momentum operator P and insert the result into the Schrödinger equation:

$$\begin{aligned} i\hbar \left|\dot{\psi}\right\rangle &= H\left|\psi\right\rangle & (2)\\ &= \frac{P^2}{2m}\left|\psi\right\rangle & (3) \end{aligned}$$

Since H is time-independent, the solution can be written using a propagator:

$$\left|\psi\left(t\right)\right\rangle = U\left(t\right)\left|\psi\left(0\right)\right\rangle \tag{4}$$

To find U, we need to solve the eigenvalue equation for the stationary states

$$\frac{P^2}{2m}\left|E\right\rangle = E\left|E\right\rangle \tag{5}$$

where E is an eigenvalue representing the allowable energies. Since the Hamiltonian is $P^2/2m$, and an eigenstate of P with eigenvalue p is also an eigenstate of P^2 with eigenvalue p^2, we can write this equation in terms of the momentum eigenstates $\left|p\right\rangle$:

$$\frac{P^2}{2m}\left|p\right\rangle = E\left|p\right\rangle \tag{6}$$

Using $P^2\left|p\right\rangle = p^2\left|p\right\rangle$ this gives

$$\left(\frac{p^2}{2m} - E\right)\left|p\right\rangle = 0 \tag{7}$$

Assuming that $\left|p\right\rangle$ is not a null vector gives the relation between momentum and energy:

$$p = \pm\sqrt{2mE} \tag{8}$$

Thus each allowable energy E has two possible momenta. Once we specify the momentum, we also specify the energy and since each energy state is two-fold degenerate, we can eliminate the ambiguity by specifying only the momentum. Therefore the propagator can be written as

$$U\left(t\right) = \int_{-\infty}^{\infty} e^{-ip^2t/2m\hbar}\left|p\right\rangle\left\langle p\right| dp \tag{9}$$

We can convert this to an integral over the energy by using 8 to change variables, and by splittling the integral into two parts. For $p > 0$ we have

$$dp = \sqrt{\frac{m}{2E}}dE \tag{10}$$

and for $p < 0$ we have

$$dp = -\sqrt{\frac{m}{2E}}dE \tag{11}$$

Therefore, we get

$$U\left(t\right) = \int_0^{\infty} e^{-iEt/\hbar}\left|E,+\right\rangle\left\langle E,+\right|\sqrt{\frac{m}{2E}}dE + \int_{\infty}^{0} e^{-iEt/\hbar}\left|E,-\right\rangle\left\langle E,-\right|\left(-\sqrt{\frac{m}{2E}}\right)dE \tag{12}$$

$$= \int_0^{\infty} e^{-iEt/\hbar}\left|E,+\right\rangle\left\langle E,+\right|\sqrt{\frac{m}{2E}}dE + \int_0^{\infty} e^{-iEt/\hbar}\left|E,-\right\rangle\left\langle E,-\right|\sqrt{\frac{m}{2E}}dE \tag{13}$$

$$= \sum_{\alpha=\pm}\int_0^{\infty}\frac{m}{\sqrt{2mE}}e^{-iEt/\hbar}\left|E,\alpha\right\rangle\left\langle E,\alpha\right| dE \tag{14}$$

Here, $\left|E,+\right\rangle$ is the state with energy E and momentum $p = +\sqrt{2mE}$ and similarly for $\left|E,-\right\rangle$. In the first line, the first integral is for $p > 0$ and corresponds to the $\int_0^{\infty}$ part of 9. The second integral is for $p < 0$ and corresponds

to the $\int_{-\infty}^{0}$ part of 9, which is why the limits on the second integral have ∞ at the bottom and 0 at the top. Reversing the order of integration cancels out the minus sign in $-\sqrt{\frac{m}{2E}}$, which allows us to add the two integrals together to get the final answer.

PINGBACKS

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Pingback: Path integral formulation of quantum mechanics: free particle propagator

FREE PARTICLE IN THE POSITION BASIS

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References: Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 5.1, Exercise 5.1.2.

Post date: 4 Jan 2017

In quantum mechanics, the free particle has degenerate energy eigenstates for each energy

$$E = \frac{p^2}{2m} \tag{1}$$

where p is the momentum. The degeneracy arises because the momentum can be either positive (for a particle moving to the right) or negative (to the left):

$$p = \pm\sqrt{2mE} \tag{2}$$

Thus the most general energy eigenstate is a linear combination of the two momentum states:

$$|E\rangle = \beta \left| p = \sqrt{2mE} \right\rangle + \gamma \left| p = -\sqrt{2mE} \right\rangle \tag{3}$$

This bizarre feature of quantum mechanics means that a particle in such a state could be moving either left or right, and if we make a measurement of the momentum we force the particle into one or other of the two momentum states.

We obtained this solution by working in the momentum basis, but we can also find the solution in the position basis. In that basis, the momentum operator has the form

$$P = -i\hbar\frac{d}{dx} \tag{4}$$

The matrix elements of this operator in the position basis are

$$\left\langle x \left| P \right| x' \right\rangle = -i\hbar\delta'\left(x - x'\right) \tag{5}$$

where $\delta'\left(x - x'\right)$ is the derivative of the delta function with respect to the x, not the x'. We can use the properties of this derivative to get a solution in the X basis. To be completely formal about it, the derivation of the matrix elements of P^2 in the X basis is:

$$\left\langle x\left|P^2\right|\psi\right\rangle = \int\int \left\langle x\left|P\right|x'\right\rangle \left\langle x'\left|P\right|x''\right\rangle \left\langle x''\left|\psi\right.\right\rangle dx'dx'' \tag{6}$$

$$= \int\int \left\langle x\left|P\right|x'\right\rangle \left(-i\hbar\delta'\left(x'-x''\right)\right)\psi\left(x''\right)dx'dx'' \tag{7}$$

$$= -i\hbar\int \left\langle x\left|P\right|x'\right\rangle \frac{d\psi\left(x'\right)}{dx'}dx' \tag{8}$$

$$= -i\hbar\int\int \left(-i\hbar\delta'\left(x-x'\right)\right)\frac{d\psi\left(x'\right)}{dx'}dx' \tag{9}$$

$$= -\hbar^2\frac{d^2}{dx^2}\psi\left(x\right) \tag{10}$$

In this basis, the Schrödinger equation is therefore the familiar one:

$$\frac{P^2}{2m}\left|\psi\right\rangle = E\left|\psi\right\rangle \tag{11}$$

$$\left\langle x\left|\frac{P^2}{2m}\right|\psi\right\rangle = E\psi\left(x\right) \tag{12}$$

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi\left(x\right) = E\psi\left(x\right) \tag{13}$$

$$\frac{d^2}{dx^2}\psi\left(x\right) = -\frac{2mE}{\hbar^2}\psi\left(x\right) \tag{14}$$

This has the general solution

$$\psi\left(x\right) = \beta e^{ix\sqrt{2mE}/\hbar} + \gamma e^{-ix\sqrt{2mE}/\hbar} \tag{15}$$

[Shankar extracts a factor of $1/\sqrt{2\pi\hbar}$ but as he notes, this is arbitrary and can be absorbed into the constants β and γ as we've done here.]

In this derivation we've implicitly assumed that $E > 0$, since there is no potential so a free particle can't really have a negative energy. However, if you follow through the derivation, you'll see that it works even if $E < 0$. In that case, we'd get

$$\psi\left(x\right) = \beta e^{-x\sqrt{2m|E|}/\hbar} + \gamma e^{x\sqrt{2m|E|}/\hbar} \tag{16}$$

That is, the exponents in both terms are now real instead of imaginary. The problem with this is that the first term blows up for $x \to -\infty$ while the second blows up for $x \to +\infty$. Thus this function is not normalizable, even to a delta function (as was the case when $E > 0$), so functions such as these when $E < 0$ are not in the Hilbert space.

PROPAGATOR FOR A GAUSSIAN WAVE PACKET FOR THE FREE PARTICLE

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

References: Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 5.1, Exercise 5.1.3.

Post date: 5 Jan 2017

The propagator for the free particle is

$$U(t) = \int_{-\infty}^{\infty} e^{-ip^2 t/2m\hbar} |p\rangle \langle p| \, dp \tag{1}$$

We can find its matrix elements in position space by using the position space form of the momentum

$$\langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar} \tag{2}$$

Taking the matrix element of 1 we have

$$\begin{aligned} U\left(x,t;x'\right) &= \left\langle x\left|U(t)\right|x'\right\rangle && (3)\\ &= \int \langle x|p\rangle \left\langle p\left|x'\right.\right\rangle e^{-ip^2 t/2m\hbar} dp && (4)\\ &= \frac{1}{2\pi\hbar} \int e^{ip(x-x')/\hbar} e^{-ip^2 t/2m\hbar} dp && (5)\\ &= \sqrt{\frac{m}{2\pi\hbar i t}} e^{im(x-x')^2/2\hbar t} && (6) \end{aligned}$$

The final integral can be done by combining the exponents in the third line, completing the square and using the standard formula for Gaussian integrals. We won't go through that here, as our main goal is to explore the evolution of an initial wave packet using the propagator. Given 6, we can in principle find the wave function for all future times given an initial wave function, by using the propagator:

$$\psi(x,t) = \int U\left(x,t;x'\right) \psi\left(x',0\right) dx' \tag{7}$$

Here, we're assuming that the initial time is $t = 0$. Shankar uses the standard example where the initial wave packet is a Gaussian:

$$\psi\left(x',0\right)=e^{ip_0x'/\hbar}\frac{e^{-x'^2/2\Delta^2}}{\left(\pi\Delta^2\right)^{1/4}} \tag{8}$$

This is a wave packet distributed symmetrically about the origin, so that $\langle X\rangle=0$, and with mean momentum given by $\langle P\rangle=p_0$. By plugging this and 6 into 7, we can work out the time-dependent version of the wave packet, which Shankar gives as

$$\psi\left(x,t\right)=\left[\sqrt{\pi}\left(\Delta+\frac{i\hbar t}{m\Delta}\right)\right]^{-1/2}\exp\left[\frac{-\left(x-p_0t/m\right)^2}{2\Delta^2\left(1+i\hbar t/m\Delta^2\right)}\right]\exp\left[\frac{ip_0}{\hbar}\left(x-\frac{p_0t}{2m}\right)\right] \tag{9}$$

Again, we won't go through the derivation of this result as it involves a messy calculation with Gaussian integrals again. The main problem we want to solve here is to use our alternative form of the propagator in terms of the Hamiltonian:

$$U\left(t\right)=e^{-iHt/\hbar} \tag{10}$$

For the free particle

$$H=-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} \tag{11}$$

so if we expand $U\left(t\right)$ as a power series, we have

$$U\left(t\right)=\sum_{s=0}^{\infty}\frac{1}{s!}\left(\frac{i\hbar t}{2m}\right)^s\frac{d^{2s}}{dx^{2s}} \tag{12}$$

To see how we can use this form to generate the time-dependent wave function, we'll consider a special case of 8 with $p_0=0$ and $\Delta=1$, so that

$$\psi_0\left(x\right) = \frac{e^{-x^2/2}}{\pi^{1/4}} \tag{13}$$

$$= \frac{1}{\pi^{1/4}}\sum_{n=0}^{\infty}\frac{\left(-1\right)^n x^{2n}}{2^n n!} \tag{14}$$

We therefore need to apply one power series 12 to the other 14. This is best done by examining a few specific terms and then generalizing to the main result. To save writing, we'll work with the following

$$\alpha \equiv \frac{i\hbar t}{m} \tag{15}$$

$$\psi_\pi\left(x\right) \equiv \pi^{1/4}\psi_0\left(x\right) \tag{16}$$

The $s = 0$ term in 12 is just 1, so we'll look at the $s = 1$ term and apply it to 14:

$$\frac{\alpha}{2}\frac{d^2}{dx^2}\left[\sum_{n=0}^{\infty}\frac{(-1)^n x^{2n}}{2^n n!}\right] = \frac{\alpha}{2}\sum_{n=1}^{\infty}\frac{(-1)^n (2n)(2n-1)x^{2n-2}}{2^n n!} \tag{17}$$

$$= \frac{\alpha}{2}\sum_{n=1}^{\infty}\frac{(-1)^n (2n)! x^{2n-2}}{2^n n!(2n-2)!} \tag{18}$$

We can simplify this by using an identity involving factorials:

$$\frac{(2n)!}{n!} = \frac{(2n)(2n-1)(2n-2)(2n-3)\ldots(2)(1)}{n(n-1)(n-2)\ldots(2)(1)} \tag{19}$$

$$= \frac{2^n [n(n-1)(n-2)\ldots(2)(1)][(2n-1)(2n-3)\ldots(3)(1)]}{n!} \tag{20}$$

$$= \frac{2^n n!(2n-1)!!}{n!} \tag{21}$$

$$= 2^n (2n-1)!! \tag{22}$$

The 'double factorial' notation is defined as

$$(2n-1)!! \equiv (2n-1)(2n-3)\ldots(3)(1) \tag{23}$$

That is, it's the product of every other term from n down to 1. Using this result, we can write 18 as

$$\frac{\alpha}{2}\sum_{n=1}^{\infty}\frac{(-1)^n (2n)! x^{2n-2}}{2^n n!(2n-2)!} = \alpha\sum_{n=1}^{\infty}\frac{(-1)^n (2n-1)!! x^{2n-2}}{2(2n-2)!} \tag{24}$$

Now look at the $s = 2$ term from 12.

$$\frac{1}{2!}\frac{\alpha^2}{2^2}\frac{d^4}{dx^4}\left[\sum_{n=0}^{\infty}\frac{(-1)^n x^{2n}}{2^n n!}\right] = \frac{1}{2!}\frac{\alpha^2}{2^2}\sum_{n=2}^{\infty}\frac{(-1)^n (2n)(2n-1)(2n-2)(2n-3)x^{2n-4}}{2^n n!} \tag{25}$$

$$= \frac{1}{2!}\frac{\alpha^2}{2^2}\sum_{n=2}^{\infty}\frac{(-1)^n (2n)! x^{2n-4}}{2^n n!(2n-4)!} \tag{26}$$

$$= \frac{\alpha^2}{2^2 2!}\sum_{n=2}^{\infty}\frac{(-1)^n (2n-1)!! x^{2n-4}}{(2n-4)!} \tag{27}$$

We can see the pattern for the general term for arbitrary s from 12 (we could prove it by induction, but hopefully the pattern is fairly obvious):

$$\frac{1}{s!}\frac{\alpha^s}{2^s}\frac{d^{2s}}{dx^{2s}}\left[\sum_{n=0}^{\infty}\frac{(-1)^n x^{2n}}{2^n n!}\right] = \frac{1}{s!}\frac{\alpha^s}{2^s}\sum_{n=s}^{\infty}\frac{(-1)^n (2n)! x^{2n-2s}}{2^n n!(2n-2s)!} \tag{28}$$

$$= \frac{\alpha^s}{2^s s!}\sum_{n=s}^{\infty}\frac{(-1)^n (2n-1)!! x^{2n-2s}}{(2n-2s)!} \tag{29}$$

Now we can collect terms for each power of x. The constant term (for x^0) is the first term from each series for each value of s, so we have, using the general term 29 and taking the first term where $n = s$:

$$\sum_{s=0}^{\infty}\frac{(-1)^s \alpha^s (2s-1)!!}{2^s s!} = 1 - \frac{\alpha}{2} + \frac{\alpha^2}{2!}\frac{3}{2}\frac{1}{2} - \frac{\alpha^3}{3!}\frac{5}{2}\frac{3}{2}\frac{1}{2} + \ldots \tag{30}$$

[The $(2s-1)!!$ factor is 1 when $s = 0$ as we can see from the result 22.] The series on the RHS is the Taylor expansion of $(1+\alpha)^{-1/2}$, as can be verified using tables.

In general, to get the coefficient of x^{2r} (only even powers of x occur in the series), we take the term where $n = s + r$ from 29 and sum over s. This gives

$$\sum_{s=0}^{\infty}\frac{\alpha^s}{2^s s!}\frac{(-1)^{s+r}(2s+2r-1)!!}{(2r)!} = \frac{(-1)^r}{2^r r!}\sum_{s=0}^{\infty}\frac{\alpha^s}{2^s s!}\frac{(-1)^s (2s+2r-1)!!}{(2r-1)!!} \tag{31}$$

where we used 22 to get the RHS. Expanding the sum gives

$$\sum_{s=0}^{\infty}\frac{\alpha^s}{2^s s!}\frac{(-1)^s (2s+2r-1)!!}{(2r-1)!!} = 1 - \alpha\frac{2r+1}{2} + \frac{\alpha^2}{2!}\left(\frac{2r+3}{2}\right)\left(\frac{2r+1}{2}\right) - \ldots \tag{32}$$

$$= 1 - \alpha\left(r+\frac{1}{2}\right) + \frac{\alpha^2}{2!}\left(r+\frac{3}{2}\right)\left(r+\frac{1}{2}\right) - \ldots \tag{33}$$

$$= (1+\alpha)^{-r-\frac{1}{2}} \tag{34}$$

where again we've used a standard series from tables (given by Shankar in the problem) to get the last line. Combining this with 31, we see that the coefficient of x^{2r} is

$$\frac{(-1)^r}{2^r r!}(1+\alpha)^{-r-\frac{1}{2}} \tag{35}$$

Thus the time-dependent wave function can be written as a single series as:

$$\psi(x,t) = U(t)\,\psi(x,0) \tag{36}$$

$$= e^{-iHt/\hbar}\psi(x,0) \tag{37}$$

$$= \frac{1}{\pi^{1/4}} \sum_{r=0}^{\infty} \frac{(-1)^r}{2^r r!} (1+\alpha)^{-r-\frac{1}{2}} x^{2r} \tag{38}$$

$$= \frac{1}{\pi^{1/4}\sqrt{1+\alpha}} \sum_{r=0}^{\infty} \frac{(-1)^r}{2^r (1+\alpha)^r r!} x^{2r} \tag{39}$$

$$= \frac{1}{\pi^{1/4}\sqrt{1+\alpha}} \exp\left[\frac{-x^2}{2(1+\alpha)}\right] \tag{40}$$

$$= \frac{1}{\pi^{1/4}\sqrt{1+i\hbar t/m}} \exp\left[\frac{-x^2}{2(1+i\hbar t/m)}\right] \tag{41}$$

This agrees with 9 when $p_0 = 0$ and $\Delta = 1$, though it does take a fair bit of work!

INFINITE SQUARE WELL - EXPANDING WELL

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To leave a comment or report an error, please use the auxiliary blog.

References: Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 5.2, Exercise 5.2.1.

Post date: 8 Jan 2017

Shankar's treatment of the infinite square well is similar to that of Griffiths, which we've already covered, so we won't go through the details again. The main difference is that Shankar places the potential walls at $x = \pm\frac{L}{2}$ while Griffiths places them at $x = 0$ and $x = a$. As a result, the stationary states found by Shankar are shifted to the left, with the result

$$\psi_n(x) = \begin{cases} \sqrt{\frac{2}{L}}\cos\frac{n\pi x}{L} & n = 1,3,5,7,\ldots \\ \sqrt{\frac{2}{L}}\sin\frac{n\pi x}{L} & n = 2,4,6,\ldots \end{cases} \tag{1}$$

These results can be obtained from the form given by Griffiths (where we take the width of the well to be L rather than a):

$$\psi_n(x) = \sqrt{\frac{2}{L}}\sin\frac{n\pi\left(x+\frac{L}{2}\right)}{L} \tag{2}$$

$$= \sqrt{\frac{2}{L}}\left[\sin\frac{n\pi x}{L}\cos\frac{n\pi}{2} + \cos\frac{n\pi x}{L}\sin\frac{n\pi}{2}\right] \tag{3}$$

Choosing n to be even or odd gives the results in 1.

The specific problem we're solving here involves a particle that starts off in the ground state ($n = 1$) of a square well of width L. The well then suddenly expands to a width of $2L$ symmetrically, that is, it now extends from $x = -L$ to $x = +L$. We are to find the probability that the particle will be found in the ground state of the new well.

We solved a similar problem before, but in that case the well expanded by moving its right-hand wall to the right while keeping the left-hand wall fixed, so that the particle found itself in the left half of the new, expanded well. In the present problem, the particle finds itself centred in the new expanded well. You might think that this shouldn't matter, but it turns out to make quite a difference. To calculate this probability, we need to express the original wave function in terms of the stationary states of the expanded well, which we'll refer to as $\phi_n(x)$. That is

$$\psi_1(x) = \sum_{n=1}^{\infty} c_n \phi_n(x) \tag{4}$$

Working with Shankar's functions 1 we find ϕ_n by replacing L by $2L$:

$$\phi_n(x) = \begin{cases} \frac{1}{\sqrt{L}} \cos \frac{n\pi x}{2L} & n = 1,3,5,7,\ldots \\ \frac{1}{\sqrt{L}} \sin \frac{n\pi x}{2L} & n = 2,4,6,\ldots \end{cases} \tag{5}$$

Using the orthonormality of the wave functions, we have

$$\begin{aligned} c_1 &= \int_{-L}^{L} \psi_1(x)\, \phi_1(x)\, dx && (6)\\ &= \int_{-L/2}^{L/2} \sqrt{\frac{2}{L}} \cos\frac{\pi x}{L} \frac{1}{\sqrt{L}} \cos\frac{\pi x}{2L} dx && (7)\\ &= \frac{\sqrt{2}}{L} \int_{-L/2}^{L/2} \cos\frac{\pi x}{L} \cos\frac{\pi x}{2L} dx && (8)\\ &= \frac{\sqrt{2}}{L} \int_{-L/2}^{L/2} \left(1 - 2\sin^2\frac{\pi x}{2L}\right) \cos\frac{\pi x}{2L} dx && (9)\\ &= \frac{8}{3\pi} && (10) \end{aligned}$$

The limits of integration are reduced in the second line since $\psi_1(x) = 0$ if $x > \left|\frac{L}{2}\right|$.

Thus the probability of finding the particle in the new ground state is

$$|c_1|^2 = \frac{64}{9\pi^2} \tag{11}$$

Note that in the earlier problem where the well expanded to the right, the probability was $\frac{32}{9\pi^2}$, so the new probability is twice as much when the wave function remains centred in the new well.

We could have also done the calculation using Griffiths's well which extended from $x = 0$ to $x = L$. If this well expands symmetrically, it now runs from $x = -\frac{L}{2}$ to $x = \frac{3L}{2}$, and the stationary states of this new well are obtained by replacing $L \to 2L$ and $x \to x + \frac{L}{2}$, so we have

$$\phi_n(x) = \frac{1}{\sqrt{L}} \sin\frac{n\pi\left(x + \frac{L}{2}\right)}{2L} \tag{12}$$

We then get

$$c_1 = \int_{-L/2}^{3L/2} \psi_1(x)\,\phi_1(x)\,dx \tag{13}$$

$$= \frac{\sqrt{2}}{L}\int_0^L \sin\frac{\pi x}{L}\sin\frac{\pi\left(x+\frac{L}{2}\right)}{2L}dx \tag{14}$$

$$= \frac{8}{3\pi} \tag{15}$$

The integral can be done by expanding the second sine using the sine addition formula. (I just used Maple.)

INFINITE SQUARE WELL - FORCE TO DECREASE WELL WIDTH

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To leave a comment or report an error, please use the auxiliary blog.

References: Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 5.2, Exercise 5.2.4.

Post date: 9 Jan 2017

One way of comparing the classical and quantum pictures of a particle in an infinite square well is to calculate the force exerted on the walls by the particle. If a particle is in state $|n\rangle$, its energy is

$$E_n = \frac{(n\pi\hbar)^2}{2mL^2} \tag{1}$$

If the particle remains in this state as the walls are slowly pushed in, so that L slowly decreases, then its energy E_n will increase, meaning that work is done on the system. The force is the change in energy per unit distance, so the force required is

$$F = -\frac{\partial E_n}{\partial L} = \frac{(n\pi\hbar)^2}{mL^3} \tag{2}$$

If we treat the system classically, then a particle with energy E_n between the walls is effectively a free particle in this region (since the potential $V = 0$ there), so all its energy is kinetic. That is

$$\begin{aligned} E_n &= \frac{1}{2}mv^2 && (3)\\ v &= \sqrt{\frac{2E_n}{m}} && (4)\\ &= \frac{n\pi\hbar}{mL} && (5) \end{aligned}$$

The classical particle bounces elastically between the two walls, which means its velocity is exactly reversed at each collision. The momentum transfer in such a collision is

$$\Delta p = 2mv = \frac{2n\pi\hbar}{L} \tag{6}$$

The time between successive collisions on the same wall is

$$\Delta t = \frac{2L}{v} = \frac{2mL^2}{n\pi\hbar} \tag{7}$$

Thus the average force exerted on one wall is

$$\bar{F} = \frac{\Delta p}{\Delta t} = \frac{(n\pi\hbar)^2}{mL^3} \tag{8}$$

Comparing with 2, we see that the quantum and classical forces in this case are the same.

PROBABILITY CURRENT WITH COMPLEX POTENTIAL

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To leave a comment or report an error, please use the auxiliary blog.

References: Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 5.3, Exercise 5.3.1.

Post date: 11 Jan 2017

Shakar's derivation of the probability current in 3-d is similar to the one we reviewed earlier, so we don't need to repeat it here. We can, however, look at a slight variant where the potential has a constant imaginary part, so that

$$V(\mathbf{r}) = V_r(\mathbf{r}) - iV_i \tag{1}$$

where $V_r(\mathbf{r})$ is a real function of position and V_i is a real constant. A Hamiltonian containing such a complex potential is not Hermitian.

To see what effect this has on the total probability of finding a particle in all space, we can repeat the derivation of the probability current. From the Schrödinger equation and its complex conjugate, we have

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi + V_r\psi - iV_i\psi \tag{2}$$

$$-i\hbar\frac{\partial\psi^*}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi^* + V_r\psi^* + iV_i\psi^* \tag{3}$$

Multiply the first equation by ψ^* and the second by ψ and subtract to get

$$i\hbar\frac{\partial}{\partial t}(\psi\psi^*) = -\frac{\hbar^2}{2m}\left(\psi^*\nabla^2\psi - \psi\nabla^2\psi^*\right) - 2iV_i\psi\psi^* \tag{4}$$

As in the case with a real potential, the first term on the RHS can be written as the divergence of a vector:

$$\mathbf{J} = \frac{\hbar}{2mi}(\Psi^*\nabla\Psi - \Psi\nabla\Psi^*) \tag{5}$$

$$\nabla\cdot\mathbf{J} = \frac{\hbar}{2mi}\left(\psi^*\nabla^2\psi - \psi\nabla^2\psi^*\right) \tag{6}$$

$$\frac{\partial}{\partial t}(\psi\psi^*) = -\nabla\cdot\mathbf{J} - \frac{2V_i}{\hbar}\psi\psi^* \tag{7}$$

If we define the total probability of finding the particle anywhere in space as

$$P \equiv \int \psi^* \psi d^3\mathbf{r} \tag{8}$$

then we can integrate 4 over all space and use Gauss's theorem to convert the volume integral of a divergence into a surface integral:

$$\frac{\partial}{\partial t}\left(\int \psi\psi^* d^3\mathbf{r}\right) = -\int \nabla\cdot\mathbf{J} d^3\mathbf{r} - \frac{2V_i}{\hbar}\int \psi\psi^* d^3\mathbf{r} \tag{9}$$

$$\frac{\partial P}{\partial t} = -\int_S \mathbf{J}\cdot d\mathbf{a} - \frac{2V_i}{\hbar}P \tag{10}$$

We make the usual assumption that the probability current $\mathbf{J}$ tends to zero at infinity fast enough for the first integral on the RHS to be zero, and we get

$$\frac{\partial P}{\partial t} = -\frac{2V_i}{\hbar}P \tag{11}$$

This has the solution

$$P(t) = P(0)\, e^{-2V_i t/\hbar} \tag{12}$$

That is, the probability of the particle existing decays exponentially. Although Shankar says that such a potential can be used to model a system where particles are absorbed, it's not clear how realistic it is since the Hamiltonian isn't hermitian, so technically the energies in such a system are not observables.

PROBABILITY CURRENT: A FEW EXAMPLES

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References: Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 5.3, Exercises 5.3.2 - 5.3.4.

Post date: 12 Jan 2017

Here are a few examples of probability current.

Example 1. Suppose the wave function has the form

$$\psi(\mathbf{r},t) = c\tilde{\psi}(\mathbf{r},t) \tag{1}$$

where c is a complex constant and $\tilde{\psi}(\mathbf{r},t)$ is a real function of position and time. Then the probability current is

$$\begin{aligned}
\mathbf{j} &= \frac{\hbar}{2mi}\left(\psi^*\nabla\psi - \psi\nabla\psi^*\right) && (2)\\
&= \frac{\hbar}{2mi}\left(cc^*\left(\tilde{\psi}\nabla\tilde{\psi}\right) - \tilde{\psi}\nabla\tilde{\psi}\right) && (3)\\
&= 0 && (4)
\end{aligned}$$

In particular, if ψ itself is real, the probability current is always zero, so all the stationary states of systems like the harmonic oscillator and hydrogen atom that we've studied show no flow of probability, which is what we'd expect since they are, after all, stationary states.

Example 2. Now the wave function is

$$\psi_{\mathbf{p}} = \frac{1}{(2\pi\hbar)^{3/2}}e^{i\mathbf{p}\cdot\mathbf{r}/\hbar} \tag{5}$$

where the momentum $\mathbf{p}$ is constant. In this case we have

$$\begin{aligned}
\nabla\psi_{\mathbf{p}} &= \frac{i}{(2\pi\hbar)^{3/2}\hbar}e^{i\mathbf{p}\cdot\mathbf{r}/\hbar}\mathbf{p} && (6)\\
\nabla\psi^*_{\mathbf{p}} &= \frac{-i}{(2\pi\hbar)^{3/2}\hbar}e^{-i\mathbf{p}\cdot\mathbf{r}/\hbar}\mathbf{p} && (7)\\
\psi^*_{\mathbf{p}} &= \frac{1}{(2\pi\hbar)^{3/2}}e^{-i\mathbf{p}\cdot\mathbf{r}/\hbar} && (8)
\end{aligned}$$

This gives a probability current of

$$\mathbf{j} = \frac{\hbar}{2mi}(\psi^*_{\mathbf{p}}\nabla\psi_{\mathbf{p}} - \psi_{\mathbf{p}}\nabla\psi^*_{\mathbf{p}}) \tag{9}$$

$$= \frac{1}{(2\pi\hbar)^3 2m}(\mathbf{p}+\mathbf{p}) \tag{10}$$

$$= \frac{1}{(2\pi\hbar)^3 m}\mathbf{p} \tag{11}$$

The probability density is

$$P = \psi^*_{\mathbf{p}}\psi_{\mathbf{p}} = \frac{1}{(2\pi\hbar)^3} \tag{12}$$

Thus the current can be written as

$$\mathbf{j} = \frac{P}{m}\mathbf{p} \tag{13}$$

Classically, the momentum is $\mathbf{p} = mv$, so the current has the same form as $\mathbf{j} = P\mathbf{v}$. This is similar to the electromagnetic case where the electric current density $\mathbf{J} = \rho\mathbf{v}$ where ρ is the charge density and $\mathbf{v}$ is the velocity of that charge. The probability density can be viewed as "probability" moving with velocity $\mathbf{v}$.

Example 3. Now consider a one-dimensional problem where the wave function consists of two oppositely-moving plane waves:

$$\psi = Ae^{ipx/\hbar} + Be^{-ipx/\hbar} \tag{14}$$

In this case, we have

$$\frac{2mi}{\hbar}j = \psi^*\nabla\psi - \psi\nabla\psi^* \tag{15}$$

$$= \left(A^*e^{-ipx/\hbar} + B^*e^{ipx/\hbar}\right)\frac{ip}{\hbar}\left(Ae^{ipx/\hbar} + Be^{-ipx/\hbar}\right) - \left(Ae^{ipx/\hbar} + Be^{-ipx/\hbar}\right)\frac{ip}{\hbar}\left(-A^*e^{-ipx/\hbar} + B^*e^{ipx/\hbar}\right) \tag{16}$$

$$= \frac{2ip}{\hbar}\left(|A|^2 - |B|^2\right) \tag{17}$$

$$j = \frac{p}{m}\left(|A|^2 - |B|^2\right) \tag{18}$$

The probability current separates into two terms, one for each direction of momentum.

FREE PARTICLE: GAUSSIAN WAVE PACKET

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

Post date: 28 Jul 2012.

Reference: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Problem 2.22.

While analyzing the free particle, we saw that we could construct a normalizable combination of stationary states by writing

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k) e^{ikx} e^{-i\hbar k^2 t/2m} dk \tag{1}$$

Given the initial wave function, we can find $\phi(k)$ via Plancherel's theorem:

$$\phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \Psi(x,0) e^{-ikx} dx \tag{2}$$

The integral 1 cannot usually be done in closed form, but one case where it can is if the initial wave function is a Gaussian, of the form

$$\Psi(x,0) = Ae^{-ax^2} \tag{3}$$

To find A, we normalize:

$$A^2 \int_{-\infty}^{\infty} e^{-2ax^2} dx = 1 \tag{4}$$

The integral comes out to $\sqrt{\pi/2a}$ from which we get

$$A = \left(\frac{2a}{\pi}\right)^{1/4} \tag{5}$$

Finding $\Psi(x,t)$ requires finding $\phi(k)$ via equation 2. So we get (using Maple to do the integral):

$$\begin{aligned} \phi(k) &= \frac{1}{\sqrt{2\pi}} \left(\frac{2a}{\pi}\right)^{1/4} \int_{-\infty}^{\infty} e^{-ax^2 - ikx} dx & (6) \\ &= \left(\frac{1}{2\pi a}\right)^{1/4} e^{-k^2/4a} & (7) \end{aligned}$$

We can now use 1 again using Maple to do the integral:

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\phi(k)e^{ikx}e^{-i\hbar k^2 t/2m}dk \tag{8}$$

$$= \frac{1}{\sqrt{2\pi}}\left(\frac{1}{2\pi a}\right)^{1/4}\int_{-\infty}^{\infty}e^{-k^2/4a}e^{ikx}e^{-i\hbar k^2 t/2m}dk \tag{9}$$

$$= \left(\frac{2a}{\pi}\right)^{1/4}\frac{e^{-ax^2/(1+2i\hbar at/m)}}{\sqrt{1+2i\hbar at/m}} \tag{10}$$

where Maple was used for the integral.

Calculating $|\Psi(x,t)|^2$ can be done using Maple, but it seems to require a bit of help. First we write out the complex conjugate:

$$\Psi^*(x,t) = \left(\frac{2a}{\pi}\right)^{1/4}\frac{e^{-ax^2/(1-2i\hbar at/m)}}{\sqrt{1-2i\hbar at/m}} \tag{11}$$

Then we calculate $\Psi^*\Psi$ using the Maple command *simplify(evalc($\Psi^*\Psi$)) assuming positive* and we get

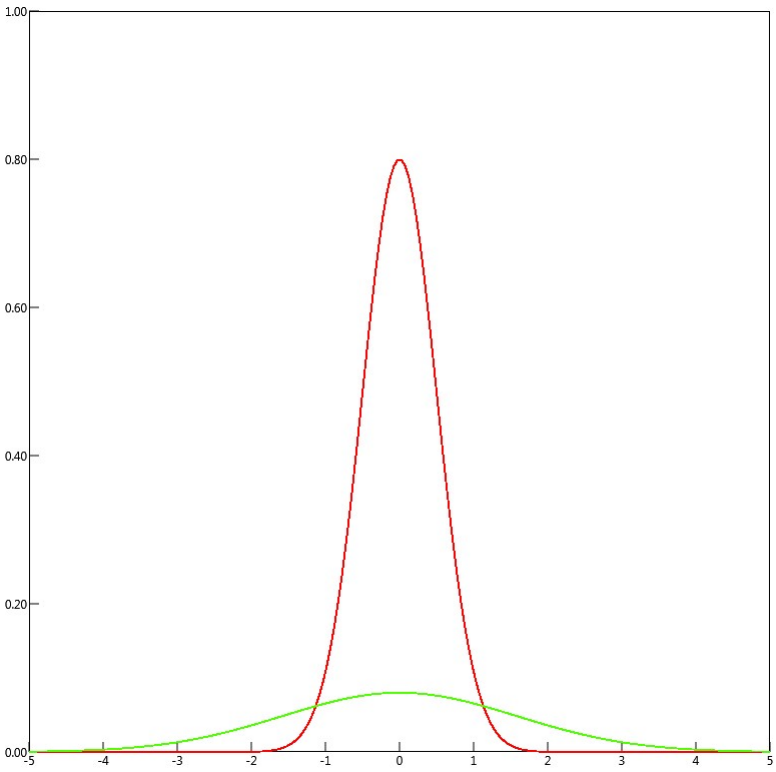
$$|\Psi(x,t)|^2 = \sqrt{\frac{2a}{\pi}}\frac{e^{-2ax^2/\left[1+(2\hbar at/m)^2\right]}}{\sqrt{1+(2\hbar at/m)^2}} \tag{12}$$

$$= \sqrt{\frac{2}{\pi}}we^{-2w^2x^2} \tag{13}$$

with

$$w \equiv \left(\frac{a}{1+(2\hbar at/m)^2}\right)^{1/2} \tag{14}$$

At $t=0$, $w=\sqrt{a}$, so $|\Psi(x,t)|^2 = \sqrt{2a/\pi}e^{-2ax^2}$ which is correct. The wave packet at $t=0$ is therefore a Gaussian centred at $x=0$. As t increases, w gets smaller but the centre of the Gaussian does not move from $x=0$ so the packet spreads out. A couple of plots show this behaviour. We've set $a=1$ in both plots. In the red plot $t=0$ so $w=1$ and in the green plot t is larger, at a value such that $w=0.1$.



We can get the mean values of position and momentum by integration, although it takes a bit of work. By symmetry, $\langle x \rangle = \langle p \rangle = 0$. To get the other two average values, we use integration with Maple.

$$\langle x^2 \rangle = \int_{-\infty}^{\infty} x^2 |\Psi(x,t)|^2 dx \tag{15}$$

$$= \frac{1}{4w^2} \tag{16}$$

$$= \frac{1 + (2\hbar a t/m)^2}{4a} \tag{17}$$

This shows that the wave function spreads out with time. At $t = 0$ $\left\langle x^2 \right\rangle = 1/4a$, but it then increases quadratically with t.

Calculating $\langle p^2 \rangle$ starts with:

$$\langle p^2 \rangle = -\hbar^2 \int_{-\infty}^{\infty} \Psi^* \frac{\partial^2}{\partial x^2} \Psi dx \tag{18}$$

This can be evaluated with the Maple command *simplify(evalc(int(-h^2*simplify(evalc(psixtconj*(di x$2)))), x = -infinity .. infinity))) assuming positive* where *psixtconj* and *psixt* are the Maple expressions for Ψ^* and Ψ respectively. The result is:

$$\langle p^2 \rangle = a\hbar^2 \tag{19}$$

The uncertainty principle thus becomes

$$\begin{aligned} \sigma_x \sigma_p &= \sqrt{\langle x^2 \rangle \langle p^2 \rangle} && (20) \\ &= \frac{\hbar}{2}\sqrt{1 + (2\hbar a t/m)^2} && (21) \end{aligned}$$

The system has the least uncertainty at $t = 0$. Uncertainty increases with time as the wave packet spreads out.

PINGBACKS

Pingback: Free particle - travelling wave packet
Pingback: Free particle in momentum space

FINITE SQUARE WELL: BOUND STATES & ODD WAVE FUNCTIONS

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

Post date: 5 Mar 2011.

Reference: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Problem 2.29.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 5.2, Exercise 5.2.6.

To complete our analysis of the finite square well, we'll have a look at the solutions where the spatial wave function $\psi(x)$ is an odd function. In our analysis of the problem where $\psi(x)$ was even, we began with the potential:

$$V(x) = \begin{cases} 0 & x < -a \\ -V_0 & -a \leq x \leq a \\ 0 & x > a \end{cases} \tag{1}$$

where V_0 is a positive constant energy, and a is a constant location on the x axis.

For bound states, we have $-V_0 < E < 0$, (the total energy has to be greater than the minimum value of the potential, as we proved before) which results in bound states in which we would expect $\psi(x)$ to oscillate within the well and decay exponentially outside the well.

Following the same procedure as in the even function case, we divide the solution into separate regions and try to solve for the various constants that pop up by applying boundary conditions. The equation to be solved can be split into three regions:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi \qquad (x < -a) \tag{2}$$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} - V_0\psi = E\psi \qquad (-a \leq x \leq a) \tag{3}$$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi \qquad (x > a) \tag{4}$$

The general solutions in these three regions are easy enough to write down. We get

$$\psi(x) = \begin{cases} Ae^{-\kappa x} + Be^{\kappa x} & x < -a \\ C\sin(\mu x) + D\cos(\mu x) & -a \leq x \leq a \\ Fe^{-\kappa x} + Ge^{\kappa x} & x > a \end{cases} \tag{5}$$

where as usual we've introduced some convenience parameters:

$$\kappa \equiv \frac{\sqrt{-2mE}}{\hbar} \tag{6}$$

$$\mu \equiv \frac{\sqrt{2m(E+V_0)}}{\hbar} \tag{7}$$

Note that both these parameters are real and can be taken as positive, since $-V_0 < E < 0$ for bound states. Note that we've also expressed the solution in the middle section in terms of sin and cos rather than in terms of $e^{i\mu x}$ and $e^{-i\mu x}$. The latter is also valid, but as we'll see in the next paragraph, using sin and cos is easier.

So now we have six constants to deal with. First, we can use the theorem that says that if the potential function is even (as this one is: $V(-x) = V(x)$), then $\psi(x)$ is even or odd. We now require $\psi(x)$ to be odd, so that $\psi(-x) = -\psi(x)$. Since the cosine is an even function, we must have $D = 0$. In the outer regions, the requirement of an odd function means that $A = -G$ and $B = -F$.

Next, we can impose the requirement that $\psi(x) \to 0$ at $\pm\infty$, so this means that $A = G = 0$. We therefore get

$$\psi(x) = \begin{cases} Be^{\kappa x} & x < -a \\ C\sin(\mu x) & -a \leq x \leq a \\ -Be^{-\kappa x} & x > a \end{cases} \tag{8}$$

Now we can apply the boundary conditions. Since there are no infinite energies involved (the potential is finite everywhere), we apply Born's conditions and require that both ψ and ψ' are continuous at both boundaries. Because of the symmetry of the wave function, we can consider only one boundary; the other one won't give us anything new. Therefore these two conditions give us (using the fact that sine is odd and cosine is even):

$$Be^{-\kappa a} = -C\sin(\mu a) \tag{9}$$

$$\kappa Be^{-\kappa a} = \mu C\cos(\mu a) \tag{10}$$

Dividing these two equations together, we can get rid of B and C:

$$\frac{1}{\kappa} = -\frac{1}{\mu}\tan(\mu a) \tag{11}$$

This is actually a condition that will give us the allowed energies, since both κ and μ are functions of E. Unfortunately, this equation cannot be solved explicitly for E (it's what is known as *transcendental*, which means that the variable we're trying to solve for occurs both inside and outside of a function such as the tan). The only way such equations can be solved is numerically, but we can get an idea of the solutions by plotting the two sides of the equation on the same graph and seeing where these plots intersect.

We can rewrite this equation as

$$\tan(\mu a) = -\frac{\mu}{\kappa} \tag{12}$$

From the definitions of κ and μwe can eliminate κ as follows:

$$\kappa^2 + \mu^2 = 2mV_0/\hbar^2 \tag{13}$$

$$\kappa = \sqrt{2mV_0/\hbar^2 - \mu^2} \tag{14}$$

$$\frac{\mu}{\kappa} = \frac{1}{\sqrt{2mV_0/\mu^2\hbar^2 - 1}} \tag{15}$$

$$\tan(\mu a) = -\frac{1}{\sqrt{2mV_0/\mu^2\hbar^2 - 1}} \tag{16}$$

$$= -\frac{1}{\sqrt{2ma^2V_0/(\mu a)^2\hbar^2 - 1}} \tag{17}$$

Defining the variable $z \equiv \mu a$, we can now write this equation as a transcendental equation in the single variable z:

$$\tan z = -\left(\frac{2ma^2V_0/\hbar^2}{z^2} - 1\right)^{-1/2} \tag{18}$$

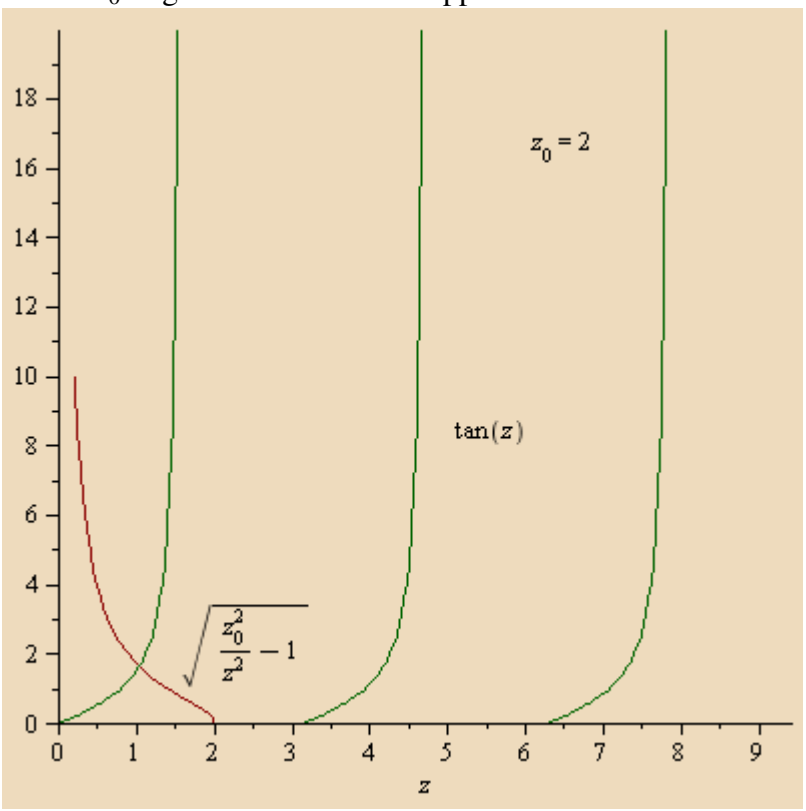
To solve this equation graphically or numerically for a given particle, we clearly need to specify values for a and V_0. However, we can treat the combination of parameters as a single parameter z_0:

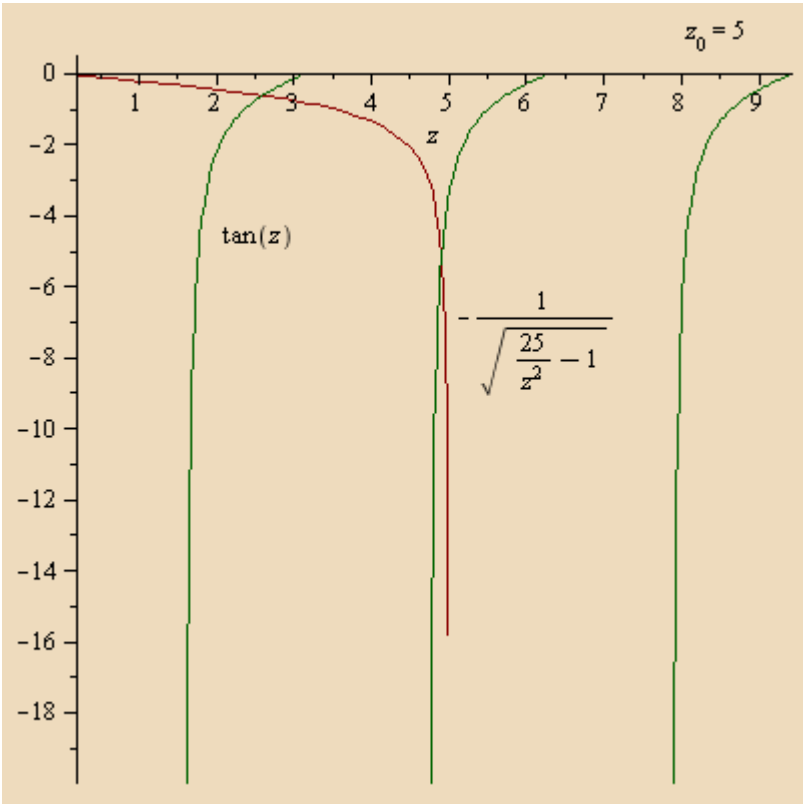
$$z_0^2 \equiv \frac{2ma^2V_0}{\hbar^2} \tag{19}$$

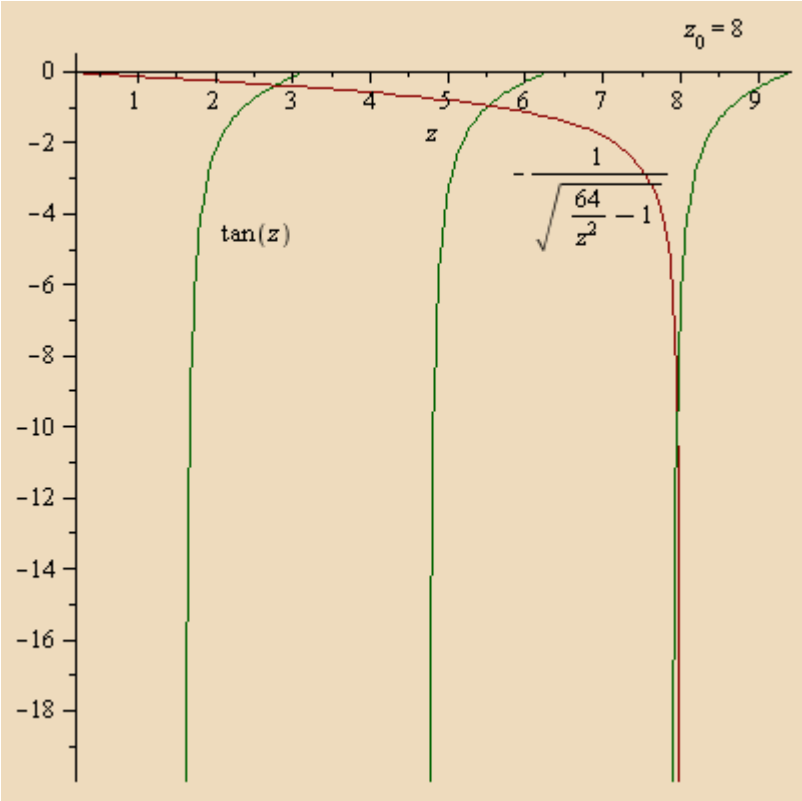
so we have the equation

$$\tan z = -\left(\frac{z_0^2}{z^2} - 1\right)^{-1/2} \tag{20}$$

We can plot both sides of this equation on the same graph for various values of z_0 to get an idea of what happens.



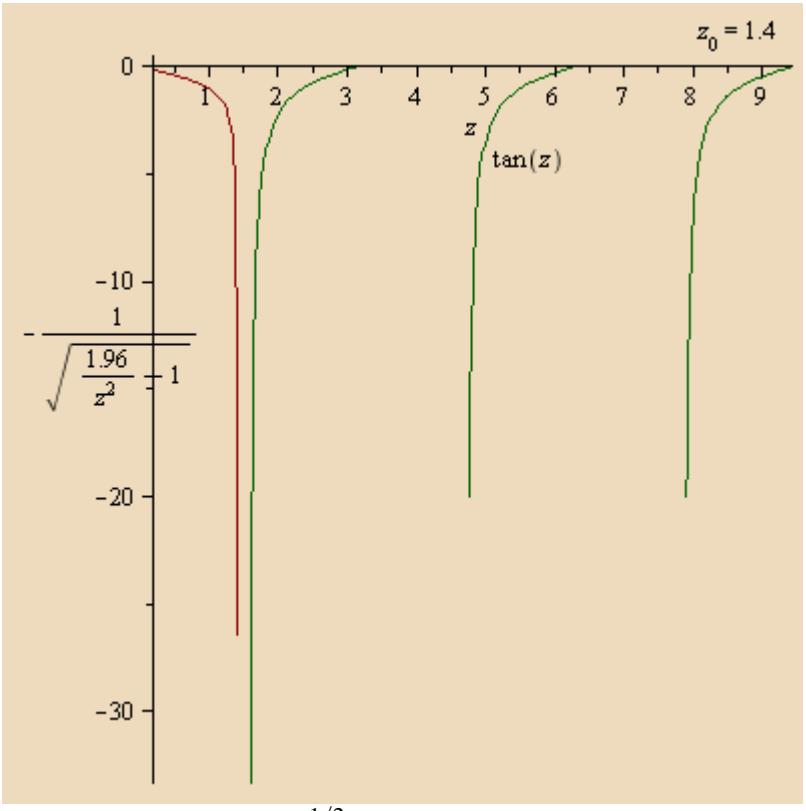

$z_0 = 5$
0
-2
-4
-6
-8
-10
-12
-14
-16
-18
1
2
3
4
5
6
7
8
9
z
tan(z)
$-\frac{1}{\sqrt{\frac{25}{z^2}-1}}$



In these plots, we show what happens for three different values of z_0. The green curves show the plot of $\tan z$; the red curves that of $-\left(\frac{z_0^2}{z^2}-1\right)^{-1/2}$. In the first graph, with $z_0 = 2$, we get only one intersection between the two plots, around $z = 2$. Thus for $z_0 = 2$, there is only one bound state, with an energy that can be worked out from $z = \mu a = \frac{\sqrt{2m(E+V_0)}a}{\hbar} \approx 2$. A more accurate value can be obtained by numerical solution of the equation, but this requires a computer (well, actually, the graphs were drawn on a computer too, but never mind).

The second and third graphs show what happens as we increase z_0 to 5 and then 8. In each case we pick up an extra intersection between the two graphs, so we add an extra bound state.

In this case, we see that if we reduce z_0 to a value less than $\pi/2$, there will be no bound states, since the tangent is asymptotic to the line $z = \pi/2$. We can see the situation in the following plot, in which $z_0 = 1.4 < \pi/2$:



The curve $-\left(\frac{z_0^2}{z^2}-1\right)^{-1/2}$ is here asymptotic to the line $z = 1.4$, so it will never intersect the tangent curve.

At the other extreme, as $V_0 \to \infty$, we would expect to get the infinite square well states. To see this, note that the graph of $-\left(\frac{z_0^2}{z^2}-1\right)^{-1/2}$ is asymptotic to the line $z = z_0$, so as $V_0 \to \infty$, $z_0 \to \infty$ and the asymptote gets further and further along the axis, so the number of intersections with branches of the tangent gets larger. Thus the *number* of energy states gets larger and larger, eventually becoming infinite. As to the locations of these intersections, we can notice that for any fixed, finite value of z, the quantity $-\left(\frac{z_0^2}{z^2}-1\right)^{-1/2}$ tends to zero as $z_0 \to \infty$, so that means that the entire curve approaches the horizontal axis, so the intersections with the tangent curve will occur very near those locations where the tangent curve meets the horizontal axis, that is, where $\tan z = 0$. These points are at $z = n\pi$. This means that

$$z^2 = \frac{2ma^2(E+V_0)}{\hbar^2} \tag{21}$$

$$\approx n^2\pi^2 \tag{22}$$

$$E+V_0 \approx \frac{n^2\pi^2\hbar^2}{2ma^2} \tag{23}$$

$$= \frac{(2n)^2\pi^2\hbar^2}{2m(2a)^2} \tag{24}$$

Since $E+V_0$ is the height of the bound state above the bottom of the well, we can see that this formula does indeed give us the expected energy levels for an infinite square well of width $2a$, for even quantum numbers $2n$. The other ones, for odd n came from a solution where we assume $\psi(x)$ is an even function.

PINGBACKS

Pingback: Finite square well - normalization
Pingback: Hybrid infinite-finite square well
Pingback: Finite square well - numerical solution
Pingback: Finite spherical well
Pingback: Klein-Gordon equation with finite square well - numerical solution

FINITE SQUARE BARRIER - SCATTERING

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

Post date: 6 Aug 2012.

Reference: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Problem 2.33.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 5.4, Exercise 5.4.2 (a).

We've analyzed the scattering problem in the finite square well, and we can use similar techniques to analyze a finite square barrier, which has the potential

$$V(x) = \begin{cases} 0 & x < -a \\ V_0 & -a \le x \le a \\ 0 & x > a \end{cases} \tag{1}$$

where V_0 is a positive constant energy, and a is a constant location on the x axis.

There are three distinct cases here:

(1) Energy below the barrier: $0 \le E < V_0$
(2) Energy exactly equal to the barrier: $E = V_0$
(3) Energy greater than the barrier: $E > V_0$

In all three cases, the wave function away from the barrier on either side has the same form; it is only within the barrier that the three cases differ. We'll consider first the case where $0 \le E < V_0$.

In this case, the Schrödinger equation within the barrier is

$$-\frac{\hbar^2}{2m}\psi'' + V_0\psi = E\psi \tag{2}$$

$$\psi'' = \mu^2\psi \tag{3}$$

where

$$\mu = \frac{\sqrt{2m(V_0 - E)}}{\hbar} \tag{4}$$

This has solution

$$\psi(x) = Ce^{\mu x} + De^{-\mu x} \tag{5}$$

Outside the barrier, the Schrödinger equation is

$$\psi'' = E\psi \tag{6}$$

Outside the barrier on the left, the solution is the sum of travelling waves (assuming particles are incident from the left only), while to the right we have right propagating waves only. Thus

$$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & x < -a \\ Fe^{ikx} & x > a \end{cases} \tag{7}$$

where

$$k = \frac{\sqrt{2mE}}{\hbar} \tag{8}$$

Since the potential is finite everywhere, both ψ and ψ' are continuous everywhere, which gives us four boundary conditions.

At $x = -a$ we have

$$\begin{aligned} Ae^{-ika} + Be^{ika} &= Ce^{-\mu a} + De^{\mu a} & (9) \\ ik\left(Ae^{-ika} - Be^{ika}\right) &= \mu\left(Ce^{-\mu a} - De^{\mu a}\right) & (10) \end{aligned}$$

At $x = a$:

$$\begin{aligned} Ce^{\mu a} + De^{-\mu a} &= Fe^{ika} & (11) \\ \mu\left(Ce^{\mu a} - De^{-\mu a}\right) &= ikFe^{ika} & (12) \end{aligned}$$

We can solve these linear equations to get the other four constants in terms of A. The results are

$$B = \frac{e^{-2ika}\left(k^2+\mu^2\right)\left(e^{2\mu a}-e^{-2\mu a}\right)}{2ik\mu\left(e^{2\mu a}+e^{-2\mu a}\right)+\left(k^2-\mu^2\right)\left(e^{2\mu a}-e^{-2\mu a}\right)}A \quad (13)$$

$$= \frac{e^{-2ika}\left(k^2+\mu^2\right)\sinh(2\mu a)}{2ik\mu\cosh(2\mu a)+\left(k^2-\mu^2\right)\sinh(2\mu a)}A \quad (14)$$

$$C = \frac{e^{-a\mu-iak}\left(-k^2+k\mu i\right)}{2ik\mu\cosh(2\mu a)+\left(k^2-\mu^2\right)\sinh(2\mu a)}A \quad (15)$$

$$D = \frac{e^{-a\mu-iak}\left(k^2+k\mu i\right)}{2ik\mu\cosh(2\mu a)+\left(k^2-\mu^2\right)\sinh(2\mu a)}A \quad (16)$$

$$F = \frac{2e^{-2ika}k\mu i}{2ik\mu\cosh(2\mu a)+\left(k^2-\mu^2\right)\sinh(2\mu a)}A \quad (17)$$

From here we can get the transmission coefficient as

$$T = \frac{|F|^2}{|A|^2} \quad (18)$$

$$= \frac{4\mu^2k^2}{\left[\mu^4+2\mu^2k^2+k^4\right]\sinh^2(2\mu a)+4\mu^2k^2} \quad (19)$$

$$= \frac{1}{\left(\mu^2+k^2\right)^2\sinh^2(2\mu a)/4\mu^2k^2+1} \quad (20)$$

The reciprocal of T is then, substituting to get the physical quantities back:

$$T^{-1} = 1+\frac{\left(\mu^2+k^2\right)^2\sinh^2(2\mu a)}{4\mu^2k^2} \quad (21)$$

$$= 1+\frac{V_0^2}{4E\left(V_0-E\right)}\sinh^2\left(\frac{2a}{\hbar}\sqrt{2m\left(V_0-E\right)}\right) \quad (22)$$

The second case is where $E = V_0$. In this case, the outer two solutions are the same as before, but in the barrier region we have

$$\psi'' = 0 \quad (23)$$

which has the solution

$$\psi = Cx+D \quad (24)$$

Applying the boundary conditions we have, at $x = -a$

$$Ae^{-ika} + Be^{ika} = -Ca + D \tag{25}$$
$$ik\left(Ae^{-ika} - Be^{ika}\right) = C \tag{26}$$

At $x = a$ we have

$$Ca + D = Fe^{ika} \tag{27}$$
$$C = ikFe^{ika} \tag{28}$$

Solving these equations we get

$$B = \frac{kae^{-2ika}}{ka+i}A \tag{29}$$
$$C = \frac{ke^{-ika}}{-ka-i}A \tag{30}$$
$$D = e^{-ika}A \tag{31}$$
$$F = \frac{e^{-2ika}}{1-ika}A \tag{32}$$

In this case the transmission coefficient is

$$T = \frac{|F|^2}{|A|^2} \tag{33}$$
$$= \frac{1}{1+k^2a^2} \tag{34}$$
$$= \frac{1}{1+2mEa^2/\hbar^2} \tag{35}$$

Finally, for $E > V_0$ the Schrödinger equation within the barrier is

$$-\frac{\hbar^2}{2m}\psi'' = (E - V_0)\,\psi \tag{36}$$
$$\psi'' = -\frac{2m\,(E-V_0)}{\hbar^2}\psi \tag{37}$$
$$= -\lambda^2\psi \tag{38}$$

where

$$\lambda = \frac{\sqrt{2m\,(E-V_0)}}{\hbar} \tag{39}$$

The solution within the barrier is thus

$$\psi(x) = Ce^{i\lambda x} + De^{-i\lambda x} \tag{40}$$

Boundary conditions give at $x = -a$

$$\begin{aligned} Ae^{-ika} + Be^{ika} &= Ce^{-i\lambda a} + De^{i\lambda a} && (41)\\ ik\left(Ae^{-ika} - Be^{ika}\right) &= i\lambda\left(Ce^{-i\lambda a} - De^{i\lambda a}\right) && (42) \end{aligned}$$

At $x = a$:

$$\begin{aligned} Ce^{i\lambda a} + De^{-i\lambda a} &= Fe^{ika} && (43)\\ i\lambda\left(Ce^{i\lambda a} - De^{-i\lambda a}\right) &= ikFe^{ika} && (44) \end{aligned}$$

Solving these four equations gives

$$\begin{aligned} B &= \frac{e^{-2ika}\left(k^2-\lambda^2\right)\sin(2\lambda a)}{\left(k^2+\lambda^2\right)\sin(2\lambda a) + 2i\lambda k\cos(2\lambda a)}A && (45)\\ C &= \frac{e^{-ia(\lambda+k)}(\lambda+k)k}{-i\left(k^2+\lambda^2\right)\sin(2\lambda a) + 2\lambda k\cos(2\lambda a)}A && (46)\\ D &= \frac{e^{-ia(k-\lambda)}(k-\lambda)k}{i\left(k^2+\lambda^2\right)\sin(2\lambda a) - 2\lambda k\cos(2\lambda a)}A && (47)\\ F &= \frac{2k\lambda e^{-2ika}}{-i\left(k^2+\lambda^2\right)\sin(2\lambda a) + 2\lambda k\cos(2\lambda a)}A && (48) \end{aligned}$$

The transmission coefficient is

$$\begin{aligned} T &= \frac{|F|^2}{|A|^2} && (49)\\ &= \frac{4\lambda^2k^2}{\left(\lambda^4 - 2\lambda^2k^2 + k^4\right)\sin^2(2\lambda a) + 4\lambda^2k^2} && (50)\\ &= \frac{1}{1 + \left(\lambda^2-k^2\right)^2\sin^2(2\lambda a)/4\lambda^2k^2} && (51) \end{aligned}$$

The reciprocal is

$$T^{-1} = 1 + \frac{\left(\lambda^2 - k^2\right)^2 \sin^2(2\lambda a)}{4\lambda^2 k^2} \tag{52}$$

$$= 1 + \frac{V_0^2}{4E(E - V_0)} \sin^2\left(\frac{2a}{\hbar}\sqrt{2m(E - V_0)}\right) \tag{53}$$

PINGBACKS

Pingback: WKB approximation
Pingback: WKB approximation: tunneling

THE VARIATIONAL PRINCIPLE IN QUANTUM MECHANICS

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References: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Problem 7.1.

Post date: 4 Jan 2014.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 5.2, Exercise 5.2.2a.

We've used the calculus of variations to derive the geodesic equation in general relativity, but a similar approach can be used in quantum mechanics to get an upper bound on the ground state energy for a given hamiltonian. The technique rests on the following theorem:

Theorem. *If ψ is any normalized function and H is a hamiltonian, then the ground state energy E_0 of this hamiltonian has an upper bound given by*

$$\boxed{E_0 \leq \langle \psi | H | \psi \rangle \equiv \langle H \rangle} \tag{1}$$

Although we don't know the eigenfunctions or eigenvalues of H, we do know that the eigenfunctions satisfy $H\psi_n = E_n\psi_n$ and form a complete orthonormal set, so we can expand ψ in terms of them:

$$\psi = \sum_n c_n \psi_n \tag{2}$$

Therefore

$$\langle \psi | H | \psi \rangle = \sum_{n,m} c_m^* c_n \langle \psi_m | H | \psi_n \rangle \tag{3}$$

$$= \sum_{n,m} c_m^* c_n E_n \langle \psi_m | \psi_n \rangle \tag{4}$$

$$= \sum_n |c_n|^2 E_n \tag{5}$$

Since $E_n \geq E_0$ for all n, we get

$$\langle \psi | H | \psi \rangle \geq E_0 \sum_n |c_n|^2 = E_0 \tag{6}$$

This theorem is usually applied by choosing the function ψ such that it depends on one or more parameters which can then be varied to find the minimum value for $\langle H \rangle$.

Example 1. We'll use a Gaussian trial function to get an upper bound on the ground state energy for the potential

$$V(x) = \alpha |x| \tag{7}$$

The trial function is

$$\psi = Ae^{-bx^2} \tag{8}$$

The parameter A is determined by normalization:

$$|A|^2 \int_{-\infty}^{\infty} e^{-2bx^2} dx = 1 \tag{9}$$

$$A = \left(\frac{2b}{\pi}\right)^{1/4} \tag{10}$$

We get

$$\langle H \rangle = \sqrt{\frac{2b}{\pi}} \int_{-\infty}^{\infty} \left[-\frac{\hbar^2}{2m} e^{-bx^2} \frac{d^2}{dx^2} \left(e^{-bx^2} \right) + e^{-2bx^2} \alpha |x| \right] dx \tag{11}$$

The integrand is an even function of x, so this is equivalent to

$$\langle H \rangle = 2\sqrt{\frac{2b}{\pi}} \int_{0}^{\infty} \left[-\frac{\hbar^2}{2m} e^{-bx^2} \frac{d^2}{dx^2} \left(e^{-bx^2} \right) + e^{-2bx^2} \alpha x \right] dx \tag{12}$$

$$= \frac{1}{2\sqrt{2\pi} m} \left(\hbar^2 b \sqrt{2\pi} + \frac{2\alpha m}{\sqrt{b}} \right) \tag{13}$$

where we did the integral using Maple.

We want to vary the parameter b to find the minimum of this expression, so we take the derivative and set it to zero:

$$\frac{d\langle H \rangle}{db} = \frac{1}{2\sqrt{2\pi} m} \left(\hbar^2 \sqrt{2\pi} - \frac{\alpha m}{b^{3/2}} \right) = 0 \tag{14}$$

$$b = \frac{(\alpha m)^{2/3}}{(2\pi)^{1/3} \hbar^{4/3}} \tag{15}$$

This gives the upper bound on E_0 as

$$\boxed{E_0 \leq \frac{3(2\alpha\hbar)^{2/3}}{4(\pi m)^{1/3}}} \tag{16}$$

—-

Example 2. Now we'll use the potential

$$V(x) = \alpha x^4 \tag{17}$$

Doing the calculations yields (since the potential is again an even function):

$$\langle H \rangle = 2\sqrt{\frac{2b}{\pi}} \int_0^\infty \left[-\frac{\hbar^2}{2m} e^{-bx^2} \frac{d^2}{dx^2} \left(e^{-bx^2} \right) + e^{-2bx^2} \alpha x^4 \right] dx \tag{18}$$

$$= \frac{1}{16} \frac{8\hbar^2 b^3 + 3\alpha m}{b^2 m} \tag{19}$$

$$= \frac{\hbar^2 b}{2m} + \frac{3\alpha}{16 b^2} \tag{20}$$

Finding the parameter value that minimizes $\langle H \rangle$ we get

$$\frac{d\langle H \rangle}{db} = \frac{\hbar^2}{2m} - \frac{3\alpha}{8b^3} = 0 \tag{21}$$

$$b = \frac{(6\alpha m)^{1/3}}{2\hbar^{2/3}} \tag{22}$$

$$E_0 \leq \frac{3}{8} \left(\frac{6\hbar^4 \alpha}{m^2} \right)^{1/3} \tag{23}$$

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DELTA-FUNCTION WELL - BOUND STATE

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

Post date: 24 Feb 2011.

Reference: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Sec 2.5.2.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 5.2, Exercise 5.2.3.

If the potential function in the Schrödinger equation goes to infinity at infinite distance (as is the case in the infinite square well and the harmonic oscillator), then the only allowed energies of a particle in such a system are discrete, quantized energy states. A particle moving in such a potential can exist only in a bound state, where the probability of finding the particle tends to zero beyond some finite distance. In the infinite square well, the particle is bounded by the infinitely high walls, and the probability of finding it outside these walls is rigorously zero. In the harmonic oscillator, where the potential tends to infinity gradually, the particle can exist at greater distances if its energy is higher (just as in classical physics, a mass with higher energy will have a larger range of oscillation on a spring), but for any given energy state, the probability of finding the particle in any region where the potential is greater than the energy drops rapidly to zero.

Such potentials offer insurmountable barriers to the particle, so the notions of scattering from, or transmission through a region do not arise (in a scattering experiment, the particle is assumed to travel in from infinity in one direction and scatter back to infinity in the opposite direction; with an infinite potential, this is not possible). The only way we can talk about scattering or transmission of particles is to deal with cases where the particle has the possibility of travelling arbitrarily far. In such cases, infinitely high barriers cannot appear.

Unfortunately, the mathematics for such cases tends to get a bit more complicated than in those cases with infinite barriers (and as we've seen in the case of the harmonic oscillator, the mathematics is adquately hard even there!). One case that is often analyzed as an introduction to scattering and transmission is that of the *delta-function well*. The Dirac delta-function $\delta(x)$ is a mathematical curiosity in that it is zero everywhere except at $x = 0$, is infinite at that one point, and has an integral equal to 1 provided that the interval of integration includes the point $x = 0$ (the integral is zero otherwise).

Clearly the delta-function doesn't describe any real physical situation, since no known potential function is a delta-function. However, the function does have its uses as an approximation in many areas of physics, notably electrodynamics (where in fact the representation of an electron as a point charge just might actually be realistic - electrons have what appears to be zero size, or something very close to it). The delta-function does allow one of the simpler analyses of scattering and transmission, however, so it's useful to have a look at it before tackling more realistic cases.

The potential we'll consider is

$$V(x) = -\alpha\delta(x) \tag{1}$$

where α is a positive constant, so this represents a potential well of infinite depth at the origin, but with infinitestimally small width. Note that, from the properties of the delta-function, this is the same as writing

$$V(x) = -\delta(x/\alpha) \tag{2}$$

Since $\delta(x)$ is infinite at $x = 0$, no matter what the value of α, α does not measure the depth of the well; rather it might be thought of more as measuring the 'strength' of the potential in some sense. As we'll see, α *does* turn up in the energy levels and in the probabilities of scattering and transmission, so it's not an irrelevant parameter.

Since $\delta(x) = 0$ everywhere except $x = 0$, the Schrödinger equation at these points reduces to

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi \tag{3}$$

We'll consider bound states here and leave the scattering states to another post. For bound states, the energy E has to be negative, since it has to be less than the potential on either side of the (infinitesimally narrow) well, which has its top at $V(x) = 0$. So we can rewrite this as

$$\frac{d^2\psi}{dx^2} = \kappa^2\psi \tag{4}$$

where

$$\kappa \equiv \frac{\sqrt{-2mE}}{\hbar} \tag{5}$$

Since E is negative, κ is real and can be assumed positive.

Now we have to be careful here. The general solution of 4 is quite simple:

$$\psi(x) = Ae^{-\kappa x} + Be^{\kappa x} \tag{6}$$

as can be checked by direct substitution. The constants A and B, one might think, can be determined by some boundary conditions or by normalization. But we have in fact two distinct regions in which we have to find the solution: $x < 0$ and $x > 0$ (we'll get to what happens at $x = 0$ in a moment). Clearly if we want the solution to be normalizable, we can't use the same solution in both regions, since for $x < 0$, the $Ae^{-\kappa x}$ term tends to infinity for large negative x, and for $x > 0$, the *other* term $Be^{\kappa x}$ tends to infinity for large positive x. So we need a separate solution in each area. If we take 6 as the solution for $x < 0$, then we can propose another function with different constants as the solution for $x > 0$:

$$\begin{aligned} \psi_-(x) &= Ae^{-\kappa x} + Be^{\kappa x} & (7)\\ \psi_+(x) &= Ce^{-\kappa x} + De^{\kappa x} & (8) \end{aligned}$$

We can dispose of two of the constants immediately by requiring the wave functions tend to zero at infinity. This gives us $A = 0$ and $D = 0$, so we have

$$\begin{aligned} \psi_-(x) &= Be^{\kappa x} & (9)\\ \psi_+(x) &= Ce^{-\kappa x} & (10) \end{aligned}$$

Somehow we have to join up these functions across $x = 0$. We can refer to Born's conditions on the wave function and note that if the wave function is continuous at $x = 0$, then we must have $B = C$, so we're now down to

$$\begin{aligned} \psi_-(x) &= Be^{\kappa x} & (11)\\ \psi_+(x) &= Be^{-\kappa x} & (12) \end{aligned}$$

However, since the potential is infinite at $x = 0$, we can't require that the derivative of the wave function be continuous.

So what can we say about B? The trick here is to try integrating the Schrödinger equation across the boundary. Putting the delta-function potential into the Schrödinger equation we get

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} - \alpha\delta(x)\psi = E\psi \tag{13}$$

Now if we integrate this equation term by term across the boundary, we get, for some value of ϵ:

$$-\frac{\hbar^2}{2m}\int_{-\epsilon}^{\epsilon}\frac{d^2\psi}{dx^2}dx-\alpha\int_{-\epsilon}^{\epsilon}\delta(x)\psi dx = E\int_{-\epsilon}^{\epsilon}\psi dx \quad (14)$$

$$-\frac{\hbar^2}{2m}\frac{d\psi}{dx}\Big|_{-\epsilon}^{\epsilon}-\alpha\psi(0) = E\int_{-\epsilon}^{\epsilon}\psi dx \quad (15)$$

If we take the limit as $\epsilon \to 0$, the integral on the right tends to zero, since it is the integral of a continuous function over an infinitesimally small interval. The first term on the left, however, will *not* be zero, since derivative of the wave function is not continuous when the potential is infinite. However, it does give us a relation which ends up determining the bound state energy. So if we take the limit as $\epsilon \to 0$, we get

$$-\frac{\hbar^2}{2m}\left[\frac{d\psi}{dx}\Big|_{\epsilon\downarrow 0}-\frac{d\psi}{dx}\Big|_{-\epsilon\uparrow 0}\right] = \alpha B \quad (16)$$

$$\frac{\hbar^2}{m}B\kappa = \alpha B \quad (17)$$

$$\kappa = \frac{m\alpha}{\hbar^2} \quad (18)$$

$$E = -\frac{\hbar^2\kappa^2}{2m} \quad (19)$$

$$= -\frac{m\alpha^2}{2\hbar^2} \quad (20)$$

Just as in the infinite square well, our analysis ends up giving a condition on the energy E rather than on the constant B. B is in fact easily determined by normalizing the wave function:

$$\int_{-\infty}^{\infty}|\psi(x)|^2dx = |B|^2\left(\int_{-\infty}^{0}e^{2\kappa x}dx+\int_{0}^{\infty}e^{-2\kappa x}dx\right) \quad (21)$$

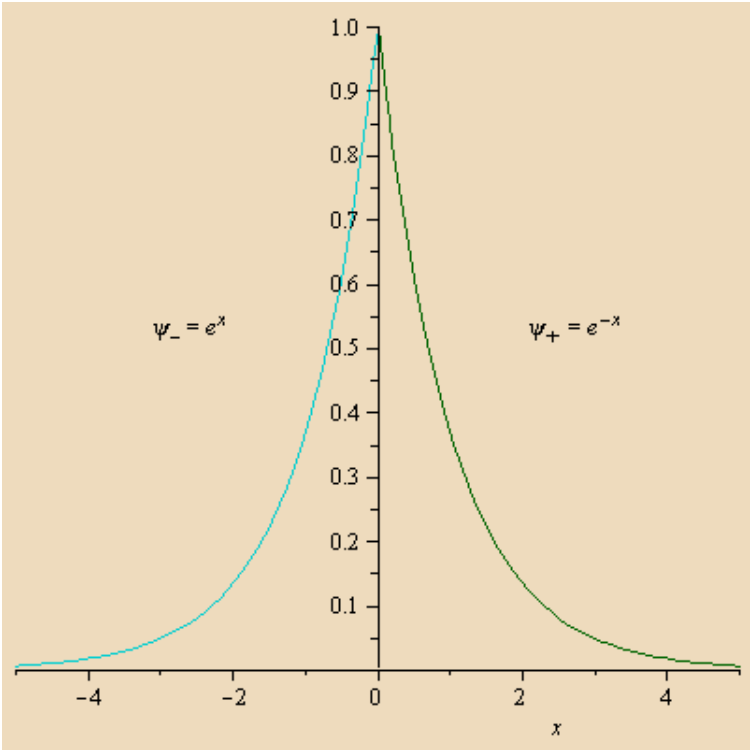
$$= \frac{1}{\kappa}|B|^2 = 1 \quad (22)$$

$$B = \sqrt{\kappa} \quad (23)$$

$$= \frac{\sqrt{m\alpha}}{\hbar} \quad (24)$$

Thus a delta-function well has precisely one bound state, and the energy does depend on the parameter α: the larger α is, the lower (more negative) the energy E is. This is why it makes sense to consider α as the strength of the potential; it regulates how deeply bound the particle in a stationary state is within the well.

The wave function for the bound state looks like this (here we've taken $\kappa = 1$ but it's just the general shape of the curve that's important):



The probability of finding the particle is maximum at $x = 0$ and falls off exponentially on either side. Since the exponent is $\pm\kappa x$ and $\kappa = m\alpha/\hbar^2$, the rate of exponential fall-off depends on the strength of the delta-function. This behaviour is consistent with other bound states. The infinite square well is essentially a well with infinite strength, so the fall off at the boundaries is absolute - there is no exponential decay. With the harmonic oscillator, the wave function oscillates (in space) within the well (although mathematically, the oscillation is due to Legendre polynomials rather than trigonometric functions), but in the regions where the potential is greater than the energy, there is again an exponential decay. In the case of a delta function, since the well itself is infinitesimally narrow, there is no region where the wave nature of the particle is displayed - the exponential fall-off starts immediately either side of the well.

PINGBACKS

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DELTA-FUNCTION WELL - SCATTERING

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

Post date: 25 Feb 2011.

Reference: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Sec 2.5.2.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 5.4, Exercise 5.4.2 (b).

The delta-function well always has exactly one bound state, where the energy of the particle is less than zero. If we consider states where the energy is greater than zero, we can investigate the phenomenon of scattering.

The potential function we are using is

$$V(x) = -\alpha\delta(x) \tag{1}$$

where α is a positive constant that gives the strength of the well. In this case, the Schrödinger equation is

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} - \alpha\delta(x)\psi = E\psi \tag{2}$$

At all points except $x = 0$ this equation becomes

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi \tag{3}$$

With $E > 0$, we can write this as

$$\frac{d^2\psi}{dx^2} = -k^2\psi \tag{4}$$

where

$$k \equiv \frac{\sqrt{2mE}}{\hbar} \tag{5}$$

Since $E > 0$, k is real and can be taken to be positive. As in the case of the bound state, because of the singularity at $x = 0$ we need to consider solutions on either side of this point separately.

The general solution of 4 is

$$\psi(x) = Ae^{ikx} + Be^{-ikx} \tag{6}$$

so we can take this as the solution for $x < 0$ and call it $\psi_-(x)$:

$$\psi_-(x) = Ae^{ikx} + Be^{-ikx} \tag{7}$$

For $x > 0$, we can write

$$\psi_+(x) = Ce^{ikx} + De^{-ikx} \tag{8}$$

Because the potential is zero in these two regions, the solutions are those of the free particle and, as we saw when we considered that case, these solutions are not normalizable so cannot, on their own, represent a physically realizable state. However, because any linear combination of solutions is also a solution, we found in the case of the free particle that we could create a wave packet and that such a packet, although not itself a stationary state, *was* normalizable and represented a particle travelling through space.

Unfortunately, we also saw that the mathematics rapidly becomes pretty horrible when we attempt to work with wave packets, so much of what is known about them is derived through computer simulations. When dealing with scattering problems, the same problems arise, and realistic problems (that is, ones involving wave packets rather than single, non-normalizable functions) can be solved only by simulation.

We will work through the problem using stationary states to see how scattering problems are handled, but it should always be kept in mind that this is not a physically realizable situation. The problem is that we will be doing the analysis for only a single value of k (and hence, of E), whereas a wave packet consists of contributions from many different values of k, and thus from many different energies. As we will see, the probabilities of reflection from the potential and of transmission through it both depend on k, so each value of k behaves differently. A proper wave packet therefore scatters in quite a complex manner, and it's a non-trivial problem to work this out in detail.

With that warning, let's see how we solve a scattering problem for a single value of k. The idea behind a scattering experiment is that we imagine a particle coming in from one direction (say, coming in from the left, so moving towards the positive x direction). When this particle hits the potential well, it may bounce back towards $-x$, or it may go through the $x = 0$ point and emerge on the other side, still travelling in the direction of $+x$.

Remember that the full solution of the Schrödinger equation in this case is

$$\Psi(x,t) = \psi(x)e^{-iEt/\hbar} \tag{9}$$

For $x < 0$, this becomes

$$\Psi_-(x,t) = Ae^{i(kx-Et/\hbar)} + Be^{i(-kx-Et/\hbar)} \tag{10}$$

and for $x > 0$:

$$\Psi_+(x,t) = Ce^{i(kx-Et/\hbar)} + De^{i(-kx-Et/\hbar)} \tag{11}$$

In each of these functions, the first term represents a wave travelling to the right, and the second term a wave travelling to the left. (A reminder of how to see this: consider the motion of a fixed point on the wave, where the exponent is a constant, and consider how x must change as t increases to see which way the wave is moving. If $kx - Et/\hbar =$constant, then x must increase as t increases; just the opposite is true if $-kx - Et/\hbar =$constant.)

Therefore, to represent the experiment we described above, with a particle coming in from the left and possibly reflecting back from or passing through the potential well, we need to include terms with waves travelling in both directions for $x < 0$ and only one direction (travelling to the right) for $x > 0$. Therefore, we can say that $D = 0$ since there are no waves travelling to the left when $x > 0$.

Requiring the wave function to be continuous at $x = 0$ gives us one more condition:

$$A + B = C \tag{12}$$

We can get another condition by using the same integration technique that we applied in the case of the bound state. Integrating the Schrödinger equation across the origin we get:

$$-\frac{\hbar^2}{2m}\int_{-\epsilon}^{\epsilon}\frac{d^2\psi}{dx^2}dx - \alpha\int_{-\epsilon}^{\epsilon}\delta(x)\psi dx = E\int_{-\epsilon}^{\epsilon}\psi dx \tag{13}$$

$$-\frac{\hbar^2}{2m}\frac{d\psi}{dx}\Big|_{-\epsilon}^{\epsilon} - \alpha\psi(0) = E\int_{-\epsilon}^{\epsilon}\psi dx \tag{14}$$

Taking the limit as $\epsilon \to 0$ gives us

$$-\frac{\hbar^2 ik}{2m}(C - A + B) - \alpha C = 0 \tag{15}$$

We can now use 12 and 15 to eliminate two of the three constants, and we can express C and B in terms of A:

$$B = \frac{i\beta}{1-i\beta}A \tag{16}$$

$$C = \frac{1}{1-i\beta}A \tag{17}$$

$$\beta \equiv \frac{m\alpha}{\hbar^2 k} \tag{18}$$

It might look as though we're stuck at this point, since we can't normalize the wave function, so we can't determine A. However, what we really want is the probability that the particle will be reflected or transmitted, and we can get that by comparing B and C with A. Remember that the term $Ae^{i(kx-Et/\hbar)}$ represents the incoming particle, $Be^{i(-kx-Et/\hbar)}$ the reflected particle and $Ce^{i(kx-Et/\hbar)}$ the transmitted particle. For the region $x < 0$, the probability that the particle is travelling to the left *relative* to the probability that it is travelling to the right should give the probability that it has been reflected. Comparing the probability that the particle is found in the region $x > 0$ to the probability that it is travelling to the right in the region $x < 0$ should give the probability that it has been transmitted.

At this point, you might be thinking there is something wrong with the logic here. After all, the particle can't be *both* travelling to the right *and* to the left at the same time in the region $x < 0$, nor can it be on both sides of the origin at the same time. Not only that, but we are analyzing an explicitly time-dependent problem using only stationary states, and these states are just waves of constant amplitude that extend out to infinity, rather than wave packets describing real particles. There is no honest way around this problem; essentially we are fudging the answer since we are analyzing a non-physical system anyway. One way of thinking about it that might make you feel a bit better is, instead of imagining a single particle travelling in and either bouncing off or passing through the well, imagine a steady stream of particles being beamed at the well from the left. In that case, we would reach a steady state in which a certain fraction of particles would get reflected and the remainder would get transmitted. This situation at least gets rid of any explicit time dependence, although the problem of non-normalizability of the wave function is still there.

In the final analysis, the only honest way of analyzing this problem is by constructing a wave packet out of multiple values of k, doing the normalization properly and then working out the probabilities. However, as you might imagine, that is far from easy.

In the meantime, we can get expressions for our steady state reflection and transmission probabilities R and T by finding the appropriate ratios:

$$R = \frac{|B|^2}{|A|^2} \tag{19}$$

$$= \frac{\beta^2}{1+\beta^2} \tag{20}$$

$$= \frac{1}{1+2\hbar^2 E/m\alpha^2} \tag{21}$$

$$T = \frac{|C|^2}{|A|^2} \tag{22}$$

$$= \frac{1}{1+\beta^2} \tag{23}$$

$$= \frac{1}{1+m\alpha^2/2\hbar^2 E} \tag{24}$$

after substituting for β and then for k in terms of E. Note that $R+T=1$ so the particle must be either reflected or transmitted.

The derivation of R and T is also valid for a delta function barrier if we set $\alpha < 0$, since nothing in the derivation relied on α being positive, and the final values of R and T depend only on α^2.

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EVERY ATTRACTIVE 1-DIMENSIONAL POTENTIAL HAS A BOUND STATE

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

Post date: 1 Oct 2016.

Reference: Lecture by Barton Zwiebach in MIT course 8.05.1x, week 1, Deep Dive 2 (not in the PDF notes).

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 5.2, Exercise 5.2.2b.

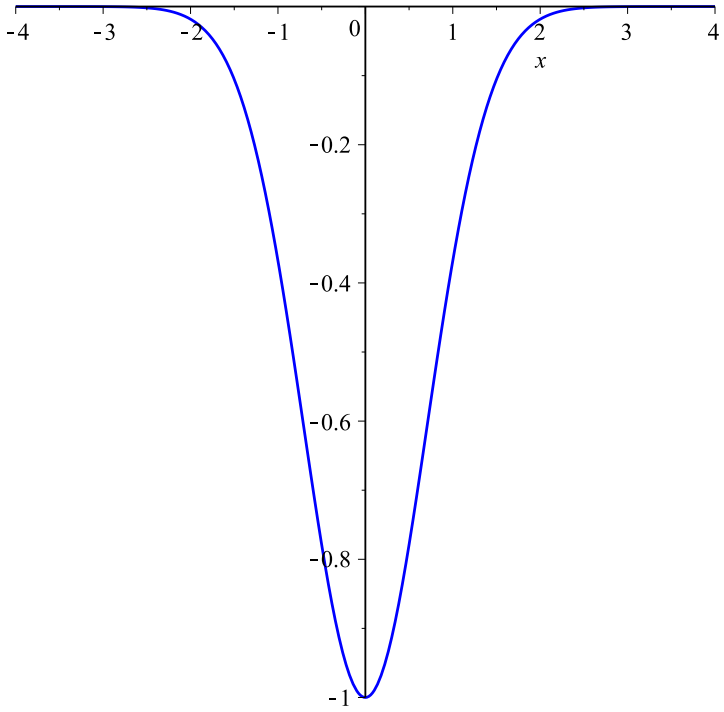
An interesting application of the variational principle in quantum mechances is the following theorem:

Theorem. ***Every 1-dimensional attractive potential has at least one bound state.***

To prove this, we need first to define what we mean by an attractive potential $V(x)$. $V(x)$ must satisfy the following conditions:

- $V(x) \to 0$ as $x \to \pm\infty$.
- $V(x) < 0$ everywhere.
- $V(x)$ is piecewise continuous. This means that it may have a finite number of jump discontinuities.

One possible form for $V(x)$ is as shown:



This is a particularly simple potential that satisfies the above conditions. We could introduce a few step functions, multiple local maxima and minima, and so on, provided we don't violate any of the 3 conditions above.

Since $V(x) < 0$ everywhere, we can write it as

$$V(x) = -|V(x)| \tag{1}$$

What we would like to prove is that for any hamiltonian of the form

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} - |V(x)| \tag{2}$$

the ground state E_0 is a bound state, that is

$$E_0 < 0 \tag{3}$$

We can apply the variational principle, which states

If ψ is any normalized function and H is a hamiltonian, then the ground state energy E_0 of this hamiltonian has an upper bound given by

$$E_0 \leq \langle \psi | H | \psi \rangle \equiv \langle H \rangle \tag{4}$$

The use of the variational principle to prove the above theorem involves a bit of a convoluted argument, but the mathematics involved is fairly simple.

Our goal is to find some wave function ψ_α (where α is some parameter that we can vary) so that

$$E_0 \leq \langle \psi_\alpha | H | \psi_\alpha \rangle = \langle H \rangle_{\psi_\alpha} < 0 \tag{5}$$

From 2 we have

$$\begin{aligned} \left\langle \hat{H} \right\rangle_{\psi_\alpha} &= \int dx\, \psi_\alpha(x)\, \hat{H} \psi_\alpha(x) & (6) \\ &= \langle T \rangle_{\psi_\alpha} - \langle |V(x)| \rangle_{\psi_\alpha} & (7) \end{aligned}$$

where

$$\langle T \rangle_{\psi_\alpha} = -\int dx\, \psi_\alpha(x) \frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi_\alpha(x) \tag{8}$$

$$\langle |V(x)| \rangle_{\psi_\alpha} = \int dx\, \psi_\alpha(x) |V(x)| \psi_\alpha(x) \tag{9}$$

We can integrate 8 by parts once to get

$$\begin{aligned} \langle T \rangle_{\psi_\alpha} &= -\int dx\, \psi_\alpha(x) \frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi_\alpha(x) & (10) \\ &= -\frac{\hbar^2}{2m} \psi_\alpha(x) \frac{d}{dx} \psi_\alpha(x) \Big|_{-\infty}^{\infty} + \frac{\hbar^2}{2m} \int dx \left(\frac{d}{dx} \psi_\alpha(x) \right)^2 & (11) \\ &= \frac{\hbar^2}{2m} \int_{-\infty}^{\infty} dx \left(\frac{d}{dx} \psi_\alpha(x) \right)^2 & (12) \end{aligned}$$

where we invoke the usual requirement that ψ_α and its first derivative vanish at infinity.

We therefore see that since the integrand in the last line is always positive (we're assuming that ψ_α is not zero everywhere), that $\langle T \rangle_{\psi_\alpha} > 0$. Likewise, from 9, $\langle |V(x)| \rangle_{\psi_\alpha} > 0$. Thus in order that $\langle H \rangle_{\psi_\alpha} < 0$, we must have

$$\langle T \rangle_{\psi_\alpha} < \langle |V(x)| \rangle_{\psi_\alpha} \tag{13}$$

To get any further, we need to choose a test function $\psi_\alpha(x)$. We'll pick (because it works!)

$$\psi_\alpha = \left(\frac{\alpha}{\pi} \right)^{1/4} e^{-\frac{1}{2}\alpha x^2} \tag{14}$$

The factor of $\left(\frac{\alpha}{\pi}\right)^{1/4}$ is required so that ψ_α is normalized. The integral in 12 can be done using standard methods; I'll just use Maple, and we find

$$\langle T \rangle_{\psi_\alpha} = \frac{\hbar^2 \alpha}{4m} \tag{15}$$

The integral 9 of course can't be done exactly if we don't know what V is, so we have just

$$\langle |V(x)| \rangle_{\psi_\alpha} = \int dx \, \psi_\alpha^2(x) \, |V(x)| \tag{16}$$

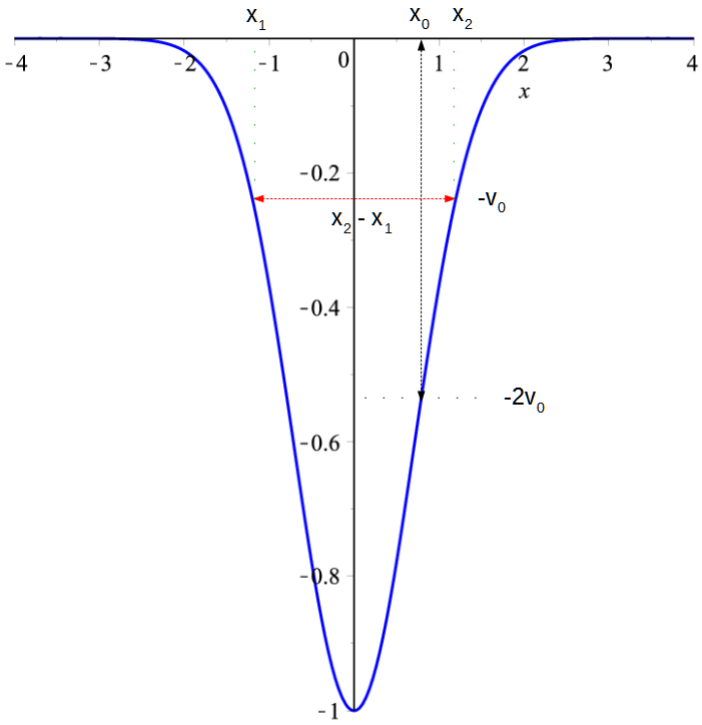
(No need for modulus signs around ψ_α since the function 14 is real.) To progress further, we need to start invoking some inequalities to get where we want to go. The argument consists of several steps, so watch carefully as we go along.

From 13 through 15 we have to show that we can satisfy the condition

$$\frac{\langle |V(x)| \rangle_{\psi_\alpha}}{\langle T \rangle_{\psi_\alpha}} = \frac{4m}{\hbar^2 \sqrt{\pi}} \frac{1}{\sqrt{\alpha}} \int_{-\infty}^{\infty} e^{-\alpha x^2} \, |V(x)| \, dx > 1 \tag{17}$$

Since V is arbitrary subject to the 3 conditions above, the only thing we can legitimately fiddle with is the value of α. We can see that if we choose α small enough, we should be able to satisfy this inequality, since for small α, the $1/\sqrt{\alpha}$ term gets large, while the $e^{-\alpha x^2}$ term in the integrand is bounded between 0 and 1. We need to find some upper limit for α.

In what follows, you'll need to refer to the following diagram:



First, we choose some point x_0 at which $V(x_0)$ is continuous (that is, we ensure that x_0 isn't at one of the points where $V(x)$ has a discontinuity, or jump). The value of $V(x_0)$ is defined as $-2v_0$ where $v_0 > 0$. Because $V \to 0$ at $x \to \pm\infty$, there must be points x_1 and x_2 on either side of x_0 where V has the value $-v_0$ (actually, I'm not sure this is strictly true, because, as V is allowed a few jumps, it might jump over the point where it's equal to $-v_0$. However, as the number of jumps is required to be finite, there must be *some* points x_1 and x_2 on either side of x_0 where V attains a value that is between $-2v_0$ and 0, and I think the argument below still works if we choose those points instead.)

Now for the first inequality. We know that, because the integrand is positive

$$\int_{-\infty}^{\infty} e^{-\alpha x^2} |V(x)|\, dx > \int_{x_1}^{x_2} e^{-\alpha x^2} |V(x)|\, dx \tag{18}$$

Second inequality: in the interval x_1 to x_2, $|V(x)| > v_0$ (see the diagram!), so we have

$$\int_{x_1}^{x_2} e^{-\alpha x^2} |V(x)|\, dx > v_0 \int_{x_1}^{x_2} e^{-\alpha x^2} dx \tag{19}$$

The last integral has no closed form solution, but we know that in the interval x_1 to x_2

$$e^{-\alpha x^2} > e^{-\alpha \max\left(x_1^2, x_2^2\right)} \tag{20}$$

Therefore

$$v_0 \int_{x_1}^{x_2} e^{-\alpha x^2} dx > v_0 \int_{x_1}^{x_2} e^{-\alpha \max\left(x_1^2, x_2^2\right)} dx \tag{21}$$

$$= v_0 \left(x_2 - x_1\right) e^{-\alpha \max\left(x_1^2, x_2^2\right)} \tag{22}$$

Now suppose we choose α to be

$$\alpha < \frac{1}{\max\left(x_1^2, x_2^2\right)} \tag{23}$$

Then

$$e^{-\alpha \max\left(x_1^2, x_2^2\right)} > e^{-1} \tag{24}$$

We can now summarize as follows:

$$\int_{-\infty}^{\infty} e^{-\alpha x^2} \left|V\left(x\right)\right| dx > v_0 \left(x_2 - x_1\right) e^{-1} \tag{25}$$

provided we choose α according to 23. Plugging this back into 17 we have

$$\frac{\left\langle \left|V\left(x\right)\right| \right\rangle_{\psi_\alpha}}{\left\langle T \right\rangle_{\psi_\alpha}} > \frac{4m}{\hbar^2 \sqrt{\pi}} \frac{v_0 \left(x_2 - x_1\right)}{e} \frac{1}{\sqrt{\alpha}} \tag{26}$$

This expression will now be greater than 1 provided that

$$\sqrt{\alpha} < \frac{4m}{\hbar^2 \sqrt{\pi}} \frac{v_0 \left(x_2 - x_1\right)}{e} \tag{27}$$

$$\alpha < \left[\frac{4m}{\hbar^2 \sqrt{\pi}} \frac{v_0 \left(x_2 - x_1\right)}{e}\right]^2 \tag{28}$$

Comparing 23 and 28, we see that we can satisfy both conditions if we take

$$\alpha < \min\left\{ \frac{1}{\max\left(x_1^2, x_2^2\right)}, \left[\frac{4m}{\hbar^2 \sqrt{\pi}} \frac{v_0 \left(x_2 - x_1\right)}{e}\right]^2 \right\} \tag{29}$$

This condition depends on x_1 and x_2 but that doesn't matter, since both quantities in the RHS of 29 are positive, so there is always some positive

value of α that satisfies the condition. In other words, going right back to 17 and then to 7, we can always find a value of α so that $\langle H \rangle < 0$ which means that the ground state of H must be negative, which makes it a bound state.

FINITE SQUARE WELL: BOUND STATES & EVEN WAVE FUNCTIONS

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

Post date: 5 Mar 2011.

Reference: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Sec. 2.6.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 5.2, Exercise 5.2.6.

A general rule when solving the Schrödinger equation in one dimension is that in those regions where the total energy E is less than the potential V the spatial part of the wave function $\psi(x)$ decays exponentially, while if $E > V$, the wave function $\psi(x)$ oscillates in some fashion. In the case of the infinite square well, ψ is zero outside the well since the potential is infinite there, so there is zero chance of finding the particle outside the well. Within the well, the oscillation follows the pattern of a sine wave, which must be zero at the boundaries. This boundary condition is responsible for the quantization of the energy levels.

For the delta-function well, $\psi(x)$ peaks at $x = 0$ (the only place where $\delta(x) \neq 0$), and decays exponentially on either side. A kind of hybrid of these two extreme examples (the delta-function and the infinite square well) is the finite square well, in which the potential follows the rule

$$V(x) = \begin{cases} 0 & x < -a \\ -V_0 & -a \leq x \leq a \\ 0 & x > a \end{cases} \tag{1}$$

where V_0 is a positive constant energy, and a is a constant location on the x axis.

With such a potential, we have two main possibilities. First, $-V_0 < E < 0$, (the total energy has to be greater than the minimum value of the potential, as we proved before) which results in bound states in which we would expect $\psi(x)$ to oscillate within the well and decay exponentially outside the well. Second, $E > 0$, in which we would expect $\psi(x)$ to oscillate everywhere. In the first case, we also expect the energy levels to be quantized due to the boundary conditions within the well, so we can try to find the allowed states. In the second case, as with the delta-function, we can study the behaviour of an incoming beam of particles as it hits the barrier, and calculate

the reflection and transmission coefficients (while keeping in mind that any real particle is composed of a combination of pure waves in the form of a wave packet, so that calculations with single energy states are at best an approximation).

The mathematics for the bound state case of the finite square well turns out to be more complicated than in the case of the delta-function, and in fact we can't get an exact formula for the allowed energies. However, the process of solving the Schrödinger equation is fairly straightforward, if a bit messy.

As usual, we divide the solution into separate regions and try to solve for the various constants that pop up by applying boundary conditions. The equation to be solved can be split into three regions:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi \qquad (x < -a) \tag{2}$$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} - V_0\psi = E\psi \qquad (-a \le x \le a) \tag{3}$$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi \qquad (x > a) \tag{4}$$

The general solutions in these three regions are easy enough to write down. We get

$$\psi(x) = \begin{cases} Ae^{-\kappa x} + Be^{\kappa x} & x < -a \\ C\sin(\mu x) + D\cos(\mu x) & -a \le x \le a \\ Fe^{-\kappa x} + Ge^{\kappa x} & x > a \end{cases} \tag{5}$$

where as usual we've introduced some convenience parameters:

$$\kappa \equiv \frac{\sqrt{-2mE}}{\hbar} \tag{6}$$

$$\mu \equiv \frac{\sqrt{2m(E+V_0)}}{\hbar} \tag{7}$$

Note that both these parameters are real and can be taken as positive, since $-V_0 < E < 0$ for bound states. Note that we've also expressed the solution in the middle section in terms of sin and cos rather than in terms of $e^{i\mu x}$ and $e^{-i\mu x}$. The latter is also valid, but as we'll see in the next paragraph, using sin and cos is easier.

So now we have six constants to deal with. First, we can use the theorem that says that if the potential function is even (as this one is: $V(-x) = V(x)$), then $\psi(x)$ is even or odd. Unfortunately, we need to work out these

two cases separately, but in each case, it does allow us to eliminate three of the constants. We'll deal with the even solutions first, so that we require $\psi(-x) = \psi(x)$. (We deal with the odd functions in another post.) Since the sine is an odd function, we must have $C = 0$. In the outer regions, the requirement of an even function means that $A = G$ and $B = F$.

Next, we can impose the requirement that $\psi(x) \to 0$ at $\pm\infty$, so this means that $A = G = 0$. We therefore get

$$\psi(x) = \begin{cases} Be^{\kappa x} & x < -a \\ D\cos(\mu x) & -a \leq x \leq a \\ Be^{-\kappa x} & x > a \end{cases} \tag{8}$$

Now we can apply the boundary conditions. Since there are no infinite energies involved (the potential is finite everywhere), we apply Born's conditions and require that both ψ and ψ' are continuous at both boundaries. Because of the symmetry of the wave function, we can consider only one boundary; the other one won't give us anything new. Therefore these two conditions give us (using the fact that cos is even):

$$Be^{-\kappa a} = D\cos(\mu a) \tag{9}$$

$$-\kappa Be^{-\kappa a} = -\mu D\sin(\mu a) \tag{10}$$

Dividing these two equations together, we can get rid of B and D:

$$\kappa = \mu\tan(\mu a) \tag{11}$$

This is actually a condition that will give us the allowed energies, since both κ and μ are functions of E. Unfortunately, this equation cannot be solved explicitly for E (it's what is known as *transcendental*, which means that the variable we're trying to solve for occurs both inside and outside of a function such as the tan). The only way such equations can be solved is numerically, but we can get an idea of the solutions by plotting the two sides of the equation on the same graph and seeing where these plots intersect.

We can rewrite this equation as

$$\tan(\mu a) = \frac{\kappa}{\mu} \tag{12}$$

From the definitions of κ and μwe can eliminate κ as follows:

$$\begin{aligned}
\kappa^2 + \mu^2 &= 2mV_0/\hbar^2 && (13)\\
\kappa &= \sqrt{2mV_0/\hbar^2 - \mu^2} && (14)\\
\frac{\kappa}{\mu} &= \sqrt{2mV_0/\mu^2\hbar^2 - 1} && (15)\\
\tan(\mu a) &= \sqrt{2mV_0/\mu^2\hbar^2 - 1} && (16)\\
&= \sqrt{2ma^2V_0/(\mu a)^2\hbar^2 - 1} && (17)
\end{aligned}$$

Defining the variable $z \equiv \mu a$, we can now write this equation as a transcendental equation in the single variable z:

$$\tan z = \sqrt{\frac{2ma^2V_0/\hbar^2}{z^2} - 1} \tag{18}$$

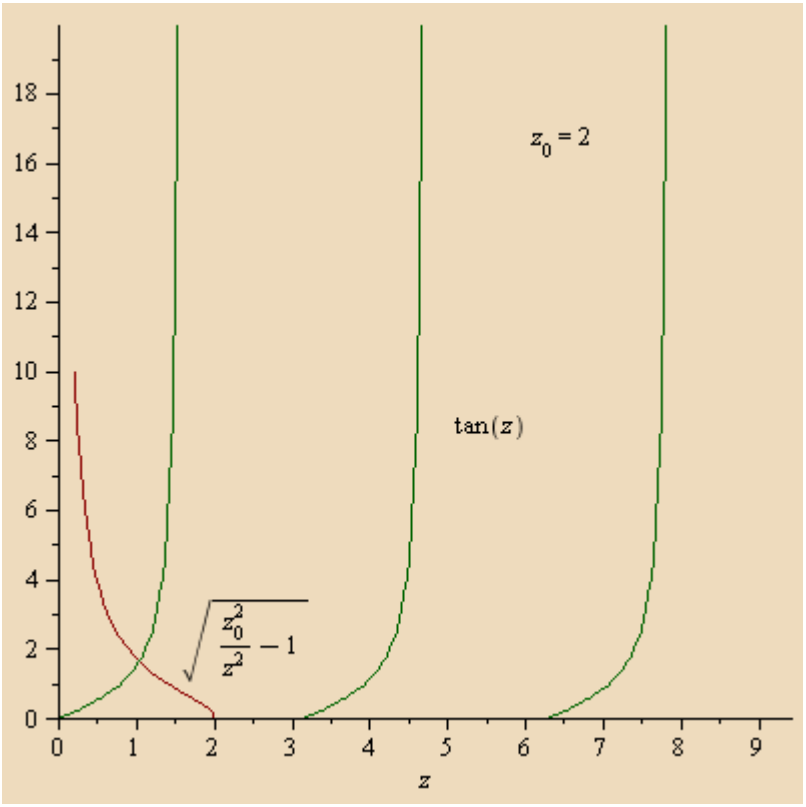
To solve this equation graphically or numerically for a given particle, we clearly need to specify values for a and V_0. However, we can treat the combination of parameters as a single parameter z_0:

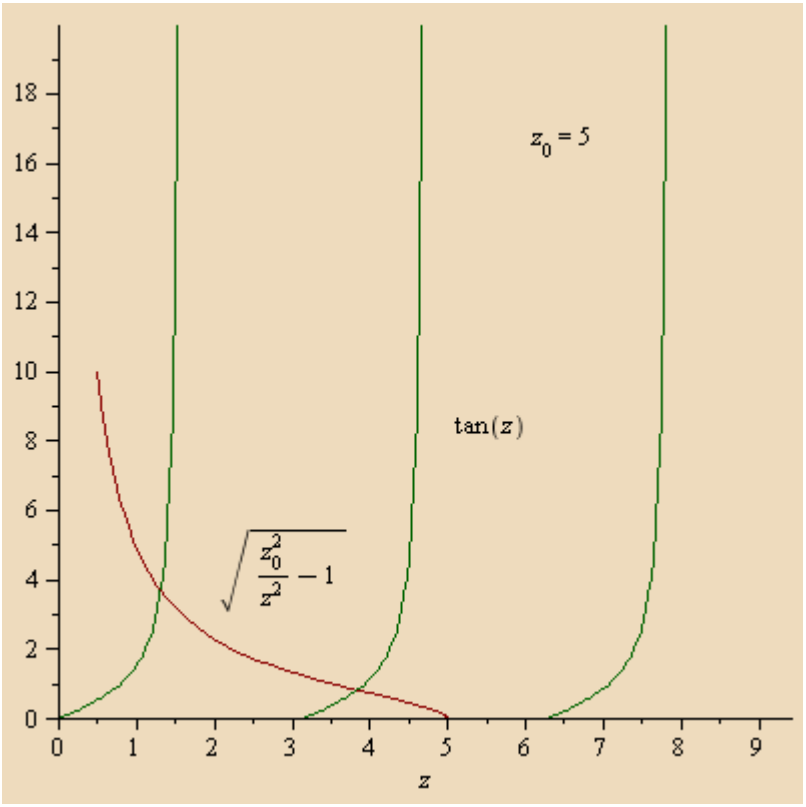
$$z_0^2 \equiv \frac{2ma^2V_0}{\hbar^2} \tag{19}$$

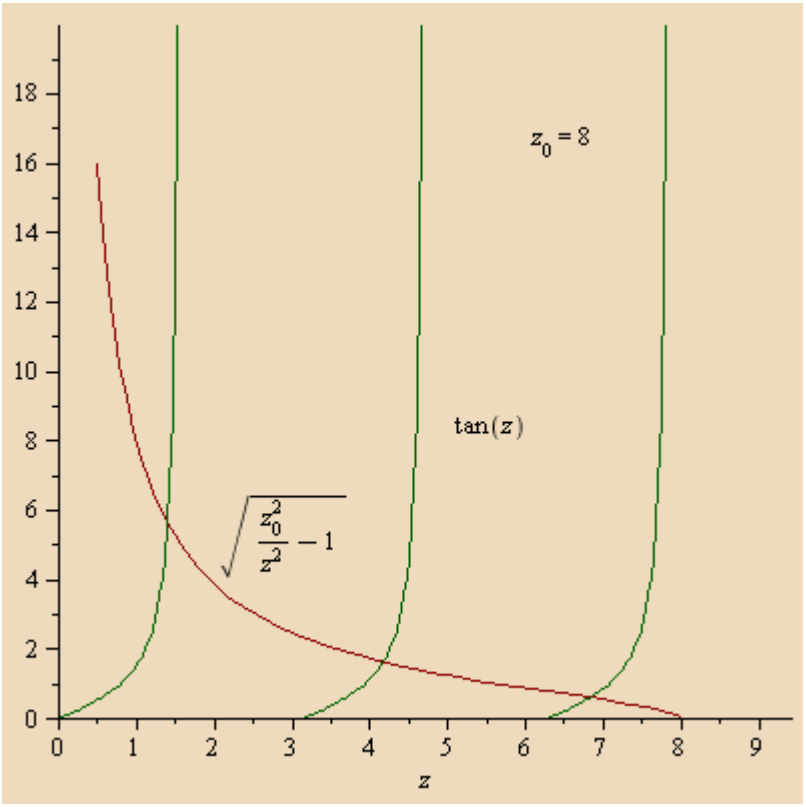
so we have the equation

$$\tan z = \sqrt{\frac{z_0^2}{z^2} - 1} \tag{20}$$

We can plot both sides of this equation on the same graph for various values of z_0 to get an idea of what happens.


$z_0 = 2$
$\tan(z)$
$\sqrt{\frac{z_0^2}{z^2} - 1}$
0
2
4
6
8
10
12
14
16
18
0
1
2
3
4
5
6
7
8
9
z


$z_0 = 5$
$\tan(z)$
$\sqrt{\frac{z_0^2}{z^2} - 1}$
0
2
4
6
8
10
12
14
16
18
0
1
2
3
4
5
6
7
8
9
z



In these plots, we show what happens for three different values of z_0. The green curves show the plot of $\tan z$; the red curves that of $\sqrt{\frac{z_0^2}{z^2} - 1}$. In the first graph, with $z_0 = 2$, we get only one intersection between the two plots, around $z = 1$. Thus for $z_0 = 2$, there is only one bound state, with an energy that can be worked out from $z = \mu a = \frac{\sqrt{2m(E+V_0)}a}{\hbar} \approx 1$. A more accurate value can be obtained by numerical solution of the equation, but this requires a computer (well, actually, the graphs were drawn on a computer too, but never mind).

The second and third graphs show what happens as we increase z_0 to 5 and then 8. In each case we pick up an extra intersection between the two graphs, so we add an extra bound state.

In this case, we can see that no matter how small we make z_0, we will always have at least one bound state (since the $\tan z$ graph starts off from the origin). As $V_0 \to 0$, we would expect the situation to tend to that of the free particle, so the presence of this bound state might be a bit worrying. However, if $V_0 = 0$ exactly, then the quantity $\sqrt{\frac{z_0^2}{z^2} - 1}$ has no values of z which give a real value, so there are no intersections on the graph, thus there

are no bound states. However, if there is any potential well at all, no matter how shallow, there will be at least one bound state.

At the other extreme, as $V_0 \to \infty$, we would expect to get the infinite square well states. To see this, note that the graph of $\sqrt{\frac{z_0^2}{z^2} - 1}$ intersects the horizontal axis at $z = z_0$, so as $V_0 \to \infty$, $z_0 \to \infty$ and the intersection point gets further and further along the axis, so the number of intersections with branches of the tangent gets larger. Thus the *number* of energy states gets larger and larger, eventually becoming infinite. As to the locations of these intersections, we can notice that for any fixed, finite value of z, the quantity $\sqrt{\frac{z_0^2}{z^2} - 1}$ tends to infinity as $z_0 \to \infty$, so that means that the entire curve gets higher, so the intersections with the tangent curve will occur at higher locations. The tangent is asymptotic to the vertical lines $n\pi/2$ for odd n, so we would expect the intersection points to eventually become $z = n\pi/2$. This means that

$$z^2 = \frac{2ma^2(E+V_0)}{\hbar^2} \tag{21}$$

$$\approx \frac{n^2\pi^2}{4} \tag{22}$$

$$E + V_0 \approx \frac{n^2\pi^2\hbar^2}{2m(2a)^2} \tag{23}$$

Since $E + V_0$ is the height of the bound state above the bottom of the well, we can see that this formula does indeed give us the expected energy levels for an infinite square well of width $2a$, or at least those corresponding to odd n. The other ones, for even n come from a solution where we assume $\psi(x)$ is an odd function.

PINGBACKS

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THE INFINITE SQUARE WELL (PARTICLE IN A BOX)

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Reference: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Sec 2.2.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 5.2, Exercise 5.2.5.

Post date: 26 Jan 2011.

To get the feel of how to solve the time-independent Schrödinger equation in one dimension, the most commonly used example is that of the infinite square well, sometimes known as the 'particle in a box' problem. First, recall the Schrödinger equation itself:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2}+V(x)\Psi = i\hbar\frac{\partial\Psi}{\partial t} \tag{1}$$

Remember that the 'time-independent' bit refers to the potential function V which is taken to be a function of position only; the wave function itself, which is the solution of the equation, will in general be time-dependent.

The infinite square well is defined by a potential function as follows:

$$V(x)=\begin{cases}0 & 0<x<a\\ \infty & \text{otherwise}\end{cases} \tag{2}$$

An area with an infinite potential means simply that the particle is not allowed to exist there. In classical physics, you can think of an infinite potential as an infinitely high wall, which no matter how much kinetic energy a particle has, it can never leap over. Although examples from classical physics frequently break down when applied to quantum mechanics, in this case, the comparison is still valid: an infinitely high potential barrier is an absolute barrier to a particle in both cases.

We saw in our study of the time independent Schrödinger equation that separation of variables reduces the problem to solving the spatial part of the equation, which is

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}+V(x)\psi = E\psi \tag{3}$$

where the constant E represents the possible energies that the system can have. It is important to note that both E and $V(x)$ are unknown before we solve the equation. In classical physics, we would be allowed to specify E since it is just the kinetic energy that the particle has inside the well. Classically, E can be any positive quantity, and the particle would just bounce around inside the well without ever changing its speed (assuming the walls were perfectly elastic and there was no friction). In quantum physics, as we will see, E can have only certain discrete values, and these values arise in the course of solving the equation.

In an infinite square well, the infinite value that the potential has outside the well means that there is zero chance that the particle can ever be found in that region. Since the probability density for finding the particle at a given location is $|\Psi|^2$, this condition can be represented in the mathematics by requiring $\psi(x) = 0$ if $x < 0$ or $x > a$. This condition is forced from the Schrödinger equation since if $V(x) = \infty$, any non-zero value for $\psi(x)$ would result in an infinite term in the equation. However, it is certainly not rigorous mathematics, since multiplying infinity by zero can be done properly only by using a limiting procedure, which we haven't done here. A proper treatment of the infinite square well is as a limiting case of the *finite* square well, where $V(x)$ can have a large but finite value outside the well. However, the mathematics for solving the finite square well is considerably more complicated and tends to obscure the physics. Readers who are worried, however, can be reassured that the energy levels in the finite square well do become those in the infinite square well when the proper limit is taken.

Inside the well, $V(x) = 0$ so the Schrödinger equation becomes

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi \tag{4}$$

$$\frac{d^2\psi}{dx^2} = -k^2\psi \tag{5}$$

$$\text{with } k \equiv \frac{\sqrt{2mE}}{\hbar} \tag{6}$$

This differential equation has the general solution

$$\psi(x) = A\sin(kx) + B\cos(kx) \tag{7}$$

for unspecified (yet) constants A and B. If you don't believe this, just substitute the solution back into the equation.

How can we determine A and B? To do this, we need to appeal to Born's conditions on the wave function. Born's first condition is clearly satisfied here: ψ is single-valued. The second condition of ψ being square integrable we'll leave for a minute. The third condition is that ψ must be continuous. We have argued above that $\psi = 0$ outside the well, so in particular, this means that at the boundaries $x = 0$ and $x = a$ we must have $\psi = 0$. If we impose that condition on our general solution above, we get:

$$\begin{aligned}
\psi(0) &= 0 && (8)\\
A\sin(0) + B\cos(0) &= 0 && (9)\\
B &= 0 && (10)\\
\psi(a) &= 0 && (11)\\
A\sin(ka) &= 0 && (12)\\
ka &= n\pi && (13)\\
\frac{\sqrt{2mE}}{\hbar} &= \frac{n\pi}{a} && (14)\\
E &= \frac{n^2\pi^2\hbar^2}{2ma^2} && (15)
\end{aligned}$$

where n is an integer. The useful values of n are just the positive integers. To see this, note that if $n = 0$, then $\psi(x) = 0$ everywhere which besides being very boring, is also no good as a probability density since its square modulus cannot integrate to 1. Negative integers don't really give new solutions, since $\sin(-x) = -\sin x$, so the negative sign can be absorbed into the (still undetermined) constant A. Also, the energies depend only on the square of n so the sign of n doesn't matter physically.

We can now return to the square-integrable condition and use it to determine A. Remember that the integral is over all space in which the particle can be found, so in this case we are interested in $0 \leq x \leq a$.

$$\int_0^a |\psi|^2 dx = 1 \tag{16}$$

$$A^2 \int_0^a \sin^2 kx = 1 \tag{17}$$

$$= A^2 \frac{1}{2} \int_0^a [1 - \cos(2kx)]\, dx \tag{18}$$

$$= \frac{A^2}{2} \left[x - \frac{1}{2k} \sin(2kx) \right]_0^a \tag{19}$$

$$= A^2 \frac{a}{2} \tag{20}$$

$$A = \pm\sqrt{\frac{2}{a}} \tag{21}$$

where we used 13 in 19 to eliminate the sine term.

Since it is only the square modulus of the wave function that has physical significance, we can ignore the negative root and take the final form of the wave function as

$$\psi(x) = \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a} \tag{22}$$

Notice what has happened here. Applying the first boundary condition at $x = 0$ allowed us to eliminate B. But the other boundary condition at $x = a$ ended up giving us a condition on E rather than A. (Well, ok, we *could* have used the second boundary condition to set $A = 0$ but then we would have $\psi(x) = 0$ everywhere again.) Not only that, but the energy levels are discrete; thus the infinite square well is the first case in which the Schrödinger equation has actually *predicted* quantization in a system.

So the boundary conditions on the differential equation have put restrictions on the allowable energies. The acceptable solutions for ψ are determined by the condition $ka = n\pi$ and so the various ψ functions are just lobes of the sine function. The lowest energy, called the *ground state*, occurs when $n = 1$ and ψ is half a sine wave, consisting of the bit between $x = 0$ and $x = \pi$. The next state at $n = 2$ corresponds to a single complete cycle of the sine wave; $n = 3$ contains 1.5 cycles and so on.

Eagle-eyed readers will have noticed that in all the excitement over discovering quantization, we have neglected to look at Born's fourth condition: that of continuous first derivatives. Clearly this condition is violated, since the derivative of ψ outside the well is 0 (since $\psi = 0$ outside the well), but inside the derivative is $kA\cos(kx)$,which is kA at $x = 0$ and $\pm kA$ at $x = a$

(the sign depends on whether n is odd or even). Neither of these derivatives is zero.

The reason is, of course, because of the infinite potential function which is not physically realistic. In fact, what happens in the (real-world) finite square well is that the wave function inside the potential barrier (that is, just off the ends of the well) is *not* zero, but a decaying exponential which tends to zero the further into the barrier you go. In that case, it *is* possible to make both the wave function and its first derivative continuous at both ends of the well (and it is precisely that condition which makes the mathematics so much more complicated in the finite square well).

In fact, this effect happens in any potential where the energy of the particle is less than that of a (finite) potential barrier: the particle's wave function extends into the barrier region. So does that mean that the particle has a probability of appearing *inside* a barrier? Technically yes, but in practice it usually doesn't do the particle much good, since the probability of being outside the barrier is usually a lot greater. However, there is one case where this barrier penetration effect does occur, and that is if the barrier is thin enough for the wave function to have a significant magnitude on the *other* side of the barrier. That is, if we have a particle in a finite well, but the wall of the well is fairly thin and there is another well (or just open space) on the other side of the barrier, then the wave function starts off with a respectable magnitude inside the main well, extends into the barrier (but gets attentuated exponentially in doing so), but before the attenuation gets so severe that the wave function becomes very small, it bursts through to the other side of the barrier. *That* means that, yes, there is a definite probability that the particle can spontaneously appear *outside* the well *without* having to jump over the barrier. In effect, it tunnels through the barrier and escapes. The effect, not surprisingly, is known as *quantum tunneling* and is one of the main causes of some forms of radioactive decay. But that's a topic for another post.

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THE CLASSICAL LIMIT OF QUANTUM MECHANICS; EHRENFEST'S THEOREM

Link to: physicspages home page.

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Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 6.

Post date: 16 Jan 2017

We've met Ehrenfest's theorem while studying Griffiths's book, where the theorem had the form

$$\frac{\partial \langle p \rangle}{\partial t} = -\left\langle \frac{\partial V}{\partial x} \right\rangle \tag{1}$$

This says that, in one dimension, the rate of change of the mean momentum equals the negative of the mean of the derivative of the potential V, which is assumed to depend on x only. In this case, the behaviour of the means of the quantum variables reduces to the corresponding classical relation, in this case, Newton's law $F = \frac{dp}{dt}$, where the force is defined in terms of the gradient of the potential: $F = -\frac{dV}{dx}$.

Shankar treats Ehrenfest's theorem a bit more generally. For an operator Ω we can use the product rule to state that

$$\begin{aligned} \frac{d}{dt} \langle \Omega \rangle &= \frac{d}{dt} \langle \psi | \Omega | \psi \rangle & (2) \\ &= \langle \dot{\psi} | \Omega | \psi \rangle + \langle \psi | \Omega | \dot{\psi} \rangle + \langle \psi | \dot{\Omega} | \psi \rangle & (3) \end{aligned}$$

where a dot indicates a time derivative. If Ω does not depend explicitly on time, we have

$$\frac{d}{dt} \langle \Omega \rangle = \langle \dot{\psi} | \Omega | \psi \rangle + \langle \psi | \Omega | \dot{\psi} \rangle \tag{4}$$

The time derivative of ψ can be found from the Schrödinger equation:

$$\begin{aligned} | \dot{\psi} \rangle &= -\frac{i}{\hbar} H | \psi \rangle & (5) \\ \langle \dot{\psi} | &= \frac{i}{\hbar} \langle \psi | H & (6) \end{aligned}$$

The second equation follows since H is hermitian, so $H^\dagger = H$. Plugging these into 4 we have

$$\frac{d}{dt}\langle\Omega\rangle = \frac{i}{\hbar}\left[\langle\psi|H\Omega|\psi\rangle - \langle\psi|\Omega H|\psi\rangle\right] \tag{7}$$

$$= -\frac{i}{\hbar}\langle\psi|[\Omega, H]|\psi\rangle \tag{8}$$

$$= -\frac{i}{\hbar}\langle[\Omega, H]\rangle \tag{9}$$

That is, the rate of change of the mean of an operator can be found from its commutator with the Hamiltonian. It is this result that Shankar refers to as Ehrenfest's theorem. This relation is similar to that from classical mechanics, where the rate of change of a dynamical variable ω is equal to its Poisson bracket with the classical Hamiltonian. In the Hamiltonian formulation of classical mechanics, dynamical variables depend on generalized coordinates q_i and their corresponding momenta p_i, so we have:

$$\frac{d\omega}{dt} = \sum_i \left(\frac{\partial\omega}{\partial q_i}\dot{q}_i + \frac{\partial\omega}{\partial p_i}\dot{p}_i\right) \tag{10}$$

$$= \sum_i \left(\frac{\partial\omega}{\partial q_i}\frac{\partial H}{\partial p_i} - \frac{\partial\omega}{\partial p_i}\frac{\partial H}{\partial q_i}\right) \tag{11}$$

$$\equiv \{\omega, H\} \tag{12}$$

We can work out 9 for the particular cases where $\Omega = X$, the position operator and $\Omega = P$, the momentum operator. For a Hamiltonian of the form

$$H = \frac{P^2}{2m} + V(x) \tag{13}$$

and using the commutation relation

$$[X, P] = i\hbar \tag{14}$$

we have

$$\frac{d\langle X\rangle}{dt} = -\frac{i}{\hbar}\langle[X, H]\rangle \tag{15}$$

$$= -\frac{i}{2m\hbar}\left\langle\left[X, P^2\right]\right\rangle \tag{16}$$

We can evaluate this commutator using the theorem

$$[AB, C] = A[B, C] + [A, C]B \tag{17}$$

In this case, $A = B = P$ and $C = X$, so we have

$$\begin{aligned}
\left[P^2, X\right] &= P\left[P, X\right] + \left[P, X\right] P && (18)\\
&= -2i\hbar P && (19)\\
\left[X, P^2\right] &= 2i\hbar P && (20)\\
\frac{d\left\langle X\right\rangle}{dt} &= \frac{\left\langle P\right\rangle}{m} && (21)
\end{aligned}$$

This is equivalent to the classical relation $p = mv$ for velocity v. We can write this result in terms of the Hamiltonian, provided that it's legal to take the derivative of the Hamiltonian with respect to an operator (which works if we can expand the Hamiltonian as a power series):

$$\frac{d\left\langle X\right\rangle}{dt} = \frac{\left\langle P\right\rangle}{m} = \left\langle \frac{\partial H}{\partial P} \right\rangle \tag{22}$$

This looks a lot like one of Hamilton's canonical equations in classical mechanics:

$$\dot{q}_i = \frac{\partial H}{\partial p_i} \tag{23}$$

The main difference between the quantum and classical forms is that the quantum version is a relation between mean values, while the classical version is exact. We can make the correspondence exact provided that it's legal to take the averaging operation inside the derivative and apply it to each occurrence of X and P. That is, is it legal to say that

$$\left\langle \frac{\partial H}{\partial P} \right\rangle = \left\langle \frac{\partial H\left(P, X\right)}{\partial P} \right\rangle = \frac{\partial H\left(\left\langle P\right\rangle, \left\langle X\right\rangle\right)}{\partial \left\langle P\right\rangle} \tag{24}$$

This depends on the precise functional form of H. In the case 13 we're considering here, we have

$$\left\langle \frac{\partial H}{\partial P} \right\rangle = \left\langle \frac{P}{m} \right\rangle = \frac{\left\langle P\right\rangle}{m} = \frac{\partial}{\partial \left\langle P\right\rangle} \left(\frac{\left\langle P\right\rangle^2}{2m} + V\left(\left\langle X\right\rangle\right) \right) \tag{25}$$

So in this case it works. In general, if H depends on P either linearly or quadratically, then its derivative with respect to P will be either constant or linear, and we can take the averaging operation inside the function without changing anything. However, if, say, $H = P^3$ (unlikely, but just for the sake of argument), then

$$\left\langle \frac{\partial H}{\partial P} \right\rangle = \left\langle 3P^2 \right\rangle \neq 3\left\langle P\right\rangle^2 = \frac{\partial H\left(\left\langle P\right\rangle, \left\langle X\right\rangle\right)}{\partial \left\langle P\right\rangle} \tag{26}$$

since, in general, the mean of the square of a value is not the same as the square of the mean.

Shankar goes through a similar argument for $\dot{P}$. We have

$$\left\langle \dot{P} \right\rangle = -\frac{i}{\hbar} \left\langle [P, H] \right\rangle \tag{27}$$

In this case, we can use the position basis form of P which is

$$P = -i\hbar \frac{d}{dx} \tag{28}$$

and the position space version of the potential $V(x)$ to get

$$\begin{aligned} [P, H]\,\psi &= -i\hbar \left(\frac{d\,(V\psi)}{dx} - V\frac{d\psi}{dx} \right) && (29) \\ &= -i\hbar\psi \frac{dV}{dx} && (30) \end{aligned}$$

Using this in 27 we have

$$\left\langle \dot{P} \right\rangle = -\left\langle \frac{dV}{dx} \right\rangle \tag{31}$$

Writing this in terms of the Hamiltonian, we have

$$\left\langle \dot{P} \right\rangle = -\left\langle \frac{\partial H}{\partial x} \right\rangle \tag{32}$$

Again, this looks similar to the second of Hamilton's canonical equations from classical mechanics:

$$\dot{p}_i = -\frac{\partial H}{\partial q_i} \tag{33}$$

and again, we're allowed to make the correspondence exact provided we can take the averaging operation inside the derivative on the RHS of 32. This works provided that V is either linear or quadratic in x (such as in the harmonic oscillator). Other potentials such as the $\frac{1}{r}$ potential in the hydrogen atom do not allow an exact correspondence between the quantum average and the classical Hamilton equation, but this shouldn't worry us too much since the hydrogen atom is quintessentially quantum anyway, and any attempt to describe it classically will not work.

Shankar provides a lengthly discussion on when the reduction to classical mechanics is valid, and shows that in any practical experiment that we could do with a classical particle, the difference between the average quantum behaviour and the classical measurements should be so small as to be

undetectable. It is only when we deal with systems that are small enough that quantum effects dominate that we need to abandon classical mechanics.

PINGBACKS

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HARMONIC OSCILLATOR - SERIES SOLUTION REVISITED

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Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 7.3, Exercise 7.3.1.

Post date: 17 Jan 2017

Shankar's derivation of the eigenfunctions of the harmonic oscillator in the position basis is essentially the same as that in Griffiths, which we've covered before. The reader may wish to refresh their knowledge of this before reading the rest of this post.

To make the comparison we note that ϵ in Griffiths is 2ε in Shankar:

$$\varepsilon \equiv \frac{E}{\hbar\omega} \tag{1}$$

The analysis begins with the Schrödinger equation for the harmonic oscillator, which is

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \frac{1}{2}m\omega^2 x^2\psi = E\psi \tag{2}$$

Making the substitution

$$y \equiv \sqrt{\frac{m\omega}{\hbar}}x \tag{3}$$

we convert the equation to

$$\psi'' + \left(2\varepsilon - y^2\right)\psi = 0 \tag{4}$$

where a prime indicates a derivative with respect to y.

As explained in the earlier post, we further convert this equation by defining another function $u(y)$ (Griffiths calls this function $f(y)$) as

$$\psi(y) = e^{-y^2/2}u(y) \tag{5}$$

This results in a simpler differential equation for f:

$$\frac{d^2u}{dy^2} - 2y\frac{du}{dy} + (2\varepsilon - 1)u = 0 \tag{6}$$

We can solve this by proposing that u is a power series in y:

$$u(y) = \sum_{n=0}^{\infty} C_n y^n \tag{7}$$

This leads to the recursion relation for the coefficients C_n:

$$C_{n+2} = C_n \frac{2n+1-2\varepsilon}{(n+1)(n+2)} \tag{8}$$

In order that u is finite for large y, this series must terminate, which leads to the quantization condition for the energy:

$$E_n = \hbar\omega\left(n+\frac{1}{2}\right) \tag{9}$$

Shankar poses as an exercise the question as to why we didn't just try a series solution of 4, that is, we propose

$$\psi(y) = \sum_{n=0}^{\infty} A_n y^n \tag{10}$$

for some other coefficients A_n. If we try this, there are three terms with different exponents for y that result from plugging this into 4.

$$\psi'' = \sum_{n=0}^{\infty} A_n n(n-1) y^{n-2} \tag{11}$$

$$2\varepsilon\psi = 2\varepsilon \sum_{n=0}^{\infty} A_n y^n \tag{12}$$

$$-y^2\psi = -\sum_{n=0}^{\infty} A_n y^{n+2} \tag{13}$$

To compare the coefficients we reassign the summation ranges so that the powers of y are the same in all three terms.

$$\psi'' = \sum_{n=2}^{\infty} A_n n(n-1) y^{n-2} = \sum_{n=0}^{\infty} A_{n+2}(n+2)(n+1) y^n \tag{14}$$

$$2\varepsilon\psi = 2\varepsilon \sum_{n=0}^{\infty} A_n y^n \tag{15}$$

$$-y^2\psi = -\sum_{n=0}^{\infty} A_n y^{n+2} = -\sum_{n=2}^{\infty} A_{n-2} y^n \tag{16}$$

Note that the top two sums start at $n=0$ while the last sum starts at $n=2$. To satisfy 4, the coefficient of each power of y must be zero, that is

$$A_{n+2}(n+2)(n+1)+2\varepsilon A_n - A_{n-2} = 0 \tag{17}$$

There are two separate conditions here; one for even n and the other for odd n. To get either sequence started, we need to specify the first two terms. For example, in the even sequence, we need to specify A_0 and A_2 which then allows calculation of A_4 (when $n = 2$). We can then use A_2 and A_4 to get A_6 and so on. The general formula is

$$A_{n+2} = \frac{A_{n-2} - 2\varepsilon A_n}{(n+2)(n+1)} \tag{18}$$

PINGBACKS

Pingback: Harmonic oscillator - eigenfunctions in momentum space

HARMONIC OSCILLATOR: HERMITE POLYNOMIALS AND ORTHOGONALITY OF EIGENFUNCTIONS

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Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 7.3, Exercises 7.3.2 - 7.3.3.

Post date: 17 Jan 2017

The eigenfunctions of the harmonic oscillator are given by

$$\psi_n(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right) e^{-m\omega x^2/2\hbar} \tag{1}$$

where $H_n(u)$ is a Hermite polynomial. The Hermite polynomials obey the recursion relation

$$H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x) \tag{2}$$

The first few Hermite polynomials are given in Shankar's equation 7.3.21, and we may use these to verify this relation for a couple of cases. Taking $n = 2$ we have

$$\begin{aligned} H_3(x) &= 2xH_2(x) - 4H_1(x) && (3)\\ &= 2x\left[-2\left(1-2x^2\right)\right] - 4(2x) && (4)\\ &= -12x + 8x^3 && (5) \end{aligned}$$

The last line agrees with H_3 as given in Shankar.

For $n = 3$ we have

$$\begin{aligned} H_4(x) &= 2xH_3(x) - 6H_2(x) && (6)\\ &= 2x\left[-12x + 8x^3\right] - 6\left[-2\left(1-2x^2\right)\right] && (7)\\ &= 12 - 48x^2 + 16y^4 && (8) \end{aligned}$$

which again agrees with Shankar's equation.

When deriving the solution in terms of Hermite polynomials, we followed Griffiths and found that we could write the polynomials in the form

$$H_n(y) = \sum_{j=0}^{n} a_j y^j \tag{9}$$

where the coefficients a_j obey the recursion relation

$$a_{j+2} = \frac{2j+1-\varepsilon}{(j+1)(j+2)} a_j \tag{10}$$

The ε used by Griffiths is equivalent to 2ε in Shankar, so using Shankar's notation, we see that this recursion relation is the same as Shankar's equation 7.3.15:

$$C_{n+2} = C_n \frac{2n+1-2\varepsilon}{(n+1)(n+2)} \tag{11}$$

Here, we have

$$\varepsilon = \frac{E}{\hbar\omega} \tag{12}$$

where E is the energy of the oscillator state.
Looking at the polynomials in Shankar's equation 7.3.21, we have

$$H_3(y) = -12\left(y - \frac{2}{3}y^3\right) \tag{13}$$

so

$$C_1 = -12 \tag{14}$$
$$C_3 = 8 \tag{15}$$

With $n = 1$, we get from 11

$$C_3 = -12\frac{3-2\varepsilon}{6} \tag{16}$$

However, for this state, $E = \left(3+\frac{1}{2}\right)\hbar\omega$ so $2\varepsilon = 7$ and $C_3 = 8$ as required.
For H_4 we have

$$H_4(y) = 12\left(1 - 4y^2 + \frac{4}{3}y^4\right) \tag{17}$$

This means

$$C_0 = 12 \tag{18}$$
$$C_2 = -48 \tag{19}$$
$$C_4 = 16 \tag{20}$$

Here $E = \left(4+\frac{1}{2}\right)\hbar\omega$, so $2\varepsilon = 9$ and

$$C_2 = 12\frac{(-8)}{2} = -48 \tag{21}$$

$$C_4 = -48\frac{5-9}{12} = 16 \tag{22}$$

We can see from the relation 2 that, given that $H_0 = 1$ and $H_1 = 2x$, all Hermite polynomials of even index contain only even powers of x, and all polynomials of odd index contain only odd powers of x. This means that all even Hermite polynomials are even functions of x, in the sense that $H_{2n}(-x) = H_{2n}(x)$, and all odd Hermite polynomials are odd functions of x, so that $H_{2n+1}(-x) = -H_{2n+1}(x)$.

If $\psi(x)$ is even and $\phi(x)$ is odd, then

$$\psi(-x)\phi(-x) = -\psi(x)\phi(x) \tag{23}$$

That is, the product $\psi(x)\phi(x)$ is an odd function. Since the integral of any odd function over an interval symmetric about $x = 0$ is zero, we have

$$\int_{-\infty}^{\infty} \psi(x)\phi(x)\,dx = 0 \tag{24}$$

Looking at the eigenfunctions 1, we see that the exponential factor is a Gaussian centred at $x = 0$ and is therefore even, so that ψ_n will be even or odd depending on whether n is even or odd. In particular, the integral of any even ψ_n multiplied by any odd ψ_n over all x will be zero.

To show that pairs of even functions are also orthogonal is a bit trickier, but we can do it in the simplest case, where we consider the functions ψ_0 and ψ_2.

$$\int_{-\infty}^{\infty} \psi_0(x)\psi_2(x)\,dx = \sqrt{\frac{m\omega}{\pi\hbar}}\frac{1}{\sqrt{8}}\int_{-\infty}^{\infty} H_0\left(\sqrt{\frac{m\omega}{\hbar}}x\right) H_2\left(\sqrt{\frac{m\omega}{\hbar}}x\right) e^{-m\omega x^2/\hbar}dx \tag{25}$$

$$= \sqrt{\frac{m\omega}{\pi\hbar}}\frac{1}{\sqrt{8}}\int_{-\infty}^{\infty} (1)\left[-2\left(1-2\frac{m\omega}{\hbar}x^2\right)\right] e^{-m\omega x^2/\hbar}dx \tag{26}$$

$$= -\sqrt{\frac{m\omega}{\pi\hbar}}\frac{1}{\sqrt{2}}\left[\sqrt{\frac{\pi\hbar}{m\omega}} - \sqrt{\frac{\pi\hbar}{m\omega}}\right] \tag{27}$$

$$= 0 \tag{28}$$

The two Gaussian integrals can be done using standard formulas as given in Shankar's Appendix A.2. (I used Maple.)

PINGBACKS

Pingback: Harmonic oscillator - mean position and momentum

HARMONIC OSCILLATOR: MATRIX ELEMENTS USING HERMITE POLYNOMIALS

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Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 7.3, Exercise 7.3.4.

Post date: 19 Jan 2017

Earlier, we found the matrix elements of X and P of the harmonic oscillator using the raising and lowering operators. We can also find these matrix elements using the recursion relations and orthogonality of Hermite polynomials. The required relations are also given as Shankar's equations 7.3.24 - 7.3.26.

$$H_n'(y) = 2nH_{n-1}(y) \tag{1}$$

$$H_{n+1}(y) = 2yH_n(y) - 2nH_{n-1}(y) \tag{2}$$

$$\int_{-\infty}^{\infty} H_n(y)\, H_{n'}(y)\, e^{-y^2} dy = \sqrt{\pi} 2^n n! \delta_{nn'} \tag{3}$$

The energy eigenfunctions of the harmonic oscillator are

$$\psi_n(y) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} H_n(y) e^{-y^2/2} \tag{4}$$

where

$$y \equiv \sqrt{\frac{m\omega}{\hbar}} x \tag{5}$$

The matrix elements of x are therefore

$$\left\langle n' \left| X \right| n \right\rangle = \int_{-\infty}^{\infty} \psi_{n'}(x)\, x \psi_n(x)\, dx \tag{6}$$

where we've used the fact that $\psi_{n'}(x)$ is real, so its complex conjugate is the same as the original. Converting to the variable y using 5 we have

$$\langle n'|X|n\rangle = \frac{\hbar}{m\omega}\int_{-\infty}^{\infty}\psi_{n'}(y)\,y\psi_n(y)\,dy \tag{7}$$

$$= \frac{\hbar}{m\omega}\sqrt{\frac{m\omega}{\pi\hbar}}\frac{1}{\sqrt{2^{n'}2^n n'!n!}}\int_{-\infty}^{\infty}H_n(y)\,yH_{n'}(y)\,e^{-y^2}dy \tag{8}$$

$$= \sqrt{\frac{\hbar}{\pi m\omega}}\frac{1}{\sqrt{2^{n'}2^n n'!n!}}\int_{-\infty}^{\infty}\frac{1}{2}\left[H_{n+1}+2nH_{n-1}\right]H_{n'}e^{-y^2}dy \tag{9}$$

$$= \sqrt{\frac{\hbar}{m\omega}}\frac{2^{n'}n'!}{2\sqrt{2^{n'}2^n n'!n!}}\left[\delta_{n',n+1}+2n\delta_{n',n-1}\right] \tag{10}$$

$$= \sqrt{\frac{\hbar}{m\omega}}\left[\frac{2^{n+1}(n+1)!}{2\sqrt{2^{2n+1}(n+1)!n!}}\delta_{n',n+1}+\frac{2^n n(n-1)!}{2\sqrt{2^{2n-1}(n-1)!n!}}\delta_{n',n-1}\right] \tag{11}$$

$$= \sqrt{\frac{\hbar}{2m\omega}}\left[\frac{(n+1)n!}{\sqrt{(n+1)(n!)^2}}\delta_{n',n+1}+\frac{n(n-1)!}{\sqrt{n[(n-1)!]^2}}\delta_{n',n-1}\right] \tag{12}$$

$$= \sqrt{\frac{\hbar}{2m\omega}}\left[\sqrt{n+1}\delta_{n',n+1}+\sqrt{n}\delta_{n',n-1}\right] \tag{13}$$

We used 2 to get the third line and 3 to do the integrals.
For the matrix elements of P we use

$$P = -i\hbar\frac{d}{dx} = -i\sqrt{\hbar m\omega}\frac{d}{dy} \tag{14}$$

$$P\psi_n(y) = -i\sqrt{\hbar m\omega}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\frac{1}{\sqrt{2^n n!}}e^{-y^2/2}\left[H_n'(y)-yH_n(y)\right] \tag{15}$$

$$= -i\sqrt{\hbar m\omega}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\frac{1}{\sqrt{2^n n!}}e^{-y^2/2}\left[2nH_{n-1}-\frac{1}{2}\left(H_{n+1}+2nH_{n-1}\right)\right] \tag{16}$$

$$= -i\sqrt{\hbar m\omega}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\frac{1}{\sqrt{2^n n!}}e^{-y^2/2}\left[nH_{n-1}-\frac{1}{2}H_{n+1}\right] \tag{17}$$

We used 2 to get the third line.
We get, using $dx = \sqrt{\hbar/m\omega}dy$ from 5

$$\left\langle n'\left|P\right|n\right\rangle = -i\sqrt{\hbar m\omega}\sqrt{\frac{m\omega}{\pi\hbar}}\sqrt{\frac{\hbar}{m\omega}}\frac{1}{\sqrt{2^{n'}n'!2^n n!}}\int_{-\infty}^{\infty}H_{n'}\left[nH_{n-1}-\frac{1}{2}H_{n+1}\right]e^{-y^2}dy \tag{18}$$

$$= -i\sqrt{\hbar m\omega}\left[\frac{2^{n'}n'!n}{\sqrt{2^{n'}n'!2^n n!}}\delta_{n',n-1}-\frac{2^{n'-1}n'!}{\sqrt{2^{n'}n'!2^n n!}}\delta_{n',n+1}\right] \tag{19}$$

$$= -i\sqrt{\hbar m\omega}\left[\frac{2^{n-1}\left(n-1\right)!n}{\sqrt{2^{n-1}\left(n-1\right)!2^n n!}}\delta_{n',n-1}-\frac{2^n\left(n+1\right)!}{\sqrt{2^{n+1}\left(n+1\right)!2^n n!}}\delta_{n',n+1}\right] \tag{20}$$

$$= i\sqrt{\frac{\hbar m\omega}{2}}\left[\sqrt{n+1}\delta_{n',n+1}-\sqrt{n}\delta_{n',n-1}\right] \tag{21}$$

PINGBACKS

Pingback: Harmonic oscillator - mean position and momentum

HARMONIC OSCILLATOR - MEAN POSITION AND MOMENTUM

Link to: physicspages home page.

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Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 7.3, Exercise 7.3.5.

Post date: 21 Jan 2017

The energy eigenfunctions of the harmonic oscillator are

$$\psi_n(y) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} H_n(y) e^{-y^2/2} \tag{1}$$

where

$$y \equiv \sqrt{\frac{m\omega}{\hbar}} x \tag{2}$$

and H_n is the Hermite polynomial of order n. Since an even (odd) Hermite polynomial is an even (odd) function, ψ_n is even (odd) if n is even (odd), so we can use this fact to show that

$$\langle n\,|X|\,n\rangle = \int_{-\infty}^{\infty} x\psi_n^2(x)\; dx = 0 \tag{3}$$

This follows because the square of either an even or odd function gives an even function, and x itself is odd, so the integrand is the product of an odd and even function, which is odd. The integral over any interval symmetric about $x = 0$ of an odd function is odd. Thus the mean position $\langle X\rangle$ of a particle in any of the harmonic oscillator's energy eigenstates is zero.

For the momentum P, we have

$$\langle n\,|P|\,n\rangle = -i\hbar \int_{-\infty}^{\infty} \psi_n \frac{d\psi_n}{dx}\, dx \tag{4}$$

As we showed earlier

$$-i\hbar\frac{d\psi_n}{dx} = i\sqrt{\hbar m\omega}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} e^{-y^2/2}\left[nH_{n-1} - \frac{1}{2}H_{n+1}\right] \tag{5}$$

If n is even (odd), then $nH_{n-1} - \frac{1}{2}H_{n+1}$ is odd (even), so the product $\psi_n\frac{d\psi_n}{dx}$ is always the product of one odd and one even function, making it odd. Thus

$$\langle n\,|P|\,n\rangle = 0 \tag{6}$$

Thus the mean momentum $\langle P\rangle = 0$ in all energy eigenstates.

This means that the uncertainties in position and momentum are determined entirely by the mean square values:

$$\begin{aligned}(\Delta X)^2 &= \left\langle X^2\right\rangle - \langle X\rangle^2 = \left\langle X^2\right\rangle &(7)\\ (\Delta P)^2 &= \left\langle P^2\right\rangle &(8)\end{aligned}$$

We can work out these values for a couple of specific states. For $n = 1$ we have

$$\begin{aligned}\left\langle 1\left|X^2\right|1\right\rangle &= \int_{-\infty}^{\infty} x^2\psi_1^2(x)\;dx &(9)\\ &= \frac{1}{2}\sqrt{\frac{m\omega}{\pi\hbar}}\int_{-\infty}^{\infty} x^2 H_1^2(y)\,e^{-y^2}dx &(10)\\ &= \frac{1}{2}\frac{\hbar}{\sqrt{\pi}m\omega}\int_{-\infty}^{\infty} y^2 H_1^2(y)\,e^{-y^2}dy &(11)\\ &= \frac{2\hbar}{\sqrt{\pi}m\omega}\int_{-\infty}^{\infty} y^4 e^{-y^2}dy &(12)\\ &= \frac{2\hbar}{\sqrt{\pi}m\omega}\frac{3\sqrt{\pi}}{4} &(13)\\ &= \frac{3\hbar}{2m\omega} &(14)\end{aligned}$$

We've used

$$H_1(y) = 2y \tag{15}$$

and formula just before A.2.3 from the appendix in Shankar, which gives

$$\begin{aligned}I_4(\alpha) &= \int_{-\infty}^{\infty} x^4 e^{-\alpha x^2}dx &(16)\\ &= \frac{\partial^2}{\partial\alpha^2}\int_{-\infty}^{\infty} e^{-\alpha x^2}dx &(17)\\ &= \frac{\partial^2}{\partial\alpha^2}I_0(\alpha) &(18)\end{aligned}$$

From formula A.2.2

$$I_4(\alpha) = \frac{\partial^2}{\partial\alpha^2}\sqrt{\frac{\pi}{\alpha}} \tag{19}$$

$$= \frac{3\sqrt{\pi}}{4\alpha^{5/2}} \tag{20}$$

Setting $\alpha = 1$ gives

$$\int_{-\infty}^{\infty} y^4 e^{-y^2}\,dy = \frac{3\sqrt{\pi}}{4} \tag{21}$$

For P, we have

$$\left\langle 1 \left| P^2 \right| 1 \right\rangle = -\hbar^2 \int_{-\infty}^{\infty} \psi_1 \frac{d^2}{dx^2}\psi_1\,dx \tag{22}$$

The derivative is

$$\frac{d^2}{dx^2}\psi_1 = \frac{d^2\psi_1}{dy^2}\left(\frac{dy}{dx}\right)^2 \tag{23}$$

$$= \frac{1}{\sqrt{2}}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\frac{m\omega}{\hbar}\frac{d^2}{dy^2}\left[H_1(y)e^{-y^2/2}\right] \tag{24}$$

$$= \frac{1}{\sqrt{2}}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\frac{m\omega}{\hbar}\frac{d^2}{dy^2}\left[2ye^{-y^2/2}\right] \tag{25}$$

$$= \left(\frac{m\omega}{4\pi\hbar}\right)^{1/4}\frac{m\omega}{\hbar}e^{-y^2/2}\left[2y^3 - 6y\right] \tag{26}$$

We can now evaluate 22:

$$-\hbar^2\int_{-\infty}^{\infty}\psi_1\frac{d^2}{dx^2}\psi_1\,dx = -\hbar^2\sqrt{\frac{m\omega}{4\pi\hbar}}\frac{m\omega}{\hbar}\sqrt{\frac{\hbar}{m\omega}}\int_{-\infty}^{\infty}2ye^{-y^2}2\left[y^3 - 3y\right]dy \tag{27}$$

$$= -\frac{2m\omega\hbar}{\sqrt{\pi}}\int_{-\infty}^{\infty}e^{-y^2}\left[y^4 - 3y^2\right]dy \tag{28}$$

$$= -\frac{2m\omega\hbar}{\sqrt{\pi}}\left[\frac{3\sqrt{\pi}}{4} - \frac{3\sqrt{\pi}}{2}\right] \tag{29}$$

$$= \frac{3}{2}m\omega\hbar \tag{30}$$

Thus for the $n = 1$ state

$$\Delta X = \sqrt{\frac{3\hbar}{2m\omega}} \tag{31}$$

$$\Delta P = \sqrt{\frac{3}{2}m\omega\hbar} \tag{32}$$

$$\Delta X \Delta P = \frac{3}{2}\hbar > \frac{\hbar}{2} \tag{33}$$

For the $n = 0$ (ground) state, we can use $H_0 = 1$ to get

$$\left\langle X^2 \right\rangle = \int_{-\infty}^{\infty} x^2 \psi_0^2(x)\ dx \tag{34}$$

$$= \sqrt{\frac{m\omega}{\pi\hbar}} \int_{-\infty}^{\infty} x^2 H_0^2(y)\, e^{-y^2} dx \tag{35}$$

$$= \frac{\hbar}{\sqrt{\pi} m\omega} \int_{-\infty}^{\infty} y^2 e^{-y^2} dy \tag{36}$$

$$= \frac{\hbar}{2m\omega} \tag{37}$$

For P:

$$\frac{d^2}{dx^2}\psi_0 = \frac{d^2\psi_0}{dy^2}\left(\frac{dy}{dx}\right)^2 \tag{38}$$

$$= \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{m\omega}{\hbar} e^{-y^2/2}\left(y^2 - 1\right) \tag{39}$$

$$\left\langle P^2 \right\rangle = -\hbar^2 \int_{-\infty}^{\infty} \psi_0 \frac{d^2}{dx^2}\psi_0\, dx = -\hbar^2 \sqrt{\frac{m\omega}{\pi\hbar}} \frac{m\omega}{\hbar} \sqrt{\frac{\hbar}{m\omega}} \int_{-\infty}^{\infty} e^{-y^2}\left(y^2 - 1\right) dy \tag{40}$$

$$= -\frac{m\omega\hbar}{\sqrt{\pi}}\left[\frac{\sqrt{\pi}}{2} - \sqrt{\pi}\right] \tag{41}$$

$$= \frac{1}{2}m\omega\hbar \tag{42}$$

The uncertainty principle in this case gives

$$\Delta X \Delta P = \frac{\hbar}{2} \tag{43}$$

so it saturates the condition $\Delta X \Delta P \geq \frac{\hbar}{2}$.

PINGBACKS

Pingback: Harmonic oscillator - zero-point energy from uncertainty principle

HARMONIC OSCILLATOR - ZERO-POINT ENERGY FROM UNCERTAINTY PRINCIPLE

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 7.3.

Post date: 22 Jan 2017

There is a nice result derived in Shankar's section 7.3 in which he shows that we can actually derive the ground state energy and wave function for the harmonic oscillator from the uncertainty principle. Classically, the energy of a harmonic oscillator is

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 \tag{1}$$

where both p and x are continuous variables that can, in principle, take on any values. Thus classically it is possible for an oscillator to have $x = p = 0$ giving a ground state with zero energy. In quantum mechanics, because X and P don't commute, the position and momentum cannot both have precise values, which means that the ground state must have an energy greater than zero. This so-called *zero-point energy* is (as found by Solving Schrödinger's equation)

$$E_0 = \frac{\hbar\omega}{2} \tag{2}$$

To derive this without needing to solve Schrödinger's equation, we first recall that a state in which the position-momentum uncertainty is a minimum must be a gaussian of form

$$\Psi(x) = Ae^{-a(x-\langle x\rangle)^2/2\hbar}e^{i\langle p\rangle x/\hbar} \tag{3}$$

where a is a positive real constant, A is the normalization constant, $\langle x\rangle$ is the mean position and $\langle p\rangle$ is the mean momentum. For a harmonic oscillator centred at $x = 0$, we have that both $\langle x\rangle = \langle p\rangle = 0$, so we know that the ground state wave function has the form

$$\psi(x) = Ae^{-ax^2/2\hbar} \tag{4}$$

To normalize this we require (assuming A is real)

$$\int_{-\infty}^{\infty} \psi^2(x)\,dx = 1 \tag{5}$$

Using the standard result for a gaussian integral (see Appendix 2 in Shankar or use Google)

$$\begin{aligned} \int_{-\infty}^{\infty} \psi^2(x)\,dx &= A^2 \int_{-\infty}^{\infty} e^{-ax^2/\hbar} dx & (6)\\ &= A^2 \sqrt{\frac{\pi\hbar}{a}} & (7) \end{aligned}$$

Therefore

$$A = \left(\frac{a}{\pi\hbar}\right)^{1/4} \tag{8}$$

We need to find a such that $\Delta X \Delta P$ is minimized. The harmonic oscillator hamiltonian is

$$H = \frac{P^2}{2m} + \frac{1}{2} m\omega^2 X^2 \tag{9}$$

Since $\langle X \rangle = \langle P \rangle = 0$, the uncertainties become

$$\begin{aligned} (\Delta X)^2 &= \left\langle X^2 \right\rangle - \langle X \rangle^2 = \left\langle X^2 \right\rangle & (10)\\ (\Delta P)^2 &= \left\langle P^2 \right\rangle - \langle P \rangle^2 = \left\langle P^2 \right\rangle & (11) \end{aligned}$$

Averaging 9 we get

$$\begin{aligned} \langle H \rangle &= \frac{\left\langle P^2 \right\rangle}{2m} + \frac{1}{2} m\omega^2 \left\langle X^2 \right\rangle & (12)\\ &= \frac{(\Delta P)^2}{2m} + \frac{1}{2} m\omega^2 (\Delta X)^2 & (13) \end{aligned}$$

At minimum uncertainty

$$\Delta X \Delta P = \frac{\hbar}{2} \tag{14}$$

so we have

$$\begin{aligned} \Delta P &= \frac{\hbar}{2\Delta X} & (15)\\ \langle H \rangle &= \frac{\hbar^2}{8m(\Delta X)^2} + \frac{1}{2} m\omega^2 (\Delta X)^2 & (16) \end{aligned}$$

The minimum energy can now be found by finding the value of $(\Delta X)^2$ that minimizes this function. Treating $(\Delta X)^2$ (not just ΔX) as the independent variable, we have

$$\frac{\partial \langle H \rangle}{\partial (\Delta X)^2} = -\frac{\hbar^2}{8m\left[(\Delta X)^2\right]^2} + \frac{1}{2}m\omega^2 \tag{17}$$

$$= -\frac{\hbar^2}{8m(\Delta X)^4} + \frac{1}{2}m\omega^2 = 0 \tag{18}$$

$$(\Delta X)^2 = \frac{\hbar}{2m\omega} \tag{19}$$

This gives a minimum value for the mean energy of

$$\langle H \rangle_{min} = \frac{\hbar\omega}{2} \tag{20}$$

To complete the derivation, we need to find the gaussian 4 that gives the correct value 19 for $(\Delta X)^2$. That is, we need to find a such that

$$(\Delta X)^2 = \left\langle X^2 \right\rangle = \frac{\hbar}{2m\omega} \tag{21}$$

This requires doing another gaussian integral:

$$\left\langle X^2 \right\rangle = \int_{-\infty}^{\infty} x^2 \psi^2(x)\, dx \tag{22}$$

$$= \sqrt{\frac{a}{\pi\hbar}} \int_{-\infty}^{\infty} x^2 e^{-ax^2/\hbar} dx \tag{23}$$

$$= \sqrt{\frac{a}{\pi\hbar}} \sqrt{\frac{\pi\hbar}{a}} \frac{h}{2a} \tag{24}$$

$$= \frac{\hbar}{2a} \tag{25}$$

We therefore get

$$\frac{\hbar}{2a} = \frac{\hbar}{2m\omega} \tag{26}$$

$$a = m\omega \tag{27}$$

which gives a normalized minimum energy wave function

$$\psi_{min}(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-m\omega x^2/2\hbar} \tag{28}$$

This is the lowest possible value for the energy, but is it actually the ground state energy? What we have shown so far is that

$$\langle \psi_{min} | H | \psi_{min} \rangle \leq \langle \psi_0 | H | \psi_0 \rangle = E_0 \tag{29}$$

where $|\psi_0\rangle$ is the ground state energy. However, we can invoke the variational principle which states that if ψ is any normalized function, then the ground state energy E_0 of any hamiltonian H satisfies

$$E_0 \leq \langle \psi | H | \psi \rangle \tag{30}$$

Using $\psi = \psi_{min}$ we therefore have

$$E_0 \leq \langle \psi_{min} | H | \psi_{min} \rangle \tag{31}$$

Combining 29 and 31 we have

$$\langle \psi_{min} | H | \psi_{min} \rangle \leq E_0 \leq \langle \psi_{min} | H | \psi_{min} \rangle \tag{32}$$

which means that

$$E_0 = \langle \psi_{min} | H | \psi_{min} \rangle \tag{33}$$

and therefore that $|\psi_0\rangle = |\psi_{min}\rangle$, that is, 28 is actually the ground state wave function.

Although this clever little derivation gives us the ground state energy and wave function, it doesn't say anything about the higher energy states, or tell us that they are all equally spaced with a spacing of $\hbar\omega$. Nevertheless, it's a pleasant exercise.

HARMONIC OSCILLATOR - EIGENFUNCTIONS IN MOMENTUM SPACE

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Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 7.3, Exercise 7.3.7.

Post date: 23 Jan 2017

We've seen how to solve the Schrödinger equation for the harmonic oscillator in the position basis, where the independent variable is x. It's actually fairly easy to adapt this solution to find the wave functions in momentum space. (We've also found these functions by using the Fourier transform of the position functions, but the present post shows an easier way.)

The Schrödinger equation for the stationary states of the harmonic oscillator is, in operator form:

$$\frac{P^2}{2m}\psi + \frac{1}{2}m\omega^2 X^2\psi = E\psi \tag{1}$$

To work in momentum space, we use the results

$$P = p \tag{2}$$

$$X = i\hbar\frac{\partial}{\partial p} \tag{3}$$

This gives

$$\frac{p^2}{2m}\psi - \frac{1}{2}\hbar^2 m\omega^2\frac{d^2\psi}{dp^2} = E\psi \tag{4}$$

Dividing through by $(m\omega)^2$ we get

$$-\frac{\hbar^2}{2m}\psi'' + \frac{p^2}{2m^3\omega^2} = \frac{E}{(m\omega)^2}\psi \tag{5}$$

where a prime on ψ indicates a derivative with respect to p.

This is similar to the Schrödinger equation in position space:

$$-\frac{\hbar^2}{2m}\psi'' + \frac{1}{2}m\omega^2 x^2\psi = E\psi \tag{6}$$

(where a prime here indicates a derivative with respect to x). When we solved the position space equation, we introduced a dimensionless variable

$$y \equiv \sqrt{\frac{m\omega}{\hbar}}x \tag{7}$$

Using this technique to solve 5, we try a definition for y of

$$y \equiv \frac{p}{\sqrt{\hbar m\omega}} \tag{8}$$

(You can check the units of $\sqrt{\hbar m\omega}$ to see they are the units of momentum, so y is indeed dimensionless here.) Making this substitution, we get

$$\frac{d^2\psi}{dp^2} = \frac{1}{\hbar m\omega}\frac{d^2\psi}{dy^2} \tag{9}$$

$$\frac{p^2}{2m^3\omega^2} = \frac{\hbar y^2}{2m^2\omega} \tag{10}$$

Thus 5 becomes

$$-\frac{\hbar^2}{2m}\frac{1}{\hbar m\omega}\frac{d^2\psi}{dy^2} + \frac{\hbar y^2}{2m^2\omega}\psi = \frac{E}{(m\omega)^2}\psi \tag{11}$$

$$\frac{\hbar^2}{2m}\left[-\frac{d^2\psi}{dy^2} + y^2\psi\right] = \frac{\hbar E}{\omega}\psi \tag{12}$$

We can now use the same dimensionless parameter we used in the earlier derivation:

$$\varepsilon \equiv \frac{E}{\hbar\omega} \tag{13}$$

This results in the differential equation

$$\psi'' + \left(2\varepsilon - y^2\right)\psi = 0 \tag{14}$$

where a prime now indicates a derivative with respect to y. This is exactly the same differential equation that we got for the position basis, except that the independent variable y is now defined in terms of p by 8 instead of x. We can solve it in the same way, which results in the same quantization condition on the allowable energies of $E_n = \left(n + \frac{1}{2}\right)\hbar\omega$. The eigenfunctions look the same when expressed in terms of y:

$$\psi_n(y) = A\frac{1}{\sqrt{2^n n!}}H_n(y)e^{-y^2/2} \tag{15}$$

where A is a normalization constant with the value in the position basis of

$$A = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \tag{16}$$

and H_n is a Hermite polynomial. We can get the eigenfunctions in momentum space by replacing y by 8. We can see that this amounts to replacing $x \to p$ and $m\omega \to \frac{1}{m\omega}$, so we get

$$\psi_n(p) = \frac{1}{(\pi\hbar m\omega)^{1/4}} \frac{1}{\sqrt{2^n n!}} H_n\left(\frac{p}{\sqrt{\hbar m\omega}}\right) e^{-p^2/2\hbar m\omega} \tag{17}$$

In particular, the ground state is

$$\psi_0(p) = \frac{1}{(\pi\hbar m\omega)^{1/4}} e^{-p^2/2\hbar m\omega} \tag{18}$$

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Pingback: Harmonic oscillator: momentum space functions and Hermite polynomial recursion

VIRIAL THEOREM IN CLASSICAL MECHANICS; APPLICATION TO HARMONIC OSCILLATOR

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Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 7.4, Exercise 7.4.3.

Post date: 27 Jan 2017

We've seen the virial theorem in quantum mechanics, but this theorem was originally devised in classical mechanics. For a single particle, we consider the quantity

$$G = \mathbf{r} \cdot \mathbf{p} \tag{1}$$

that is, the product of position and momentum. Taking the time derivative, we have

$$\begin{aligned} \frac{dG}{dt} &= \mathbf{p} \cdot \frac{d\mathbf{r}}{dt} + \mathbf{r} \cdot \frac{d\mathbf{p}}{dt} && (2) \\ &= mv^2 + \mathbf{r} \cdot \mathbf{F} && (3) \end{aligned}$$

where $\mathbf{v} = d\mathbf{r}/dt$ is the velocity of the particle, $\mathbf{p} = m\mathbf{v}$ and $\mathbf{F} = d\mathbf{p}/dt$ is the force acting on the particle. If the force is a central force (that is, it depends only on the particle's distance from some centre point $\mathbf{r} = 0$, then the force can be written as the negative gradient of a potential V that depends only on $\mathbf{r}$. In the case where V depends only on a power of r, we have

$$\begin{aligned} V &= ar^k && (4) \\ \mathbf{F} &= -\frac{dV}{dr} = -kar^{k-1}\hat{\mathbf{r}} && (5) \end{aligned}$$

In that case, we have

$$\begin{aligned} \frac{dG}{dt} &= mv^2 - \mathbf{r} \cdot kar^{k-1}\hat{\mathbf{r}} && (6) \\ &= 2T - kar^k && (7) \\ &= 2T - kV && (8) \end{aligned}$$

where T is the kinetic energy $T = \frac{1}{2}mv^2$. If the particle is moving in a circular orbit then its average position and average momentum (averaged over one orbit) do not change with time, so $\frac{dG}{dt} = 0$ and we get

$$\begin{aligned} 2\langle T\rangle - k\langle V\rangle &= 0 \quad (9)\\ \langle T\rangle &= \frac{k}{2}\langle V\rangle \quad (10)\end{aligned}$$

Another way of seeing this is that, in a circular orbit at constant orbital speed, the only force acting is the centripetal force holding the particle in its orbit, which is

$$F_{cen} = -\frac{mv^2}{r} \quad (11)$$

where the minus sign indicates that the force acts in the opposite direction to the outward pointing radius vector.

This force is provided by the gradient of the potential, so we have

$$F_{cen} = -\frac{dV}{dr} = -kar^{k-1} \quad (12)$$

We therefore have

$$\begin{aligned} \frac{mv^2}{r} &= kar^{k-1} \quad (13)\\ mv^2 = 2T &= kar^k = kV \quad (14)\\ \langle T\rangle &= \frac{k}{2}\langle V\rangle \quad (15)\end{aligned}$$

For the case of a harmonic oscillator, $V = \frac{1}{2}m\omega^2x^2$ so the exponent is $k = 2$ and we have $T = V$. We can verify this by calculating the mean kinetic and potential energies explicitly, using earlier results. In the oscillator state $|n\rangle$ we have

$$\begin{aligned} \langle x^2\rangle &= \frac{\hbar}{m\omega}\left(n+\frac{1}{2}\right) \quad (16)\\ \langle p^2\rangle &= \hbar m\omega\left(n+\frac{1}{2}\right) \quad (17)\end{aligned}$$

The energies are

$$\langle T\rangle = \frac{\langle p^2\rangle}{2m} = \frac{\hbar\omega}{2}\left(n+\frac{1}{2}\right) \tag{18}$$

$$\langle V\rangle = \frac{1}{2}m\omega^2\langle x^2\rangle = \frac{\hbar\omega}{2}\left(n+\frac{1}{2}\right) \tag{19}$$

Therefore $\langle T\rangle = \langle V\rangle$ as required.

HARMONIC OSCILLATOR - MIXED INITIAL STATE AND EHRENFEST'S THEOREM

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Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 7.4, Exercise 7.4.5.

Post date: 29 Jan 2017

We've already done an example of a harmonic oscillator in a mixed initial state, but it's useful to do this other example from Shankar so we can see how the modified Ehrenfest's theorem fits in. In this case, we start with a particle in the mixed initial state

$$|\psi(0)\rangle = \frac{1}{\sqrt{2}}\left[|0\rangle + |1\rangle\right] \tag{1}$$

The time-dependent solution is therefore

$$\begin{aligned} |\psi(t)\rangle &= \frac{1}{\sqrt{2}}\left[e^{-iE_0\hbar t}|0\rangle + e^{-iE_1 t}|1\rangle\right] &(2)\\ &= \frac{1}{\sqrt{2}}\left[e^{-i\omega t/2}|0\rangle + e^{-3i\omega t/2}|1\rangle\right] &(3)\end{aligned}$$

since the first two energies are $E_0 = \hbar\omega/2$ and $E_1 = 3\hbar\omega/2$.

The position and momentum operators can be written in terms of the raising and lowering operators

$$\begin{aligned} X &= \sqrt{\frac{\hbar}{2m\omega}}\left(a^\dagger + a\right) &(4)\\ P &= i\sqrt{\frac{\hbar m\omega}{2}}\left(a^\dagger - a\right) &(5)\end{aligned}$$

To find the mean position and momentum, we can use these equations:

$$\begin{aligned} \langle X(0)\rangle &= \langle\psi(0)|X|\psi(0)\rangle &(6)\\ &= \frac{1}{2}\sqrt{\frac{\hbar}{2m\omega}}\left[\langle 0| + \langle 1|\right]\left(a^\dagger + a\right)\left[|0\rangle + |1\rangle\right] &(7)\end{aligned}$$

To work out the last line, remember that the stationary states are orthogonal so that $\langle 0|1\rangle = 0$, and that

$$a^\dagger |n\rangle = \sqrt{n+1}\,|n+1\rangle \quad (8)$$
$$a |n\rangle = \sqrt{n}\,|n-1\rangle \quad (9)$$

We therefore get

$$\langle X(0)\rangle = \frac{1}{2}\sqrt{\frac{\hbar}{2m\omega}}(1+1) = \sqrt{\frac{\hbar}{2m\omega}} \quad (10)$$

Doing a similar analysis for the momentum, we have

$$\langle P(0)\rangle = \langle \psi(0)|P|\psi(0)\rangle \quad (11)$$
$$= \frac{i}{2}\sqrt{\frac{\hbar m\omega}{2}}\left[\langle 0| + \langle 1|\right]\left(a^\dagger - a\right)\left[|0\rangle + |1\rangle\right] \quad (12)$$
$$= \sqrt{\frac{\hbar m\omega}{2}}\frac{1}{2i}\left[\langle 0| + \langle 1|\right]\left(a - a^\dagger\right)\left[|0\rangle + |1\rangle\right] \quad (13)$$
$$= \sqrt{\frac{\hbar m\omega}{2}}\frac{1}{2i}(1-1) \quad (14)$$
$$= 0 \quad (15)$$

We can expand these equations to give the averages of position and momentum at all times by plugging in 3:

$$\langle X(t)\rangle = \langle \psi(t)|X|\psi(t)\rangle \quad (16)$$
$$= \frac{1}{2}\sqrt{\frac{\hbar}{2m\omega}}\left[\langle 0|e^{i\omega t/2} + \langle 1|e^{3i\omega t/2}\right]\left(a^\dagger + a\right)\left[e^{-i\omega t/2}|0\rangle + e^{-3i\omega t/2}|1\rangle\right] \quad (17)$$
$$= \frac{1}{2}\sqrt{\frac{\hbar}{2m\omega}}\left(e^{-i\omega t} + e^{i\omega t}\right) \quad (18)$$
$$= \sqrt{\frac{\hbar}{2m\omega}}\cos\omega t \quad (19)$$

$$\langle P(t)\rangle = \langle\psi(t)|P|\psi(t)\rangle \tag{20}$$

$$= \frac{i}{2}\sqrt{\frac{\hbar m\omega}{2}}\left[\langle 0|e^{i\omega t/2}+\langle 1|e^{3i\omega t/2}\right]\left(a^\dagger - a\right)\left[e^{-i\omega t/2}|0\rangle + e^{-3i\omega t/2}|1\rangle\right] \tag{21}$$

$$= \sqrt{\frac{\hbar m\omega}{2}}\frac{1}{2i}\left[\langle 0|e^{i\omega t/2}+\langle 1|e^{3i\omega t/2}\right]\left(a - a^\dagger\right)\left[e^{-i\omega t/2}|0\rangle + e^{-3i\omega t/2}|1\rangle\right] \tag{22}$$

$$= \sqrt{\frac{\hbar m\omega}{2}}\frac{1}{2i}\left(e^{-i\omega t} - e^{i\omega t}\right) \tag{23}$$

$$= -\sqrt{\frac{\hbar m\omega}{2}}\sin\omega t \tag{24}$$

Although we can calculate $\left\langle \dot{X}(t)\right\rangle$ and $\left\langle \dot{P}(t)\right\rangle$ directly by taking the time derivative, we can also do it by using Ehrenfest's theorem in the form

$$\frac{d\langle\Omega\rangle}{dt} = -\frac{i}{\hbar}\langle[\Omega, H]\rangle \tag{25}$$

for some operator Ω.

Since the energy of the oscillator in state $|n\rangle$ is $\left(n+\frac{1}{2}\right)\hbar\omega$, we can write the hamiltonian as

$$H = \hbar\omega\left(a^\dagger a + \frac{1}{2}\right) \tag{26}$$

We also have the commutator

$$\left[a, a^\dagger\right] = 1 \tag{27}$$

To use this for X and P we need the commutators $[a, H]$ and $\left[a^\dagger, H\right]$, which amounts to finding

$$\left[a, a^\dagger a\right] = aa^\dagger a - a^\dagger aa \tag{28}$$

$$= \left(1 + a^\dagger a\right)a - a^\dagger aa \tag{29}$$

$$= a \tag{30}$$

$$\left[a^\dagger, a^\dagger a\right] = a^\dagger a^\dagger a - a^\dagger aa^\dagger \tag{31}$$

$$= a^\dagger a^\dagger a - a^\dagger\left(1 + a^\dagger a^\dagger a\right) \tag{32}$$

$$= -a^\dagger \tag{33}$$

Therefore we have

$$[a, H] = \hbar\omega a \tag{34}$$
$$\left[a^\dagger, H\right] = -\hbar\omega a^\dagger \tag{35}$$

Finally we get

$$\begin{aligned}
\left\langle \dot{X}(t) \right\rangle &= -\frac{i}{\hbar}\langle [X, H] \rangle && (36)\\
&= -\frac{i}{\hbar}\left\langle \left[a + a^\dagger, H\right] \right\rangle && (37)\\
&= -\frac{i}{\hbar}\hbar\omega\sqrt{\frac{\hbar}{2m\omega}}\left\langle a - a^\dagger \right\rangle && (38)\\
&= i\omega\sqrt{\frac{\hbar}{2m\omega}}\sqrt{\frac{2}{\hbar m\omega}}\frac{1}{i}\langle P(t) \rangle && (39)\\
&= -\omega\sqrt{\frac{\hbar}{2m\omega}}\sin\omega t && (40)
\end{aligned}$$

where we used 5 in the fourth line and 24 in the last line. The last line is indeed the time derivative of 19, so fortunately Ehrenfest's theorem gives the correct answer.

For the momentum, we have

$$\begin{aligned}
\left\langle \dot{P}(t) \right\rangle &= -\frac{i}{\hbar}\langle [P, H] \rangle && (41)\\
&= -\frac{i}{\hbar}\left\langle \left[a^\dagger - a, H\right] \right\rangle && (42)\\
&= -\frac{i}{\hbar}\hbar\omega\sqrt{\frac{\hbar m\omega}{2}}i\left\langle -a^\dagger - a \right\rangle && (43)\\
&= \omega\sqrt{\frac{\hbar m\omega}{2}}\sqrt{\frac{\hbar}{2m\omega}}\sqrt{\frac{2m\omega}{\hbar}}\langle -X(t) \rangle && (44)\\
&= -\omega\sqrt{\frac{\hbar m\omega}{2}}\cos\omega t && (45)
\end{aligned}$$

which is the correct derivative of 24.

PINGBACKS

Pingback: Harmonic oscillator - mixed initial state and Ehrenfest's theorem

HARMONIC OSCILLATOR - RAISING AND LOWERING OPERATORS AS FUNCTIONS OF TIME

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 7.4, Exercise 7.4.6.

Post date: 30 Jan 2017

We'll consider here the problem of finding the averages of the raising and lowering operators (from the harmonic oscillator) as functions of time, that is, we want to find $\langle a(t)\rangle$ and $\left\langle a^{\dagger}(t)\right\rangle$. At first glance we might think they are both zero, since they are defined in terms of position and momentum as

$$\begin{aligned} a^{\dagger} &= \frac{1}{\sqrt{2\hbar m\omega}}\left[-iP+m\omega X\right] && (1)\\ a &= \frac{1}{\sqrt{2\hbar m\omega}}\left[iP+m\omega X\right] && (2) \end{aligned}$$

and the averages of P and X in any of the energy eigenstates of the harmonic oscillator are all zero. However, suppose we have a mixed state $|\psi\rangle$ which can be written as a sum over the eigenstates as

$$\begin{aligned} \psi(t) &= \sum_{n=0}^{\infty} c_n e^{-iE_n t/\hbar}|n\rangle && (3)\\ &= \sum_{n=0}^{\infty} c_n e^{-i(2n+1)\omega t/2}|n\rangle && (4) \end{aligned}$$

where in the second line we used the energies of the oscillator as

$$E_n = \hbar\omega\left(n+\frac{1}{2}\right) \tag{5}$$

We now have

$$\begin{aligned}
\langle a(t)\rangle &= \langle\psi|a|\psi\rangle && (6)\\
&= \sum_{n=0}^{\infty}\sum_{m=0}^{\infty} c_m^* e^{i(2m+1)\omega t/2} c_n e^{-i(2n+1)\omega t/2} \langle m|a|n\rangle && (7)\\
&= \sum_{n=0}^{\infty}\sum_{m=0}^{\infty} c_m^* c_n e^{i(m-n)\omega t} \langle m|a|n\rangle && (8)
\end{aligned}$$

We can now use the formula

$$a|n\rangle = \sqrt{n}\,|n-1\rangle \tag{9}$$

This gives

$$\begin{aligned}
\langle a(t)\rangle &= \sum_{n=0}^{\infty}\sum_{m=0}^{\infty} c_m^* c_n e^{i(m-n)\omega t}\sqrt{n}\,\langle m|n-1\rangle && (10)\\
&= \sum_{n=0}^{\infty}\sum_{m=0}^{\infty} c_m^* c_n e^{i(m-n)\omega t}\sqrt{n}\,\delta_{m,n-1} && (11)\\
&= e^{-i\omega t}\sum_{n=0}^{\infty} c_{n-1}^* c_n \sqrt{n} && (12)\\
&= e^{-i\omega t}\langle a(0)\rangle && (13)
\end{aligned}$$

Note that if $|\psi\rangle$ is an eigenstate, then only one of the coefficients c_n is non-zero, so $\langle a(0)\rangle = 0$ as we'd expect.

The derivation for $\left\langle a^\dagger(t)\right\rangle$ is similar:

$$\begin{aligned}
\left\langle a^\dagger(t)\right\rangle &= \left\langle\psi\left|a^\dagger\right|\psi\right\rangle && (14)\\
&= \sum_{n=0}^{\infty}\sum_{m=0}^{\infty} c_m^* e^{i(2m+1)\omega t/2} c_n e^{-i(2n+1)\omega t/2}\left\langle m\left|a^\dagger\right|n\right\rangle && (15)\\
&= \sum_{n=0}^{\infty}\sum_{m=0}^{\infty} c_m^* c_n e^{i(m-n)\omega t}\left\langle m\left|a^\dagger\right|n\right\rangle && (16)
\end{aligned}$$

We can now use the formula

$$a^\dagger|n\rangle = \sqrt{n+1}\,|n+1\rangle \tag{17}$$

This gives

$$\left\langle a^{\dagger}(t)\right\rangle = \sum_{n=0}^{\infty}\sum_{m=0}^{\infty} c_m^* c_n e^{i(m-n)\omega t}\sqrt{n+1}\,\langle m\,|n+1\,\rangle \tag{18}$$

$$= \sum_{n=0}^{\infty}\sum_{m=0}^{\infty} c_m^* c_n e^{i(m-n)\omega t}\sqrt{n+1}\,\delta_{m,n+1} \tag{19}$$

$$= e^{i\omega t}\sum_{n=0}^{\infty} c_{n+1}^* c_n\sqrt{n+1} \tag{20}$$

$$= e^{i\omega t}\left\langle a^{\dagger}(0)\right\rangle \tag{21}$$

POISSON BRACKETS TO COMMUTATORS: CLASSICAL TO QUANTUM

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Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 7.4, Exercise 7.4.7.

Post date: 31 Jan 2017

The postulates of quantum mechanics that we described earlierincluded specifications for the matrix elements of position X and momentum P in position space:

$$\begin{aligned} \left\langle x\left|X\right|x'\right\rangle &= x\delta\left(x-x'\right) && (1)\\ \left\langle x\left|P\right|x'\right\rangle &= -i\hbar\delta'\left(x-x'\right) && (2) \end{aligned}$$

A more fundamental form of this postulate is to specify the commutation relation between X and P, which is independent of the basis and is

$$[X,P]=i\hbar \tag{3}$$

This allows the construction of explicit forms of the operators in other bases, such as the momentum basis, where

$$\begin{aligned} X &= i\hbar\frac{d}{dp} && (4)\\ P &= p && (5) \end{aligned}$$

We can verify this by calculating the commutator by applying it to a function $f\left(p\right)$:

$$\begin{aligned} [X,P]\,f &= i\hbar\frac{d}{dp}\left(pf\left(p\right)\right)-i\hbar p\frac{d}{dp}f\left(p\right) && (6)\\ &= i\hbar f\left(p\right)+i\hbar p\frac{d}{dp}f\left(p\right)-i\hbar p\frac{d}{dp}f\left(p\right) && (7)\\ &= i\hbar f\left(p\right) && (8) \end{aligned}$$

Thus 3 is satisfied in the momentum basis as well.

The standard recipe for converting a classical system to a quantum one is to first calculate the Poisson bracketfor two physical quantities in the classical system, which gives

$$\{\omega,\lambda\} = \sum_i \left(\frac{\partial\omega}{\partial q_i}\frac{\partial\lambda}{\partial p_i} - \frac{\partial\omega}{\partial p_i}\frac{\partial\lambda}{\partial q_i} \right) \tag{9}$$

where q_i and p_i are the canonical coordinates and momenta. To convert to a quantum commutator, we replace the classical quantities by their quantum operator equivalents and the Poisson bracket by $i\hbar$ times the corresponding commutator. That is

$$[\Omega,\Lambda] = i\hbar\{\omega,\lambda\} \tag{10}$$

For the case of X and P, we have, in classical mechanics in one dimension

$$\{x,p\} = \frac{\partial x}{\partial x}\frac{\partial p}{\partial p} - \frac{\partial x}{\partial p}\frac{\partial p}{\partial x} = 1 \tag{11}$$

so the quantum commutator is given by 3.

For other quantities, we can use the theorems on the Poisson bracketsto reduce them:

$$\begin{aligned} \{\omega,\lambda\} &= -\{\lambda,\omega\} && (12)\\ \{\omega,\lambda+\sigma\} &= \{\omega,\lambda\}+\{\omega,\sigma\} && (13)\\ \{\omega,\lambda\sigma\} &= \{\omega,\lambda\}\sigma+\{\omega,\sigma\}\lambda && (14) \end{aligned}$$

Quantum commutators obey similar rules

$$\begin{aligned} [\Omega,\Lambda] &= -[\Lambda,\Omega] && (15)\\ [\Omega,\Lambda+\Gamma] &= [\Omega,\Lambda]+[\Omega,\Gamma] && (16)\\ [\Omega\Lambda,\Gamma] &= \Omega[\Lambda,\Gamma]+[\Omega,\Gamma]\Lambda && (17) \end{aligned}$$

The main difference between Poisson brackets and commutators is that, for the latter, the order of the operators in the last equation can make a difference. That is, in 14 we could also have written

$$\{\omega,\lambda\sigma\} = \sigma\{\omega,\lambda\}+\lambda\{\omega,\sigma\} \tag{18}$$

since all three quantities are numerical (not operators), so multiplication commutes. In 17 it is *not* true in general that, for example

$$\Omega[\Lambda,\Gamma]+[\Omega,\Gamma]\Lambda = [\Lambda,\Gamma]\Omega+[\Omega,\Gamma]\Lambda \tag{19}$$

The conversion from classical to quantum mechanics can then be achieved in general by replacing

$$\{\omega(x,p),\lambda(x,p)\} = \gamma(x,p) \tag{20}$$

by

$$[\mathbf{\Omega}(X,P),\mathbf{\Lambda}(X,P)] = i\hbar\mathbf{\Gamma}(X,P) \tag{21}$$

where each of the operators in the last equation is obtained by replacing x in the first equation by X and p by P. We do need to be careful with the ordering of the operators in the quantum version, however.

As an example, suppose we have

$$\begin{aligned} \mathbf{\Omega} &= X & (22)\\ \mathbf{\Lambda} &= X^2+P^2 & (23) \end{aligned}$$

In the classical version, we calculate the Poisson bracket

$$\begin{aligned} \{\omega,\lambda\} &= \left\{x,x^2+p^2\right\} & (24)\\ &= \left\{x,x^2\right\}+\left\{x,p^2\right\} & (25)\\ &= 0+2\{x,p\}p & (26)\\ &= 2p & (27) \end{aligned}$$

Thus, by our rule above, the quantum version should be

$$[\mathbf{\Omega},\mathbf{\Lambda}] = 2i\hbar P \tag{28}$$

We can verify this using 17

$$\begin{aligned} \left[X,X^2+P^2\right] &= \left[X,X^2\right]+\left[X,P^2\right] & (29)\\ &= 0-\left[P^2,X\right] & (30)\\ &= -P[P,X]-[P,X]P & (31)\\ &= -P(-i\hbar)-(-i\hbar)P & (32)\\ &= 2i\hbar P & (33) \end{aligned}$$

In this case, there is no ordering ambiguity in the quantum version, since $[X,P]=i\hbar$ is just a number.

For a second example, suppose we have

$$\begin{aligned} \mathbf{\Omega} &= X^2 & (34)\\ \mathbf{\Lambda} &= P^2 & (35) \end{aligned}$$

The classical version gives us, using the relations 14, 11 and 27

$$\begin{aligned}\left\{x^2,p^2\right\} &= -\left\{p^2,x^2\right\} && (36)\\ &= -2\left\{p^2,x\right\}x && (37)\\ &= 2\left\{x,p^2\right\}x && (38)\\ &= 4px && (39)\end{aligned}$$

In the classical case, this result is the same as $4xp$, but because X and P don't commute in the quantum form, we need to be careful about the ordering.

We can do the calculation:

$$\left[X^2,P^2\right] = X\left[X,P^2\right] + \left[X,P^2\right]X \tag{40}$$

From 33 we have

$$\left[X,P^2\right] = 2i\hbar P \tag{41}$$

so we get

$$\left[X^2,P^2\right] = 2i\hbar\left(XP+PX\right) \tag{42}$$

Thus if the Poisson bracket involves a product of p and x, this should be replaced by

$$xp \text{ or } px \rightarrow \frac{1}{2}\left(XP+PX\right) \tag{43}$$

in the quantum version.

PINGBACKS

Pingback: Angular momentum - Poisson bracket to commutator

Pingback: Hamiltonian in non-rectangular coordinates

Pingback: Harmonic oscillator: momentum space functions and Hermite polynomial recursion

Pingback: Direct product of two vector spaces

Pingback: Nonrelativistic field theory - Schrödinger equation

ANGULAR MOMENTUM - POISSON BRACKET TO COMMUTATOR

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Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 7.4, Exercise 7.4.8.

Post date: 31 Jan 2017

The classical angular momentum components are

$$\ell_x = yp_z - zp_y \tag{1}$$
$$\ell_y = zp_x - xp_z \tag{2}$$
$$\ell_z = xp_y - yp_x \tag{3}$$

In the position basis, we can replace each coordinate by its quantum operator $x \to X$, $y \to Y$ and $z \to Z$, and each momentum component by the derivative $p_i \to -i\hbar\partial/\partial q_i$, where q_i is the ith coordinate. This gives

$$L_x = -i\hbar\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right) \tag{4}$$
$$L_y = -i\hbar\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right) \tag{5}$$
$$L_z = -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) \tag{6}$$

Because coordinates always commute with momentum components of other coordinates (x commutes with p_y and p_z, etc), there is no ordering ambiguity in making the transition from classical to quantum mechanics. That is, we could place the coordinate on either side of the momentum in each term for all components L_i.

Classically, we can calculate the Poisson brackets for the angular momentum components. For example

$$\{\ell_x, \ell_y\} = \sum_i \left(\frac{\partial \ell_x}{\partial q_i} \frac{\partial \ell_y}{\partial p_i} - \frac{\partial \ell_x}{\partial p_i} \frac{\partial \ell_y}{\partial q_i} \right) \tag{7}$$

$$= -p_y (-x) - y p_z \tag{8}$$

$$= x p_y - y p_z \tag{9}$$

$$= \ell_z \tag{10}$$

According to the rule for converting classical Poisson brackets to quantum commutators, we should get (since there is no ordering ambiguity)

$$[L_x, L_y] = i\hbar L_z \tag{11}$$

As we've seen earlier, this is verified by direct calculation using the position-momentum commutator

$$[q_i, p_j] = i\hbar \delta_{ij} \tag{12}$$

CHANGING THE POSITION BASIS WITH A UNITARY TRANSFORMATION

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Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 7.4, Exercise 7.4.9.

Post date: 30 Jan 2017

The standard representation of the position and momentum operators in the position basis is

$$X \rightarrow x \tag{1}$$

$$P \rightarrow -i\hbar\frac{d}{dx} \tag{2}$$

It turns out it's possible to modify this definition by adding some arbitrary function of position $f(x)$ to P so we have

$$X' \rightarrow x \tag{3}$$

$$P' \rightarrow -i\hbar\frac{d}{dx} + f(x) \tag{4}$$

Since any function of x commutes with X, the commutation relations remain unchanged, so we have

$$\left[X', P'\right] = i\hbar \tag{5}$$

Another way of interpreting this change in operators is by using the unitary transformation of the X basis, in the form

$$|x\rangle \rightarrow |\tilde{x}\rangle = e^{ig(X)/\hbar}|x\rangle = e^{ig(x)/\hbar}|x\rangle \tag{6}$$

where

$$g(x) \equiv \int^{x} f\left(x'\right) dx' \tag{7}$$

The last equality in 6 comes from the fact that operating on $|x\rangle$ with any function of the X operator (provided the function can be expanded in a power series) results in multiplying $|x\rangle$ by the same function, but with the operator X replaced by the numeric position value.

To verify this works, we can calcuate the matrix elements of the old X and P operators in the new basis. We have

$$\left\langle \tilde{x} \left| X \right| \tilde{x}' \right\rangle = \left\langle x \left| e^{-ig(x)/\hbar} X e^{ig(x')/\hbar} \right| x' \right\rangle \tag{8}$$

At this stage, since the two exponentials are numerical functions and not operators, we can take them outside the bracket to

$$\begin{aligned} \left\langle \tilde{x} \left| X \right| \tilde{x}' \right\rangle &= e^{-ig(x)/\hbar} e^{ig(x')/\hbar} \left\langle x \left| X \right| x' \right\rangle && (9) \\ &= e^{-ig(x)/\hbar} e^{ig(x')/\hbar} x' \delta\left(x - x'\right) && (10) \\ &= x\delta\left(x - x'\right) && (11) \end{aligned}$$

The exponentials cancel in the last line since the delta function is non-zero only when $x = x'$.

The above result can also be obtained by inserting a couple of identity operators into 8:

$$\begin{aligned} \left\langle x \left| e^{-ig(x)/\hbar} X e^{ig(x')/\hbar} \right| x' \right\rangle &= \int\int \left\langle x \left| e^{-ig(x)/\hbar} \right| y \right\rangle \left\langle y \left| X \right| z \right\rangle \left\langle z \left| e^{ig(x')/\hbar} \right| x' \right\rangle dy\, dz && (12) \\ &= \int\int \left\langle x \left| e^{-ig(x)/\hbar} \right| y \right\rangle z\delta\left(y - z\right) \left\langle z \left| e^{ig(x')/\hbar} \right| x' \right\rangle dy\, dz && (13) \\ &= \int \left\langle x \left| e^{-ig(x)/\hbar} \right| z \right\rangle z \left\langle z \left| e^{ig(x')/\hbar} \right| x' \right\rangle dz && (14) \\ &= \int e^{i[g(x') - g(x)]/\hbar} \left\langle x \left| z \right\rangle z \left\langle z \left| x' \right\rangle dz \right. && (15) \\ &= \int e^{i[g(x') - g(x)]/\hbar} \delta\left(x - z\right) z\delta\left(z - x'\right) dz && (16) \\ &= e^{i[g(x') - g(x)]/\hbar} x' \delta\left(x - x'\right) && (17) \\ &= x\delta\left(x - x'\right) && (18) \end{aligned}$$

The momentum operator works as follows. Using the original definition 2 on the modified basis we have

$$\left\langle \tilde{x} \left| P \right| \tilde{x}' \right\rangle = -i\hbar \left\langle x \left| e^{-ig(x)/\hbar} \frac{d}{dx'} e^{ig(x')/\hbar} \right| x' \right\rangle \tag{19}$$

$$= -i\hbar \left\langle x \left| e^{-ig(x)/\hbar} \frac{i}{\hbar} e^{ig(x')/\hbar} \frac{dg\left(x'\right)}{dx'} \right| x' \right\rangle - \tag{20}$$

$$i\hbar \left\langle x \left| e^{-ig(x)/\hbar} e^{ig(x')/\hbar} \frac{d}{dx'} \right| x' \right\rangle \tag{21}$$

From 7 we have

$$\frac{dg\left(x\right)}{dx} = \frac{d}{dx} \int^{x} f\left(x'\right) dx' = f\left(x\right) \tag{22}$$

This gives

$$\left\langle \tilde{x} \left| P \right| \tilde{x}' \right\rangle = \left\langle x \left| e^{i[g(x')-g(x)]/\hbar} \left[f\left(x'\right) - i\hbar \frac{d}{dx'} \right] \right| x' \right\rangle \tag{23}$$

$$= e^{i[g(x')-g(x)]/\hbar} \left[f\left(x'\right) - i\hbar \frac{d}{dx'} \right] \left\langle x \left| x' \right. \right\rangle \tag{24}$$

$$= e^{i[g(x')-g(x)]/\hbar} \left[f\left(x'\right) - i\hbar \frac{d}{dx'} \right] \delta\left(x - x'\right) \tag{25}$$

$$= \left[f\left(x\right) - i\hbar \frac{d}{dx} \right] \delta\left(x - x'\right) \tag{26}$$

This shows that by a unitary change of X basis 6, we transform the position and momentum operators (well, just the momentum operator, really) according to 3. We've multiplied the original $|x\rangle$ states by a phase factor which depends on some function $f\left(x\right)$. This doesn't change the matrix elements of X, but it does add $f\left(x\right)$ to the matrix elements of P. The commonly used definition of P is thus with $f\left(x\right) = 0$.

HAMILTONIAN IN NON-RECTANGULAR COORDINATES

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To leave a comment or report an error, please use the auxiliary blog.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 7.4, Exercise 7.4.10.

Post date: 1 Feb 2017

The standard procedure for quantizing a classical hamiltonian is to write the classical hamiltonian in terms of position and momentum variables in rectangular coordinates and then convert the position and momentum variables to operators satisfying the usual commutation relations. However, in some cases, another coordinate system makes solving the differential equation resulting from the Schrödinger equation easier (as, for example, with the hydrogen atom, where the system has spherical symmetry).

As a 2-d example, suppose we have the classical hamiltonian

$$H = \frac{p_x^2 + p_y^2}{2m} + a\sqrt{x^2+y^2} \tag{1}$$

for some constant a. Since the system has radial symmetry, polar coordinates should make things easier. That is, we'd like to transform to

$$\begin{aligned} \rho &= \sqrt{x^2+y^2} && (2)\\ \phi &= \arctan\frac{y}{x} && (3) \end{aligned}$$

In the rectangular position basis, the quantized operators are

$$\begin{aligned} P_x &= -i\hbar\frac{\partial}{\partial x} && (4)\\ P_y &= -i\hbar\frac{\partial}{\partial y} && (5)\\ X &= x && (6)\\ Y &= y && (7) \end{aligned}$$

so the quantum hamiltonian is

$$H = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) + a\sqrt{x^2+y^2} \tag{8}$$

The first term contains the Laplacian derivative operator, which can be written in polar coordinates as

$$\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}=\frac{\partial^2}{\partial \rho^2}+\frac{1}{\rho}\frac{\partial}{\partial \rho}+\frac{1}{\rho^2}\frac{\partial^2}{\partial \phi^2} \tag{9}$$

Thus the quantum hamiltonian in polar coordinates is

$$H=-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial \rho^2}+\frac{1}{\rho}\frac{\partial}{\partial \rho}+\frac{1}{\rho^2}\frac{\partial^2}{\partial \phi^2}\right)+a\rho \tag{10}$$

The question is: can we instead convert the hamiltonian 1 to polar coordinates and then quantize the result, rather than converting the rectangular coordinates after the hamiltonian is written? The answer turns out to be surprisingly complicated, and I'm not sure I follow everything Shankar says, but here's the argument anyway. Comments, as usual, are welcome.

We first convert the rectangular momentum coordinates to polar momentum coordinates by means of the substitutions

$$p_\rho = \hat{\mathbf{r}}\cdot\mathbf{p}=\frac{xp_x+yp_y}{\sqrt{x^2+y^2}} \tag{11}$$

$$p_\phi=\ell_z = xp_y-yp_x \tag{12}$$

Note that the two components of polar momentum have different units: p_ρ has the dimensions of linear momentum while p_ϕ is actually the angular momentum about the z axis ℓ_z. In terms of these new momenta, the classical hamiltonian 1 becomes

$$H=\frac{p_\rho^2}{2m}+\frac{p_\phi^2}{2m\rho^2}+a\rho \tag{13}$$

This can be verified either by inverting equations 11 and 12 to get p_x and p_y in terms of p_ρ and p_ϕ and then plugging these into 1 (very messy), or else just starting with 13 and showing it reduces to 1. We'll do the latter.

$$p_\rho^2+\frac{p_\phi^2}{\rho^2}=\left[\frac{xp_x+yp_y}{\sqrt{x^2+y^2}}\right]^2+\frac{(xp_y-yp_x)^2}{x^2+y^2} \tag{14}$$

$$=\frac{1}{\rho^2}\left(x^2p_x^2+y^2p_y^2+2xyp_xp_y+x^2p_y^2+y^2p_x^2-2xyp_xp_y\right) \tag{15}$$

$$=\frac{1}{\rho^2}\left(x^2+y^2\right)\left(p_x^2+p_y^2\right) \tag{16}$$

$$=p_x^2+p_y^2 \tag{17}$$

We can now try quantizing 13 by creating a couple of quantum momentum operators according to the standard rule:

$$P_\rho = -i\hbar\frac{\partial}{\partial\rho} \tag{18}$$

$$P_\phi = -i\hbar\frac{\partial}{\partial\phi} \tag{19}$$

These operators satisfy the usual commutation rule, in the sense that

$$[\rho, P_\rho] = \left[\phi, P_\phi\right] = i\hbar \tag{20}$$

However, substituting them into 13 gives

$$H = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial\rho^2} + \frac{1}{\rho^2}\frac{\partial^2}{\partial\phi^2}\right) + a\rho \tag{21}$$

Comparing with 10 we see that the middle term with the first order derivative is missing. The problem is due to the fact that 18 is actually not a hermitian operator, which we can see by calculating the bracket as follows:

$$\langle\psi_1|P_\rho|\psi_2\rangle = -i\hbar\int_0^{2\pi}\int_0^\infty \psi_1^*\frac{\partial\psi_2}{\partial\rho}\rho\, d\rho\, d\phi \tag{22}$$

We can do the ρ integral by parts and, assuming that $\rho\psi_1^*\psi_2 \to 0$ at both $\rho \to 0$ and $\rho \to \infty$, we have

$$\int_0^\infty \psi_1^*\frac{\partial\psi_2}{\partial\rho}\rho\, d\rho = \rho\psi_1^*\psi_2|_0^\infty - \int_0^\infty \psi_2\frac{\partial\left(\rho\psi_1^*\right)}{\partial\rho}\, d\rho \tag{23}$$

$$= -\int_0^\infty \psi_2\frac{\partial\psi_1^*}{\partial\rho}\rho\, d\rho - \int_0^\infty \psi_1^*\psi_2 d\rho \tag{24}$$

Substituting back into 22 we get

$$\langle\psi_1|P_\rho|\psi_2\rangle = i\hbar\int_0^{2\pi}\int_0^\infty\left[\psi_2\frac{\partial\psi_1^*}{\partial\rho}\rho + \psi_1^*\psi_2\right]d\rho\, d\phi \tag{25}$$

If P_ρ is to be hermitian, we need to satisfy

$$\langle\psi_1|P_\rho|\psi_2\rangle = \langle P_\rho\psi_1|\psi_2\rangle \tag{26}$$

$$= i\hbar\int_0^{2\pi}\int_0^\infty \psi_2\frac{\partial\psi_1^*}{\partial\rho}\rho\, d\rho\, d\phi \tag{27}$$

We can see that the presence of the second term in the integrand of 25 messes things up. This term arises from the presence of the extra factor of ρ that is present in a polar area integral.

We can, in fact, attempt to fix this by defining the radial momentum operator to be, instead of 18:

$$P_\rho = -i\hbar\left(\frac{\partial}{\partial\rho}+\frac{1}{2\rho}\right) \tag{28}$$

We first verify that this is hermitian:

$$\langle\psi_1|P_\rho|\psi_2\rangle = -i\hbar\int_0^{2\pi}\int_0^\infty \psi_1^*\left[\frac{\partial\psi_2}{\partial\rho}\rho+\frac{\psi_2}{2}\right]\,d\rho\,d\phi \tag{29}$$

$$= i\hbar\int_0^{2\pi}\int_0^\infty \left[\psi_2\frac{\partial\psi_1^*}{\partial\rho}\rho+\psi_1^*\psi_2-\frac{1}{2}\psi_1^*\psi_2\right]d\rho\,d\phi \tag{30}$$

$$= i\hbar\int_0^{2\pi}\int_0^\infty \left[\psi_2\frac{\partial\psi_1^*}{\partial\rho}\rho+\frac{1}{2}\psi_1^*\psi_2\right]d\rho\,d\phi \tag{31}$$

$$= \langle P_\rho\psi_1|\psi_2\rangle \tag{32}$$

In the second line we did the same integration by parts on the first term and used the result in 24. Thus this new P_ρ is indeed hermitian. If we now insert this along with the old P_ϕ from 19 into 13 we get

$$H = -\frac{\hbar^2}{2m}\left(\frac{\partial}{\partial\rho}+\frac{1}{2\rho}\right)^2+a\rho \tag{33}$$

To work out the differential part of the hamiltonian we can apply it to a test function.

$$\left(\frac{\partial}{\partial\rho}+\frac{1}{2\rho}\right)^2\psi = \left(\frac{\partial}{\partial\rho}+\frac{1}{2\rho}\right)\left(\frac{\partial\psi}{\partial\rho}+\frac{\psi}{2\rho}\right) \tag{34}$$

$$= \frac{\partial^2\psi}{\partial\rho^2}+\frac{1}{2\rho}\frac{\partial\psi}{\partial\rho}-\frac{\psi}{2\rho^2}+\frac{1}{2\rho}\frac{\partial\psi}{\partial\rho}+\frac{\psi}{4\rho^2} \tag{35}$$

$$= \frac{\partial^2\psi}{\partial\rho^2}+\frac{1}{\rho}\frac{\partial\psi}{\partial\rho}-\frac{\psi}{4\rho^2} \tag{36}$$

The hamiltonian then becomes

$$H = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial\rho^2}+\frac{1}{\rho}\frac{\partial}{\partial\rho}-\frac{1}{4\rho^2}+\frac{1}{\rho^2}\frac{\partial^2}{\partial\phi^2}\right)+a\rho \tag{37}$$

Comparing this with 10 we see that now we have an extra term $-\frac{1}{4\rho^2}$. Shankar doesn't really explain in detail what the problem is, except to state that when converting from a classical to a quantum hamiltonian, terms of order $\hbar$ or higher may be present in the quantum version that are absent in the classical version. Presumably he means terms of order $\hbar$ that don't involve

derivatives, since the entire momentum-dependent part of the hamiltonian is multiplied by a factor of $\hbar^2$. In any case, we'll have to leave it at that.

HARMONIC OSCILLATOR: MOMENTUM SPACE FUNCTIONS AND HERMITE POLYNOMIAL RECURSION RELATIONS FROM RAISING AND LOWERING OPERATORS

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 7.5, Exercises 7.5.1 - 7.5.3.

Post date: 3 Feb 2017

Earlier, we found the position space energy eigenfunctions of the harmonic oscillator to be

$$\psi_n(y) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} H_n(y) e^{-y^2/2} \tag{1}$$

$$\psi_n(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right) e^{-m\omega x^2/2\hbar} \tag{2}$$

where y in the first equation is shorthand for

$$y = \sqrt{\frac{m\omega}{\hbar}}x \tag{3}$$

It turns out that an alternative method for deriving these functions uses the lowering operator a. Shankar gives the derivation of $\psi_n(x)$ in his section 7.5, but we can use the same technique to derive the momentum space functions. We start with the ground state and use

$$a|0\rangle = 0 \tag{4}$$

In terms of X and P, we have

$$a = \sqrt{\frac{m\omega}{2\hbar}}X + i\frac{1}{\sqrt{2m\omega\hbar}}P \tag{5}$$

To find the momentum space functions, we need to express X and P in terms of p:

$$X = i\hbar\frac{d}{dp} \tag{6}$$

$$P = p \tag{7}$$

We thus have

$$\left[i\hbar\sqrt{\frac{m\omega}{2\hbar}}\frac{d}{dp}+i\frac{1}{\sqrt{2m\omega\hbar}}p\right]\psi_0(p)=0 \tag{8}$$

If we define the auxiliary variable

$$z\equiv\frac{p}{\sqrt{\hbar m\omega}} \tag{9}$$

we get

$$\left(\frac{d}{dz}+z\right)\psi_0(z)=0 \tag{10}$$

This has the solution

$$\psi_0(z)=Ae^{-z^2/2} \tag{11}$$

for some normalization constant A. Thus in terms of p we have

$$\psi_0(p)=Ae^{-p^2/2\hbar m\omega} \tag{12}$$

Normalizing in the usual way, making use of the Gaussian integral, we have

$$\int_{-\infty}^{\infty}\psi_0^2(p)\,dp = A^2\int_{-\infty}^{\infty}e^{-p^2/\hbar m\omega}dp=1 \tag{13}$$

$$A = \frac{1}{(\pi\hbar m\omega)^{1/4}} \tag{14}$$

This agrees with the earlier result which was obtained by solving a second-order differential equation.

We can also use a and $a^\dagger$ to verify a couple of recursion relations for Hermite polynomials. Reverting back to position space we have

$$X = x \tag{15}$$

$$P = -i\hbar\frac{d}{dx} \tag{16}$$

so 5 becomes

$$a=\sqrt{\frac{m\omega}{2\hbar}}x+\frac{\hbar}{\sqrt{2m\omega\hbar}}\frac{d}{dx} \tag{17}$$

Also from 5 we have, since X and P are both hermitian operators

$$a^\dagger = \sqrt{\frac{m\omega}{2\hbar}}X - i\frac{1}{\sqrt{2m\omega\hbar}}P \tag{18}$$

$$= \sqrt{\frac{m\omega}{2\hbar}}x - \frac{\hbar}{\sqrt{2m\omega\hbar}}\frac{d}{dx} \tag{19}$$

Defining

$$y \equiv \sqrt{\frac{m\omega}{\hbar}}x \tag{20}$$

we have

$$a = \frac{1}{\sqrt{2}}\left(y + \frac{d}{dy}\right) \tag{21}$$

$$a^\dagger = \frac{1}{\sqrt{2}}\left(y - \frac{d}{dy}\right) \tag{22}$$

We also recall the normalization conditions on the raising and lowering operators:

$$a\,|n\rangle = \sqrt{n}\,|n-1\rangle \tag{23}$$

$$a^\dagger\,|n\rangle = \sqrt{n+1}\,|n+1\rangle \tag{24}$$

Applying 23 to 1 we have, after cancelling common factors from each side:

$$\frac{1}{\sqrt{2}}\frac{1}{\sqrt{2^n n!}}\left(y + \frac{d}{dy}\right)\left[H_n(y)e^{-y^2/2}\right] = \frac{\sqrt{n}}{\sqrt{2^{n-1}(n-1)!}}H_{n-1}(y)\,e^{-y^2/2} \tag{25}$$

$$\frac{1}{2\sqrt{n}}\frac{1}{\sqrt{2^{n-1}(n-1)!}}e^{-y^2/2}\left[yH_n(y) - yH_n(y) + \frac{dH_n}{dy}\right] = \frac{\sqrt{n}}{\sqrt{2^{n-1}(n-1)!}}H_{n-1}(y)\,e^{-y^2/2} \tag{26}$$

$$yH_n(y) - yH_n(y) + \frac{dH_n}{dy} = 2nH_{n-1}(y) \tag{27}$$

$$H_n'(y) = 2nH_{n-1}(y) \tag{28}$$

Another recursion relation for Hermite polynomials can be found as follows. We start with 22 to get

$$a + a^\dagger = \sqrt{2}y \tag{29}$$

We now apply 23 and 24 to 1. We can cancel common factors, including $e^{-y^2/2}$, from both sides to get

$$\left(a + a^\dagger\right)\psi_n = \sqrt{2}y\psi_n \tag{30}$$

$$\frac{\sqrt{2}y}{\sqrt{2^n n!}}H_n(y) = \frac{\sqrt{n}}{\sqrt{2^{n-1}\,(n-1)!}}H_{n-1}(y) + \frac{\sqrt{n+1}}{\sqrt{2^{n+1}\,(n+1)!}}H_{n+1}(y) \tag{31}$$

$$\frac{y}{\sqrt{2^{n-1}n\,(n-1)!}}H_n(y) = \frac{\sqrt{n}}{\sqrt{2^{n-1}\,(n-1)!}}H_{n-1}(y) + \frac{1}{2\sqrt{2^{n-1}n\,(n-1)!}}H_{n+1}(y) \tag{32}$$

$$yH_n\,(y) = nH_{n-1}\,(y) + \frac{1}{2}H_{n+1}\,(y) \tag{33}$$

$$H_{n+1}\,(y) = 2yH_n\,(y) - 2nH_{n-1}\,(y) \tag{34}$$

THERMODYNAMICS OF HARMONIC OSCILLATORS - CLASSICAL AND QUANTUM

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 7.5, Exercise 7.5.4.

Post date: 4 Feb 2017

One application of harmonic oscillator theory is in the behaviour of crystals as a function of temperature. A reasonable model of a crystal is of a number of atoms that vibrate as harmonic oscillators. From statistical mechanics, the probability $P(i)$ of finding a system in a state i is given by the Boltzmann formula

$$P(i) = \frac{e^{-\beta E(i)}}{Z} \tag{1}$$

where $\beta = 1/kT$, with k being Boltzmann's constant and T the absolute temperature, and Z is the partition function

$$Z = \sum_i e^{-\beta E(i)} \tag{2}$$

The thermal average energy of the system is then

$$\begin{aligned} \bar{E} &= \sum_i E(i) P(i) && (3) \\ &= \frac{\sum_i E(i) e^{-\beta E(i)}}{Z} && (4) \\ &= -\frac{\partial (\ln Z)}{\partial \beta} && (5) \end{aligned}$$

For a classical harmonic oscillator, the energy is a continuous function of the position x and momentum p:

$$E_{cl} = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 x^2 \tag{6}$$

The classical partition function is then

$$Z_{cl} = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{-\beta p^2/2m} e^{-\beta m\omega^2 x^2/2} dp\, dx \tag{7}$$

$$= \int_{-\infty}^{\infty} e^{-\beta p^2/2m} dp \int_{-\infty}^{\infty} e^{-\beta m\omega^2 x^2/2} dx \tag{8}$$

$$= \sqrt{\frac{2\pi m}{\beta}}\sqrt{\frac{2\pi}{\beta m\omega^2}} \tag{9}$$

$$= \frac{2\pi}{\omega\beta} \tag{10}$$

Where we used the standard formula for Gaussian integrals to get the third line. The average classical energy is, from 5

$$\bar{E}_{cl} = -\frac{\partial\left(\ln Z_{cl}\right)}{\partial\beta} = \frac{1}{\beta} = kT \tag{11}$$

The average energy of a classical oscillator thus depends only on the temperature, and not on the frequency ω.

For a quantum oscillator, the energies are quantized with values of

$$E\left(n\right) = \hbar\omega\left(n + \frac{1}{2}\right) \tag{12}$$

The quantum partition function is therefore

$$Z_{qu} = e^{-\beta\hbar\omega/2}\sum_{n=0}^{\infty} e^{-\beta\hbar\omega n} \tag{13}$$

The sum is a geometric series, so we can use the standard result for $|x| < 1$:

$$\sum_{n=0}^{\infty} x^n = \frac{1}{1-x} \tag{14}$$

This gives

$$Z_{qu} = \frac{e^{-\beta\hbar\omega/2}}{1 - e^{-\beta\hbar\omega}} \tag{15}$$

The mean quantum energy is again found from 5, although this time the derivative is a bit messier, so is most easily done using Maple. However, by hand, you'd get

$$\bar{E}_{qu} = -\frac{\partial(\ln Z_{qu})}{\partial\beta} \tag{16}$$

$$= \frac{1-e^{-\beta\hbar\omega}}{e^{-\beta\hbar\omega/2}}\left[-\frac{1}{2}\frac{\hbar\omega e^{-\beta\hbar\omega/2}}{1-e^{-\beta\hbar\omega}} - \frac{\hbar\omega e^{-\beta\hbar\omega/2}e^{-\beta\hbar\omega}}{\left(1-e^{-\beta\hbar\omega}\right)^2}\right] \tag{17}$$

$$= \frac{\hbar\omega}{2}\left(\frac{1+e^{-\beta\hbar\omega}}{1-e^{-\beta\hbar\omega}}\right) \tag{18}$$

$$= \frac{\hbar\omega}{2}\left(\frac{1-e^{-\beta\hbar\omega}+2e^{-\beta\hbar\omega}}{1-e^{-\beta\hbar\omega}}\right) \tag{19}$$

$$= \hbar\omega\left(\frac{1}{2}+\frac{1}{e^{\beta\hbar\omega}-1}\right) \tag{20}$$

The average energy is the ground state energy $\hbar\omega/2$ plus a quantity that increases with increasing temperature (decreasing β). For small β we have

$$\bar{E}_{qu} \rightarrow \hbar\omega\left(\frac{1}{2}+\frac{1}{1+\beta\hbar\omega-1}\right) \tag{21}$$

$$= \frac{\hbar\omega}{2}+\frac{1}{\beta} \tag{22}$$

$$\rightarrow kT \tag{23}$$

since as $\beta \rightarrow 0$, $\frac{1}{\beta} \gg \frac{\hbar\omega}{2}$. Thus the quantum energy reduces to the classical energy 11 for high temperatures. The 'high temperature' condition is that

$$\frac{1}{\beta} \gg \frac{\hbar\omega}{2} \tag{24}$$

$$T \gg \frac{\hbar\omega}{2k} \tag{25}$$

So far, we've considered the average behaviour of only one oscillator. Suppose we now have a 3-d crystal with N_0 atoms. Assuming small oscillations we can approximate its behaviour by a system of $3N_0$ decoupled oscillators. In the classical case, the average energy is found from 11:

$$\bar{\mathcal{E}}_{cl} = 3N_0\bar{E}_{cl} = 3N_0kT \tag{26}$$

The heat capacity per atom is the amount of heat (energy) ΔE required to raise the temperature by ΔT, so

$$C_{cl} = \frac{1}{N_0}\frac{\partial \bar{\mathcal{E}}_{cl}}{\partial T} = 3k \tag{27}$$

For the quantum system, we have from 20

$$\begin{aligned} \bar{\mathcal{E}}_{qu} &= 3N_0 \bar{E}_{qu} && (28)\\ &= 3N_0\hbar\omega\left(\frac{1}{2} + \frac{1}{e^{\beta\hbar\omega}-1}\right) && (29)\end{aligned}$$

The quantum heat capacity is therefore

$$\begin{aligned} C_{qu} &= \frac{1}{N_0}\frac{\partial \bar{\mathcal{E}}_{qu}}{\partial T} && (30)\\ &= 3\hbar\omega\frac{\partial}{\partial\beta}\left(\frac{1}{e^{\beta\hbar\omega}-1}\right)\frac{d\beta}{dT} && (31)\\ &= 3\frac{\hbar^2\omega^2}{kT^2}\frac{e^{\hbar\omega/kT}}{\left(e^{\beta\hbar\omega}-1\right)^2} && (32)\end{aligned}$$

We can define the *Einstein temperature* as

$$\theta_E \equiv \frac{\hbar\omega}{k} \tag{33}$$

which gives the heat capacity as

$$C_{qu} = 3k\frac{\theta_E^2}{T^2}\frac{e^{\theta_E/T}}{\left(e^{\theta_E/T}-1\right)^2} \tag{34}$$

For large temperatures, the exponent θ_E/T becomes small, so we have

$$\begin{aligned} C_{qu} &\underset{T\gg\theta_E}{\longrightarrow} 3k\frac{\theta_E^2}{T^2}\frac{1+\theta_E/T}{(1+\theta_E/T-1)^2} && (35)\\ &\rightarrow 3k && (36)\end{aligned}$$

For low temperatures $e^{\theta_E/T} \gg 1$ so we have

$$\begin{aligned} C_{qu} &\underset{T\ll\theta_E}{\longrightarrow} 3k\frac{\theta_E^2}{T^2}\frac{e^{\theta_E/T}}{e^{2\theta_E/T}} && (37)\\ &= 3k\frac{\theta_E^2}{T^2}e^{-\theta_E/T} && (38)\end{aligned}$$

The heat capacity again reduces to the classical value for high temperatures. The observed behaviour at low temperatures is that $C_{qu} \rightarrow T^3$, so

this simple model fails for very low temperatures. However, as is shown by Shankar's figure 7.3 Einstein's quantum model is actually quite good for all but the lowest temperatures.

HARMONIC OSCILLATOR - RAISING AND LOWERING OPERATOR CALCULATIONS

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To leave a comment or report an error, please use the auxiliary blog.

Post date: 17 Jul 2012.

Reference: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Problem 2.12.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 7.4, Exercise 7.4.2.

In the study of the harmonic oscillator, we can express x and p in terms of the raising and lowering operators:

$$x = \sqrt{\frac{\hbar}{2m\omega}}(a_+ + a_-) \tag{1}$$

$$p = i\sqrt{\frac{\hbar m\omega}{2}}(a_+ - a_-) \tag{2}$$

We now have

$$\langle x\rangle = \sqrt{\frac{\hbar}{2m\omega}}\int \psi_n^*(a_+ + a_-)\psi_n dx \tag{3}$$

$$= 0 \tag{4}$$

The reason this is zero is that, as we saw when working out the normalization of the stationary states,

$$a_+\psi_n = \sqrt{n+1}\psi_{n+1} \tag{5}$$

$$a_-\psi_n = \sqrt{n}\psi_{n-1} \tag{6}$$

$$a_+a_-\psi_n = n\psi_n \tag{7}$$

$$a_-a_+\psi_n = (n+1)\,\psi_n \tag{8}$$

and since the wave functions are orthogonal, we get

$$\int \psi_n^*\psi_{n+1}dx = \int \psi_n^*\psi_{n-1}dx = 0 \tag{9}$$

Similarly:

$$\begin{aligned} \langle p \rangle &= i\sqrt{\frac{\hbar m\omega}{2}} \int \psi_n^* (a_+ - a_-)\psi_n dx && (10) \\ &= 0 && (11) \end{aligned}$$

for the same reason.

For the mean squares:

$$\begin{aligned} \langle x^2 \rangle &= \left(\frac{\hbar}{2m\omega}\right) \int \psi_n^* (a_+ + a_-)(a_+ + a_-)\psi_n dx && (12) \\ &= \left(\frac{\hbar}{2m\omega}\right) \int \psi_n^* (a_+ a_- + a_- a_+)\psi_n dx && (13) \\ &= \left(\frac{\hbar}{2m\omega}\right) (2n+1) && (14) \\ &= \frac{\hbar}{m\omega}\left(n + \frac{1}{2}\right) && (15) \end{aligned}$$

In going from the first to the second line, we've thrown out terms where we integrate two orthogonal functions. For example,

$$\begin{aligned} \int \psi_n^* a_+ a_+ \psi_n dx &= \int \psi_n^* \sqrt{(n+1)(n+2)}\psi_{n+2} dx && (16) \\ &= 0 && (17) \end{aligned}$$

We have used the relations above and the fact that ψ_n is normalized to get the third line.

Similarly:

$$\begin{aligned} \langle p^2 \rangle &= -\frac{\hbar m\omega}{2} \int \psi_n^* (-a_+ a_- - a_- a_+)\psi_n dx && (18) \\ &= \hbar m\omega \left(n + \frac{1}{2}\right) && (19) \end{aligned}$$

The uncertainty principle then becomes

$$\begin{aligned} \sigma_p \sigma_x &= \sqrt{\langle x^2 \rangle \langle p^2 \rangle} && (20) \\ &= \hbar \left(n + \frac{1}{2}\right) && (21) \end{aligned}$$

and the kinetic energy is

$$\langle T \rangle = \frac{\langle p^2 \rangle}{2m} = \frac{1}{2}\hbar\omega \left(n + \frac{1}{2} \right) \tag{22}$$

which is half the total energy, as it should be.

PINGBACKS

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Pingback: Harmonic oscillator: relativistic correction
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HALF-HARMONIC OSCILLATOR

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Post date: 18 Aug 2012.

References: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Problem 2.42.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 7.3, Exercise 7.3.6.

Suppose we modify the harmonic oscillator potential so that it becomes a half-harmonic oscillator. That is

$$V(x) = \begin{cases} \infty & x < 0 \\ \frac{1}{2}m\omega^2 x^2 & x > 0 \end{cases} \tag{1}$$

A physical interpretation of this could be a spring that can be stretched from its equilibrium position but not compressed.

We can find the allowed energies of this potential by considering its difference from the ordinary harmonic oscillator. In the ordinary case, there were no boundary conditions, and we found that the stationary states could be expressed in terms of the Hermite polynomials

$$\psi_n(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right) e^{-m\omega x^2/2\hbar} \tag{2}$$

The Hermite polynomials are even if n is even and odd if n is odd. Since all the even Hermite polynomials have a non-zero constant term, $H_n(0) \neq 0$ if n is even. Similarly, since all odd Hermite polynomials have no constant term, $H(0) = 0$ if n is odd.

From continuity of the wave function at $x = 0$ we must have $\psi(0) = 0$ (since the wave function is zero for $x < 0$). The solution above still applies for $x > 0$, but due to the boundary condition, we are allowed only the odd Hermite polynomial solutions for $x > 0$, which in turn means that the allowed energies are

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega \tag{3}$$

for n odd only.

HARMONIC OSCILLATOR: MATRIX ELEMENTS

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Post date: 11 Oct 2012.

References: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Problem 3.33.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 7.4, Exercise 7.4.1.

In analyzing the harmonic oscillator, we used the raising and lowering operators to calculate $\langle x \rangle$ and $\langle p \rangle$, finding that they are both zero for all stationary states. These quantities are really the diagonal elements of the matrices X and P. That is

$$\begin{aligned} \langle x \rangle_{nn} &= \langle n|x|n \rangle & (1) \\ &= X_{nn} & (2) \end{aligned}$$

We can use the same technique to calculate the off-diagonal elements.

We review the equations involving the raising and lowering operators first:

$$\begin{aligned} x &= \sqrt{\frac{\hbar}{2m\omega}}(a_+ + a_-) & (3) \\ p &= i\sqrt{\frac{\hbar m\omega}{2}}(a_+ - a_-) & (4) \\ a_+\psi_n &= \sqrt{n+1}\psi_{n+1} & (5) \\ a_-\psi_n &= \sqrt{n}\psi_{n-1} & (6) \end{aligned}$$

The general matrix elements for the operator x can then be calculated:

$$\begin{aligned} \langle n|x|n' \rangle &= \sqrt{\frac{\hbar}{2m\omega}}(\sqrt{n'+1}\langle n|n'+1\rangle + \sqrt{n'}\langle n|n'-1\rangle) & (7) \\ &= \sqrt{\frac{\hbar}{2m\omega}}(\sqrt{n'+1}\delta_{n,n'+1} + \sqrt{n'}\delta_{n,n'-1}) & (8) \end{aligned}$$

By similar reasoning we get the matrix elements for p:

$$\langle n|p|n'\rangle = i\sqrt{\frac{\hbar m\omega}{2}}(\sqrt{n'+1}\delta_{n,n'+1} - \sqrt{n'}\delta_{n,n'-1}) \tag{9}$$

These results agree with those found by doing the integrals involving Hermite polynomials.

We now have all the matrix elements of X and P so it would be interesting to calculate the full hamiltonian matrix, which is

$$\mathsf{H} = \frac{1}{2m}\mathsf{P}^2 + \frac{m\omega^2}{2}\mathsf{X}^2 \tag{10}$$

In order to calculate the squares of the two matrices, we observe that both X and P are *tridiagonal* matrices with the added condition that their main diagonals are all zero. That is, the two diagonals above and below the main diagonal are the only places with non-zero elements. The square of such a matrix will have non-zero elements only on the main diagonal, and on the diagonals *two* above and below the main diagonal (you can verify this by drawing out such a matrix and seeing where the non-zero elements lie, or by doing tedious calculations with indices).

We can demonstrate how these elements can be calculated by considering the diagonal elements of X^2.

$$\mathsf{X}^2_{nn} = \sum_{n'}\langle n|x|n'\rangle\langle n'|x|n\rangle \tag{11}$$

$$= \frac{\hbar}{2m\omega}\sum_{n'}[\sqrt{n'+1}\delta_{n,n'+1} + \sqrt{n'}\delta_{n,n'-1}][\sqrt{n+1}\delta_{n',n+1} + \sqrt{n}\delta_{n',n-1}] \tag{12}$$

$$= \frac{\hbar}{2m\omega}(2n+1) \tag{13}$$

The last line is obtained by noting that all the terms in the sum contain the product of two Kronecker deltas, so only in those cases where *both* deltas are non-zero is there a non-zero contribution to the sum. This happens only in the terms involving the product of the first and fourth terms (where $n' = n-1$) and the second and third terms (where $n' = n+1$).

By a similar argument, we get

$$\mathsf{P}^2_{nn} = \frac{\hbar m\omega}{2}(2n+1) \tag{14}$$

Therefore the *diagonal* elements of $(1/2m)\mathsf{P}^2 + (m\omega^2/2)\mathsf{X}^2$ are

$$\mathsf{H}_{nn} = \hbar\omega\left(n + \frac{1}{2}\right) \tag{15}$$

which is what you would expect, as these are the energy levels of the harmonic oscillator.

It remains only to show that the off-diagonal elements of H are zero.

$$\mathsf{X}^2_{nm} = \sum_{n'} \langle n|x|n'\rangle\langle n'|x|m\rangle \tag{16}$$

$$= \frac{\hbar}{2m\omega} \sum_{n'} [\sqrt{n'+1}\delta_{n,n'+1} + \sqrt{n'}\delta_{n,n'-1}][\sqrt{m+1}\delta_{n',m+1} + \sqrt{m}\delta_{n',m-1}] \tag{17}$$

To see which non-zero elements exist on row *n*, we note that for a given value of *n*, we must have either $n' = n-1$ or $n' = n+1$ in order for one of the deltas in the first term to be non-zero. If $n' = n-1$, then in the second term, we must have either $n-1 = m+1$ or $n-1 = m-1$. The second case results in a diagonal element which we have already considered, so we need consider only the case $m = n-2$. In this case, the matrix element is

$$\mathsf{X}^2_{n,n-2} = \frac{\hbar}{2m\omega}\sqrt{n(n-1)} \tag{18}$$

Similarly, if $n' = n+1$, the non-diagonal term is $n+1 = m-1$ or $m = n+2$, and we get

$$\mathsf{X}^2_{n,n+2} = \frac{\hbar}{2m\omega}\sqrt{(n+1)(n+2)} \tag{19}$$

Similar reasoning gives us the elements from P^2:

$$\mathsf{P}^2_{n,n-2} = -\frac{\hbar m\omega}{2}\sqrt{n(n-1)} \tag{20}$$

$$\mathsf{P}^2_{n,n+2} = -\frac{\hbar m\omega}{2}\sqrt{(n+1)(n+2)} \tag{21}$$

Combining these two results, we see that the *non-diagonal* elements of $(1/2m)\mathsf{P}^2 + (m\omega^2/2)\mathsf{X}^2$ are all zero.

PINGBACKS

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HARMONIC OSCILLATOR: RELATIVISTIC CORRECTION

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References: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Problem 6.14.

Post date: 15 Aug 2013.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 7.4, Exercise 7.4.4.

We can apply the relativistic correction to the one-dimensional harmonic oscillator as another example. When analyzing the hydrogen atom, we arrived at this formula for the first order correction to the energy:

$$E_{n1} = -\frac{1}{2mc^2} \langle n0| \left(E_{n0} - V\right)^2 |n0\rangle \tag{1}$$

where we've adjusted the wave functions so they apply to the harmonic oscillator.

Before applying this formula, we should check a couple of things. First, this formula was derived using non-degenerate perturbation theory. In the one-dimensional oscillator this is fine, since there are no degenerate states.

Second, we assumed that the operator p^4 was hermitian, and to check this it is easiest to use the raising and lowering operators. We have

$$p = i\sqrt{\frac{\hbar m\omega}{2}}(a_+ - a_-) \tag{2}$$

The raising and lowering operators transform one wave function into another:

$$\begin{aligned} a_+ |n0\rangle &= \sqrt{n+1}\,|n+1,0\rangle & (3)\\ a_- |n0\rangle &= \sqrt{n}\,|n-1,0\rangle & (4) \end{aligned}$$

Therefore, each application of p transforms the original wave function into a linear combination of other wave functions and since p itself must be hermitian (it represents an observable: the momentum) when applied to any oscillator wave function, any power of p is also hermitian in the same situation.

Having verified that the first order energy correction may be applied to the harmonic oscillator, we can now plug in the values. The unperturbed energies are

$$E_{n0} = \left(n + \frac{1}{2}\right)\hbar\omega \tag{5}$$

From the virial theorem we know that $\langle T\rangle = \langle V\rangle = \frac{1}{2}E_{n0}$ so

$$E_{n1} = -\frac{1}{2mc^2}\left(E_{n0}^2 - 2E_{n0}\langle V\rangle + \left\langle V^2\right\rangle\right) \tag{6}$$

$$= -\frac{1}{2mc^2}\left[\left(\left(n+\frac{1}{2}\right)\hbar\omega\right)^2 - \left(\left(n+\frac{1}{2}\right)\hbar\omega\right)^2 + \frac{1}{4}m^2\omega^4\left\langle x^4\right\rangle\right] \tag{7}$$

$$= -\frac{m\omega^4}{8c^2}\left\langle x^4\right\rangle \tag{8}$$

To calculate $\left\langle x^4\right\rangle$, we can use the raising and lowering operators again. We have

$$x = \sqrt{\frac{\hbar}{2m\omega}}(a_+ + a_-) \tag{9}$$

$$x^2 = \frac{\hbar}{2m\omega}\left(a_+^2 + a_+a_- + a_-a_+ + a_-^2\right) \tag{10}$$

Since $\left\langle x^4\right\rangle = \langle n0|\, x^4\, |n0\rangle$, the two wave functions involved in calculating the mean value are the same (both $|n0\rangle$) and $\langle n0|\, m0\rangle = \delta_{mn}$, any combination of a_+ and a_- that converts $|n0\rangle$ into a different wave function will not contribute to the overall integral, so we need consider only those terms in the operator x^4 with equal numbers of a_+ and a_-. Retaining only these terms, we get

$$x^4 = \left(\frac{\hbar}{2m\omega}\right)^2\left(a_+^2a_-^2 + a_+a_-a_+a_- + a_+a_-^2a_+ + a_-a_+a_-a_+ + a_-a_+^2a_- + a_-^2a_+^2\right) \tag{11}$$

Applying the operators according to the formulas above, we get

$$\left\langle x^4 \right\rangle = \left(\frac{\hbar}{2m\omega}\right)^2 \left[n(n-1) + n^2 + n(n+1) + (n+1)^2 + n(n+1) + (n+1)(n+2)\right] \tag{12}$$

$$= \left(\frac{\hbar}{2m\omega}\right)^2 \left(6n^2 + 6n + 3\right) \tag{13}$$

The energy correction is then

$$E_{n1} = -\frac{3\hbar^2\omega^2}{32mc^2}\left(2n^2 + 2n + 1\right) \tag{14}$$

PATH INTEGRAL FORMULATION OF QUANTUM MECHANICS: FREE PARTICLE PROPAGATOR

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Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 8.

Post date: 7 Feb 2017

Although all the non-relativistic quantum mechanics we've done so far has started with the Schrödinger equation, a different approach was devised by Richard Feynman in the 1940s. The Schrödinger method requires us to find the eigenvalues (allowed energies) and eigenstates of the hamiltonian H and then use these to construct the unitary operator known as the propagator. For discrete energies, this propagator is

$$U(t) = \sum e^{-iEt/\hbar} |E\rangle \langle E| \tag{1}$$

and for continuous energies, we have

$$U(t) = \int e^{-iEt/\hbar} |E\rangle \langle E| \, dE \tag{2}$$

Given the state of the system at an initial time $t = 0$, the general solution as a function of time is then

$$|\psi(t)\rangle = U(t) |\psi(0)\rangle \tag{3}$$

Feynman's method allows us to compute the propagator directly, without first solving the Schrödinger equation. It is known as the *path integral forumulation*.

The idea is based on the observation that the exponential $e^{-iEt/\hbar}$ that appears in the propagator contains the ratio of two quantities with the dimensions of action, that is, energy times time. In classical mechanics, the actual trajectory of a particle is found by minimizing the action S over all possible paths available to the particle. The path integral formulation of quantum mechanics works in a similar way, although at first sight, it looks like a completely impractical method.

The formulation works like this, for a single particle:

(1) Find all paths available for the particle to travel between its initial point (x', t') and its final point (x, t). This is actually similar to what we do in classical mechanics, where S is defined as $S = \int L \, dt$

where L is the Lagrangian. We then use the functional derivative to minimize S over all these paths and find the path that gives the minimum action.

(2) For each path, calculate the action S. (This is where things sound terribly impractical, since there are an infinite number of paths of all possible shape, so how can we find the action for all these paths? It turns out that, in most cases, we don't need to.)

(3) Calculate the propagator as

$$U\left(x,t;x',t'\right) = A \sum_{all\ paths} e^{iS[x(t)]/\hbar} \tag{4}$$

The notation $S\left[x\left(t\right)\right]$ indicates that S is a functional of the path $x\left(t\right)$.

The key to the success of this method is that since the action is real, the exponential $e^{iS[x(t)]/\hbar}$ is an oscillatory function, so we can expect contributions from the actions for different paths to cancel each other to some extent. Although the quantum path of a particle can't be defined precisely due to the uncertainty principle, we expect that the particle is much more likely to be found following a path that is close to the classical path, and the classical path occurs when $S\left[x\left(t\right)\right]$ is a minimum. Paths sufficiently far from this minimum will tend to cancel each other, so for practical purposes, we need calculate 4 only for paths near to the classical path.

The example given by Shankar is of a particle of mass 1 gram moving from $(x,t) = (0,0)$ to $(1,1)$ by two different paths. In the first path, the particle moves with constant speed so $x = t$. The action is

$$\begin{aligned} S &= \int_0^1 L\, dt && (5)\\ &= \int_0^1 (T-V)\, dt && (6)\\ &= \int_0^1 \frac{1}{2} m v^2 dt && (7)\\ &= \frac{m}{2}\int_0^1 \left(\frac{dx}{dt}\right)^2 dt && (8)\\ &= \frac{m}{2}\int_0^1 dt && (9)\\ &= \frac{m}{2} && (10) \end{aligned}$$

In the second path, we have $x = t^2$, so the velocity is

$$v = \frac{dx}{dt} = 2t \tag{11}$$

with associated action

$$\begin{aligned} S &= \int_0^1 \frac{1}{2} m v^2 dt && (12) \\ &= 2m \int_0^1 t^2 dt && (13) \\ &= \frac{2m}{3} && (14) \end{aligned}$$

The guideline for when the phases of the paths start to cancel each other is when $S/\hbar$ is about π out of phase with $S_{cl}/\hbar$. In this example, the second path is πout of phase with the first when

$$\left(\frac{2m}{3} - \frac{m}{2} \right) = \pi\hbar \approx 3 \times 10^{-34} \text{ m}^2\text{kg s}^{-1} \tag{15}$$

Thus for any mass larger than about $6\pi\hbar \approx 1.8 \times 10^{-33}$ kg the second path will contribute essentially nothing to 4 and can be ignored. This mass is smaller than the mass of the electron.

For the free particle, we worked out the propagator earlier and found that (where we've generalized the earlier result for an arbitrary initial time t'):

$$U\left(t, t'\right) = \int_{-\infty}^{\infty} e^{-ip^2(t-t')/2m\hbar} \left|p\right\rangle \left\langle p\right| dp \tag{16}$$

The matrix elements of U in the x basis are worked out by evaluating a Gaussian integral

$$\begin{aligned} U\left(x, t; x', t'\right) &= \int_{-\infty}^{\infty} e^{-ip^2(t-t')/2m\hbar} \left\langle x \left| p \right.\right\rangle \left\langle p \left| x' \right.\right\rangle dp && (17) \\ &= \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} e^{ip(x-x')/\hbar} e^{-ip^2(t-t')/2m\hbar} dp && (18) \\ &= \sqrt{\frac{m}{2\pi\hbar i \left(t-t'\right)}} e^{im(x-x')^2/2\hbar(t-t')} && (19) \end{aligned}$$

We can try to estimate U using the path integral approach by assuming that only the classical path contributes to the propagator. For a free particle travelling between (x', t') to (x, t), the constant velocity is

$$v = \frac{x - x'}{t - t'} \tag{20}$$

The Lagrangian is a constant

$$L = \frac{mv^2}{2} = \frac{m}{2}\left(\frac{x-x'}{t-t'}\right)^2 \tag{21}$$

The classical action is thus

$$\begin{aligned} S_{cl} &= \int_{t'}^{t} L\, dt'' && (22)\\ &= \frac{m}{2}\left(\frac{x-x'}{t-t'}\right)^2 \int_{t'}^{t} dt'' && (23)\\ &= \frac{m}{2}\left(\frac{x-x'}{t-t'}\right)^2 \left(t-t'\right) && (24)\\ &= \frac{m}{2}\frac{\left(x-x'\right)^2}{t-t'} && (25) \end{aligned}$$

The propagator in this approximation is

$$U\left(x,t;x',t'\right) = A\exp\left[\frac{im}{2\hbar}\frac{\left(x-x'\right)^2}{\left(t-t'\right)}\right] \tag{26}$$

Comparing with 19 we see that the exponential factors match; all that is left is to determine the constant A. To do this, we require $\lim_{t\to t'} U\left(x,t;x',t'\right) = \delta\left(x-x'\right)$, since if the time interval $t'-t$ goes to zero, the particle cannot move so must be in the same place. By comparing 26 with the form of a delta function as the limit of a gaussian integral, which is

$$\lim_{\Delta^2\to 0}\frac{1}{\left(\pi\Delta^2\right)^{1/2}}\int_{-\infty}^{\infty} e^{-(x-x')/\Delta^2}dx = \delta\left(x-x'\right) \tag{27}$$

we see that

$$\Delta^2 = \frac{2\hbar i\left(t-t'\right)}{m} \tag{28}$$

so the final propagator is the same as 19.

PINGBACKS

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FREE PARTICLE PROPAGATOR FROM A COMPLETE PATH INTEGRAL

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Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 8. Section 8.4.

Post date: 7 Feb 2017

We've seen that the free-particle propagator can be obtained in the path integral approach by using only the classical path in the sum over paths. It turns out that it's not too hard to calculate the propagator for a free particle properly, by summing over all possible paths. The notation used by Shankar is as follows.

We want to evaluate the path integral

$$\int_{x_0}^{x_N} e^{iS[x(t)]/\hbar} \mathfrak{D}\left[x\left(t\right)\right] \tag{1}$$

The notation $\mathfrak{D}\left[x\left(t\right)\right]$ means an integration over all possible paths from x_0 to x_N in the given time interval. This includes paths where the particle might move to the right for a while, then jog back to the left, then back to the right again and so on. This might seem like a hopeless task, but we can make sense of this method by splitting the time interval between t_0 and t_N into N small intervals, each of length ε. Thus an intermediate time $t_n = t_0 + n\varepsilon$, and the final time is $t_N = t_0 + N\varepsilon$.

For a free particle, there is no potential energy so the Lagrangian is just the kinetic energy:

$$L = \frac{1}{2} m\dot{x}^2 \tag{2}$$

We can estimate the velocity in each time slice by

$$\dot{x}_i = \frac{x_{i+1} - x_i}{\varepsilon} \tag{3}$$

Note that this assumes that the velocity within each time slice is constant, but as we make ε smaller and smaller, this is increasingly accurate. Also note that it is possible for $\dot{x}_i$ to be both positive (if the particle moves to the right in the interval) or negative (if it moves to the left).

The action for a given path is given by the integral of the Lagrangian:

$$S = \int_{t_0}^{t_N} L(t)\, dt \tag{4}$$

In our discretized approximation, we evaluate L within each time slice, and dt becomes the interval length ε, so the action becomes a sum:

$$\begin{aligned} S &= \sum_{i=0}^{N-1} L(t_i)\, \varepsilon & (5)\\ &= \frac{m}{2} \sum_{i=0}^{N-1} \left(\frac{x_{i+1} - x_i}{\varepsilon} \right)^2 \varepsilon & (6)\\ &= \frac{m}{2} \sum_{i=0}^{N-1} \frac{(x_{i+1} - x_i)^2}{\varepsilon} & (7) \end{aligned}$$

The key point here is to notice that we can label any given path by choosing values for all the x_is between the two times, and that each x_i can vary independently of the others, over a range from $-\infty$ to $+\infty$. We can therefore implement the multiple integration required by $\mathfrak{D}[x(t)]$ by integrating over all the x_i variables separately. That is,

$$\int_{x_0}^{x_N} e^{iS[x(t)]/\hbar} \mathfrak{D}[x(t)] = A \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} \exp\left[\frac{im}{2\hbar} \sum_{i=0}^{N-1} \frac{(x_{i+1} - x_i)^2}{\varepsilon} \right] dx_1 dx_2 \ldots dx_{N-1} \tag{8}$$

where A is some constant to make the scale come out right.

We don't integrate over x_0 or x_N since these are fixed as the end points of the path. To get the final version, we need to take the limit of this expression as $N \to \infty$ and $\varepsilon \to 0$. This still looks pretty scary, but in fact it is doable. We define the variable

$$\begin{aligned} y_i &\equiv \sqrt{\frac{m}{2\hbar\varepsilon}}\, x_i & (9)\\ dx_i &= \sqrt{\frac{2\hbar\varepsilon}{m}}\, dy_i & (10) \end{aligned}$$

This gives us

$$A \left(\frac{2\hbar\varepsilon}{m} \right)^{(N-1)/2} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} \exp\left[i \sum_{i=0}^{N-1} (y_{i+1} - y_i)^2 \right] dy_1 dy_2 \ldots dy_{N-1} \tag{11}$$

We can do the integral in stages in order to spot a pattern. Consider first the integral over y_1, which involves only two of the factors in the integrand:

$$\int_{-\infty}^{\infty} e^{i\left[(y_1-y_0)^2+(y_2-y_1)^2\right]} dy_1 \tag{12}$$

We first simplify the exponent

$$(y_1-y_0)^2+(y_2-y_1)^2 = y_2^2+y_0^2+2\left(y_1^2-y_0y_1-y_1y_2\right) \tag{13}$$

$$= y_2^2+y_0^2+2y_1^2-2\left(y_0+y_2\right)y_1 \tag{14}$$

We get

$$\int_{-\infty}^{\infty} e^{i\left[(y_1-y_0)^2+(y_2-y_1)^2\right]} dy_1 = e^{i\left(y_2^2+y_0^2\right)} \int_{-\infty}^{\infty} e^{2i\left[y_1^2-(y_0+y_2)y_1\right]} dy_1 \tag{15}$$

We can evaluate this using a standard Gaussian integral

$$\int_{-\infty}^{\infty} e^{-ax^2+bx} dx = e^{b^2/4a}\sqrt{\frac{\pi}{a}} \tag{16}$$

This gives

$$\int_{-\infty}^{\infty} e^{i\left[(y_1-y_0)^2+(y_2-y_1)^2\right]} dy_1 = e^{i\left(y_2^2+y_0^2\right)} e^{4(y_0+y_2)^2/8i}\sqrt{-\frac{\pi}{2i}} \tag{17}$$

$$= e^{i\left(y_2^2+y_0^2\right)} e^{(y_0+y_2)^2/2i}\sqrt{\frac{\pi i}{2}} \tag{18}$$

To simplify the exponents on the RHS:

$$i\left(y_2^2+y_0^2\right)+\frac{(y_0+y_2)^2}{2i} = \frac{1}{2i}\left[(y_0+y_2)^2-2y_2^2-2y_0^2\right] \tag{19}$$

$$= -\frac{1}{2i}\left(y_0-y_2\right)^2 \tag{20}$$

Thus we have

$$\int_{-\infty}^{\infty} e^{i\left[(y_1-y_0)^2+(y_2-y_1)^2\right]} dy_1 = \sqrt{\frac{\pi i}{2}} e^{-(y_0-y_2)^2/2i} \tag{21}$$

Having eliminated y_1 we can now do the integral over y_2:

$$\sqrt{\frac{\pi i}{2}} \int_{-\infty}^{\infty} e^{-(y_3-y_2)^2/i-(y_2-y_0)^2/2i} dy_2 \tag{22}$$

Again, we can simplify the exponent:

$$-\frac{(y_3-y_2)^2}{i}-\frac{(y_2-y_0)^2}{2i}=\frac{1}{2i}\left[-\left(2y_3^2+y_0^2\right)-3y_2^2+y_2\left(4y_3+2y_0\right)\right] \tag{23}$$

The integral now becomes

$$\sqrt{\frac{\pi i}{2}}\int_{-\infty}^{\infty}e^{-(y_3-y_2)^2/i-(y_2-y_0)^2/2i}dy_2 \;=\; \sqrt{\frac{\pi i}{2}}e^{-\left(2y_3^2+y_0^2\right)/2i}\int_{-\infty}^{\infty}e^{\left(-3y_2^2+y_2(4y_3+2y_0)\right)/2i}dy_2 \tag{24}$$

Doing the Gaussian integral on the RHS using 16:

$$\int_{-\infty}^{\infty}e^{\left(-3y_2^2+y_2(4y_3+2y_0)\right)/2i}dy_2=e^{-(4y_3+2y_0)^2i/24}\sqrt{\frac{2\pi i}{3}} \tag{25}$$

$$=e^{(2y_3+y_0)^2/6i}\sqrt{\frac{2\pi i}{3}} \tag{26}$$

Thus the combined integral over y_1 and y_2 is

$$\sqrt{\frac{\pi i}{2}}e^{-\left(2y_3^2+y_0^2\right)/2i}e^{(2y_3+y_0)^2/6i}\sqrt{\frac{2\pi i}{3}}=\sqrt{\frac{(\pi i)^2}{3}}e^{\left(-6y_3^2-3y_0^2+(2y_3+y_0)^2\right)/6i} \tag{27}$$

$$=\sqrt{\frac{(\pi i)^2}{3}}e^{-(y_3-y_0)^2/3i} \tag{28}$$

The general pattern after $N-1$ integrations is (presumably this could be proved by induction, but we'll accept the result):

$$\frac{(\pi i)^{(N-1)/2}}{\sqrt{N}}e^{-(y_N-y_0)^2/Ni}=\frac{(\pi i)^{(N-1)/2}}{\sqrt{N}}e^{-m(x_N-x_0)^2/2\hbar\varepsilon Ni} \tag{29}$$

where we reverted back to x_i using 9.

Going back to 11, we must multiply the result by $A\left(\frac{2\hbar\varepsilon}{m}\right)^{(N-1)/2}$ to get the final expression for the propagator:

$$U=A\left(\frac{2\hbar\varepsilon}{m}\right)^{(N-1)/2}\frac{(\pi i)^{(N-1)/2}}{\sqrt{N}}e^{-m(x_N-x_0)^2/2\hbar\varepsilon Ni} \tag{30}$$

$$=A\left(\frac{2\pi\hbar\varepsilon i}{m}\right)^{N/2}\sqrt{\frac{m}{2\pi\hbar iN\varepsilon}}e^{im(x_N-x_0)^2/2\hbar\varepsilon N} \tag{31}$$

In the limit as $N\to\infty$ and $\varepsilon\to 0$, $N\varepsilon=t_N-t_0$ so we have

$$U = A\left(\frac{2\pi\hbar\varepsilon i}{m}\right)^{N/2}\sqrt{\frac{m}{2\pi\hbar i\left(t_N - t_0\right)}}e^{im(x_N-x_0)^2/2\hbar(t_N-t_0)} \tag{32}$$

The expression we got earlier using the Schrödinger method is

$$U\left(x,t;x',t'\right) = \sqrt{\frac{m}{2\pi\hbar i\left(t-t'\right)}}e^{im(x-x')^2/2\hbar(t-t')} \tag{33}$$

Thus the full path integral gives the same result, with $t' = t_0$ and $t = t_N$ (similarly for x), provided that we can set

$$A = \left(\frac{m}{2\pi\hbar\varepsilon i}\right)^{N/2} \equiv B^{-N} \tag{34}$$

Shankar then says that it is conventional to associate one factor of B^{-1} with each integration over an x_i, and the remaining factor with the overall process. This seems to overlook a basic problem, in that as $N \to \infty$ and $\varepsilon \to 0$, $A \to \infty$, so we seem to be cancelling two infinities when we multiply the path integral by A.

PINGBACKS

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THE PATH INTEGRAL IS EQUIVALENT TO THE SCHRÖDINGER EQUATION

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Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 8. Section 8.5.

Post date: 10 Feb 2017

We've seen that we can produce the propagator for the free particle by means of a complete path integral over all paths between some specified initial state at (x_0, t_0) and specified final state (x_N, t_N). Here we'll show that the path integral approach is formally equivalent to the Schrödinger equation, even for an arbitrary potential V.

The Schrödinger equation is a differential equation that allows us to calculate the wave function as a function of position x and time t, when solved in the position basis. To find the same thing from the path integral, we'll consider an infinitesimal time interval ε and try to find $\psi(x, \varepsilon)$ given the wave function at $t = 0$, that is, given $\psi(x', 0)$ for some arbitrary x'. To use a path integral in this way, we're effectively asking for the contribution to the propagator from all possible paths between $t = 0$ and $t = \varepsilon$. That is, we're considering that the particle may have started at *any* position x' at $t = 0$ and stilll ended up at position x at $t = \varepsilon$. In terms of the propagator, this is

$$\psi(x, \varepsilon) = \int_{-\infty}^{\infty} U\left(x, \varepsilon; x', 0\right) \psi\left(x', 0\right) dx' \tag{1}$$

Looking at our previous derivation of the propagator, we saw that there we fixed the initial and final states and integrated over all possible paths between these two states. In this case, all we're specifying is the final state so in principle, the particle could have been anywhere at $t = 0$.

The general form for the propagator is

$$U(t) = A \int_{all\ paths} e^{iS[x(t)]/\hbar} \tag{2}$$

where A is a scale factor and $S[x(t)]$ is the action for travelling along path $x(t)$:

$$S = \int_0^{\varepsilon} L\, dt \tag{3}$$

We can approximate the action by taking the Lagrangian to be

$$L = T - V \tag{4}$$
$$= \frac{1}{2}mv^2 - V \tag{5}$$
$$= \frac{1}{2}m\frac{(x-x')^2}{\varepsilon^2} - V\left(\frac{x+x'}{2},0\right) \tag{6}$$

Here we take the velocity over the interval ε to be constant at $v = \frac{x-x'}{\varepsilon}$, and we take the potential to be constant, with its value at the midpoint between x and x' at time $t = 0$. The reason we can approximate V by its value at $t = 0$ is that in calculating the action 3, we will multiply L by ε, and we're interested only in terms of first order in ε. The action to this order is then

$$S = \varepsilon L = \frac{1}{2}m\frac{(x-x')^2}{\varepsilon} - \varepsilon V\left(\frac{x+x'}{2},0\right) \tag{7}$$

which gives a propagator of

$$U\left(x,\varepsilon;x',0\right) = A\exp\left[\frac{i}{\hbar}\left(\frac{1}{2}m\frac{(x-x')^2}{\varepsilon} - \varepsilon V\left(\frac{x+x'}{2},0\right)\right)\right] \tag{8}$$

We can try the same value for A that we had for the free particle

$$A = \left(\frac{m}{2\pi\hbar\varepsilon i}\right)^{N/2} \tag{9}$$

In this case, we have only one step so $N = 1$ and

$$U\left(x,\varepsilon;x',0\right) = \sqrt{\frac{m}{2\pi\hbar\varepsilon i}}\exp\left[\frac{i}{\hbar}\left(\frac{1}{2}m\frac{(x-x')^2}{\varepsilon} - \varepsilon V\left(\frac{x+x'}{2},0\right)\right)\right] \tag{10}$$

We now need to do some approximating. The kinetic energy term is

$$\exp\left[\frac{i}{\hbar}\left(\frac{1}{2}m\frac{(x-x')^2}{\varepsilon}\right)\right] \tag{11}$$

The exponent is pure imaginary so for infinitesimal ε, it oscillates very rapidly away from the stationary point at $x = x'$. When this term is placed in the integral 1, it multiplies $\psi(x',0)$ which we'll assume is a smooth function that doesn't oscillate much, at least over the scale at which 11 oscillates. We define

$$\eta \equiv x' - x \tag{12}$$

to be the distance from the minimum phase. Once the phase approaches π, the oscillations will be rapid enough that the contributions to the integral effectively cancel out, so we're looking at the region

$$\frac{m\eta^2}{2\hbar\varepsilon} \lesssim \pi \tag{13}$$

or

$$|\eta| \lesssim \sqrt{\frac{2\hbar\varepsilon\pi}{m}} \tag{14}$$

If we work to first order in ε we therefore must retain terms up to second order in η. In terms of η, 1 now becomes

$$\psi(x,\varepsilon) = \sqrt{\frac{m}{2\pi\hbar\varepsilon i}} \int_{-\infty}^{\infty} \exp\left(\frac{im\eta^2}{2\hbar\varepsilon}\right) \exp\left(-\frac{i\varepsilon}{\hbar} V\left(x+\frac{\eta}{2},0\right)\right) \psi(x+\eta,0)\, d\eta \tag{15}$$

We now expand the last two factors as a Taylor series in η and ε up to first order in ε or second order in η:

$$\exp\left(-\frac{i\varepsilon}{\hbar} V\left(x+\frac{\eta}{2},0\right)\right) = 1 - \frac{i\varepsilon}{\hbar} V\left(x+\frac{\eta}{2},0\right) + \ldots \tag{16}$$

$$= 1 - \frac{i\varepsilon}{\hbar} V(x,0) + \ldots \tag{17}$$

We can drop terms in the expansion of $V\left(x+\frac{\eta}{2},0\right)$ beyond $V(x,0)$ since they will be of order $\mathcal{O}(\varepsilon\eta) = \mathcal{O}\left(\varepsilon^{3/2}\right)$ or higher.

For the second term, we have

$$\psi(x+\eta,0) = \psi(x,0) + \eta\frac{\partial\psi}{\partial x} + \frac{\eta^2}{2}\frac{\partial^2\psi}{\partial x^2} + \ldots \tag{18}$$

where the partial derivatives are evaluated at $\eta = 0$.

Inserting these into the integral 15 we get

$$\psi(x,\varepsilon) = \sqrt{\frac{m}{2\pi\hbar\varepsilon i}} \int_{-\infty}^{\infty} \exp\left(\frac{im\eta^2}{2\hbar\varepsilon}\right) \times \tag{19}$$

$$\left[\psi(x,0) + \eta\frac{\partial\psi}{\partial x} + \frac{\eta^2}{2}\frac{\partial^2\psi}{\partial x^2}\right] \times \tag{20}$$

$$\left[1 - \frac{i\varepsilon}{\hbar} V(x,0)\right] d\eta \tag{21}$$

Again, retaining only terms up to first order in ε or second order in η:

$$\psi(x,\varepsilon) = \sqrt{\frac{m}{2\pi\hbar\varepsilon i}} \int_{-\infty}^{\infty} \exp\left(\frac{im\eta^2}{2\hbar\varepsilon}\right) \times \tag{22}$$

$$\left[\psi(x,0) - \frac{i\varepsilon}{\hbar} V(x,0)\,\psi(x,0) + \eta\frac{\partial\psi}{\partial x} + \frac{\eta^2}{2}\frac{\partial^2\psi}{\partial x^2}\right] d\eta \tag{23}$$

Everything in the integrand is constant with respect to η except for the first exponential and the factors of η and η^2 in the last two terms. We are therefore faced with a couple of Gaussian integrals. We have

$$\int_{-\infty}^{\infty} \exp\left(\frac{im\eta^2}{2\hbar\varepsilon}\right) d\eta = \int_{-\infty}^{\infty} \exp\left(-\frac{m\eta^2}{2\hbar i\varepsilon}\right) d\eta \tag{24}$$

$$= \sqrt{\frac{2\pi\hbar i\varepsilon}{m}} \tag{25}$$

$$\int_{-\infty}^{\infty} \eta \exp\left(\frac{im\eta^2}{2\hbar\varepsilon}\right) d\eta = 0 \tag{26}$$

$$\int_{-\infty}^{\infty} \eta^2 \exp\left(\frac{im\eta^2}{2\hbar\varepsilon}\right) d\eta = \int_{-\infty}^{\infty} \eta^2 \exp\left(-\frac{m\eta^2}{2\hbar i\varepsilon}\right) d\eta \tag{27}$$

$$= \frac{\hbar i\varepsilon}{m}\sqrt{\frac{2\pi\hbar i\varepsilon}{m}} \tag{28}$$

$$= -\frac{\hbar\varepsilon}{im}\sqrt{\frac{2\pi\hbar i\varepsilon}{m}} \tag{29}$$

Putting it all together, we have

$$\psi(x,\varepsilon) = \sqrt{\frac{m}{2\pi\hbar\varepsilon i}}\sqrt{\frac{2\pi\hbar i\varepsilon}{m}} \left[\left(1 - \frac{i\varepsilon}{\hbar}V(x,0)\right) - \frac{\hbar\varepsilon}{2im}\frac{\partial^2}{\partial x^2}\right]\psi(x,0) \tag{30}$$

$$= \psi(x,0) - \frac{i\varepsilon}{\hbar}\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x,0)\right)\psi(x,0) \tag{31}$$

Rearranging, we get

$$i\hbar\frac{\psi(x,\varepsilon) - \psi(x,0)}{\varepsilon} = \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x,0)\right)\psi(x,0) \tag{32}$$

In the limit $\varepsilon \to 0$, the LHS becomes $i\hbar\frac{\partial\psi}{\partial t}$ and we get the Schrödinger equation:

$$i\hbar\frac{\partial\psi}{\partial t}=\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V\left(x,0\right)\right)\psi\left(x,0\right) \tag{33}$$

PINGBACKS

Pingback: Path integral to Schrödinger equation for a vector potential

PATH INTEGRALS FOR SPECIAL POTENTIALS; USE OF CLASSICAL ACTION

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To leave a comment or report an error, please use the auxiliary blog.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 8. Section 8.6, Exercises 8.6.1 - 8.6.2.

Post date: 12 Feb 2017

We've seen that if we use the path integral formulation for a free particle, we get the exact propagator by considering only one path (the classical path) between the starting point (x', t') and the end point (x, t). In this case, the propagator has the form

$$U\left(x,t;x',t'\right) = A\left(t\right)e^{iS_{cl}/\hbar} \tag{1}$$

where S_{cl} is the classical action. It turns out that this form is true for a wider set of potentials, beyond just the free particle. The general form of the potential for which this is true is

$$V = a + bx + cx^2 + d\dot{x} + ex\dot{x} \tag{2}$$

where a, b, c, d and e are constants. The general expression for the propagator is (where we're taking the starting time to be $t' = 0$):

$$U\left(x,t;x'\right) = \int_{x'}^{x} e^{iS[x(t'')]/\hbar}\mathfrak{D}\left[x\left(t''\right)\right] \tag{3}$$

where the notation $\mathfrak{D}\left[x\left(t''\right)\right]$ means an integration over all possible paths from x' to x in the given time interval.

For a given path, we can write the location of the particle $x\left(t''\right)$ as composed of its position on the classical path $x_{cl}\left(t''\right)$ plus the deviation $y\left(t''\right)$ from the classical path:

$$x\left(t''\right) = x_{cl}\left(t''\right) + y\left(t''\right) \tag{4}$$

As the endpoints are fixed

$$y\left(0\right) = y\left(t\right) = 0 \tag{5}$$

Also, since for any given potential and choice of endpoints, $x_{cl}\left(t''\right)$ is fixed for all times, it is effectively a constant with regard to the path integration. Therefore

$$dx = dy \tag{6}$$

Making these substitutions into 3, we get, using Shankar's slightly misleading notation:

$$U\left(x,t;x'\right) = \int_0^0 e^{iS[x_{cl}(t'')+y(t'')]/\hbar} \mathfrak{D}\left[y\left(t''\right)\right] \tag{7}$$

Usually, when the limits on an integral are the same, the integral evaluates to zero. However, in this case, the notation $\int_0^0 \mathfrak{D}\left[y\left(t''\right)\right]$ means that y starts and ends at zero, but covers all possible paths between these endpoints.

The action is the integral of the Lagrangian which, for the potential 2 is

$$\begin{aligned} L &= T - V & (8)\\ &= \frac{1}{2}m\dot{x}^2 - a - bx - cx^2 - d\dot{x} - ex\dot{x} & (9) \end{aligned}$$

Because L is quadratic in both x and $\dot{x}$, we can expand it in a Taylor series up to second order without any approximation. That is

$$L\left(x_{cl}+y,\dot{x}_{cl}+\dot{y}\right) = L\left(x_{cl},\dot{x}_{cl}\right) + \left.\frac{\partial L}{\partial x}\right|_{x_{cl}} y + \left.\frac{\partial L}{\partial \dot{x}}\right|_{x_{cl}} \dot{y} + \tag{10}$$

$$\frac{1}{2}\left(\left.\frac{\partial^2 L}{\partial x^2}\right|_{x_{cl}} y^2 + 2\left.\frac{\partial^2 L}{\partial x \partial \dot{x}}\right|_{x_{cl}} y\dot{y} + \left.\frac{\partial^2 L}{\partial \dot{x}^2}\right|_{x_{cl}} \dot{y}^2\right) \tag{11}$$

Look first at the last two terms on the RHS of the first line. Using the equations of motion, we have

$$\left.\frac{\partial L}{\partial x}\right|_{x_{cl}} = \frac{d}{dt}\left(\left.\frac{\partial L}{\partial \dot{x}}\right|_{x_{cl}}\right) \tag{12}$$

To get the action, we need to integrate the Lagrangian over the time interval of interest. Integrating these two terms gives

$$\int_0^t \left[\left.\frac{\partial L}{\partial x}\right|_{x_{cl}} y + \left.\frac{\partial L}{\partial \dot{x}}\right|_{x_{cl}} \dot{y}\right] dt'' = \int_0^t \left[\frac{d}{dt}\left(\left.\frac{\partial L}{\partial \dot{x}}\right|_{x_{cl}}\right) y + \left.\frac{\partial L}{\partial \dot{x}}\right|_{x_{cl}} \dot{y}\right] dt'' \tag{13}$$

$$= \left(\left.\frac{\partial L}{\partial \dot{x}}\right|_{x_{cl}}\right) y\Big|_0^t - \int_0^t \left.\frac{\partial L}{\partial \dot{x}}\right|_{x_{cl}} \dot{y}dt'' + \int_0^t \left.\frac{\partial L}{\partial \dot{x}}\right|_{x_{cl}} \dot{y}dt'' \tag{14}$$

$$= 0 \tag{15}$$

where we integrated the first term by parts. The integrated term in the second line is zero because $y = 0$ at both endpoints, and the last two terms cancel each other.

Returning to 11, we can calculate the three second derivatives explicitly:

$$\frac{1}{2}\frac{\partial^2 L}{\partial x^2} = -c \tag{16}$$

$$\left.\frac{\partial^2 L}{\partial x \partial \dot{x}}\right|_{x_{cl}} = -e \tag{17}$$

$$\frac{1}{2}\frac{\partial^2 L}{\partial \dot{x}^2} = \frac{m}{2} \tag{18}$$

[Note that Shankar's equation 8.6.10 is wrong - the RHS should be $\frac{m}{2}$. However, his equation 8.6.11 appears to be correct. Thanks to commenter Alex for pointing this out.]

The integral of the first term on the RHS of 10 is just the classical action, so we get for the propagator 7:

$$U\left(x,t;x'\right) = e^{iS_{cl}/\hbar}\int_0^0 \exp\left[\frac{i}{\hbar}\int_0^t\left(\frac{m\dot{y}^2}{2} - cy^2 - ey\dot{y}\right)dt''\right]\mathfrak{D}\left[y\left(t''\right)\right] \tag{19}$$

The remaining path integral can still be difficult to evaluate, but we can observe a few properties that it has. First, for any given path in the path integral, we must be able to express both y and $\dot{y}$ as functions of time t'', so the complete path integral can depend only on the end time t (and, of course, on the constants m, c and e). That is, the propagator will always have the form 1:

$$U\left(x,t;x',t'\right) = A\left(t\right)e^{iS_{cl}/\hbar} \tag{20}$$

We have already evaluated the integral for the free particle where $c = e = 0$ and we found there that

$$U\left(x,t;x'\right) = \sqrt{\frac{m}{2\pi\hbar i t}}e^{iS_{cl}/\hbar} \tag{21}$$

Since the constant b doesn't appear in 19, the propagator must have the same form for the more general case where $V = a + bx$. For more complex potentials, such as the harmonic oscillator, the function $A\left(t\right)$ will in general have a different form and will have to be calculated explicitly in these cases.

As an example, we'll consider the case of a particle subject to a constant force in the x direction, so that the potential is given by

$$V(x) = -fx \tag{22}$$

This gives a constant force of

$$F = -\frac{dV}{dx} = f \tag{23}$$

and thus a constant acceleration of f/m. For such a particle, its classical position is (from first year physics)

$$x_{cl}\left(t''\right) = x_0 + v_0 t'' + \frac{1}{2}\frac{f}{m}t''^2 \tag{24}$$

$$\dot{x}_{cl}\left(t''\right) = v_0 + \frac{f}{m}t'' \tag{25}$$

To find x_0 and v_0, we impose boundary conditions. At $t'' = 0$

$$x_{cl}(0) = x_0 = x' \tag{26}$$

At $t'' = t$, its position is

$$x_{cl}(t) = x = x' + v_0 t + \frac{f}{2m}t^2 \tag{27}$$

This gives

$$v_0 = \frac{x - x'}{t} - \frac{f}{2m}t \tag{28}$$

The classical Lagrangian is

$$L = T - V \tag{29}$$

$$= \frac{1}{2}m\dot{x}_{cl}^2 + fx_{cl} \tag{30}$$

$$= \frac{1}{2}m\left(v_0 + \frac{f}{m}t''\right)^2 + f\left(x_0 + v_0 t'' + \frac{1}{2}\frac{f}{m}t''^2\right) \tag{31}$$

$$= \frac{1}{2}m\left(\frac{x - x'}{t} - \frac{f}{2m}t + \frac{f}{m}t''\right)^2 + f\left(x' + \left(\frac{x - x'}{t} - \frac{f}{2m}t\right)t'' + \frac{1}{2}\frac{f}{m}t''^2\right) \tag{32}$$

Note that t is a constant, as it is the time of the endpoint of the motion. To find the classical action, we must integrate this from $t'' = 0$ to t. The integral is a straightforward integral of a quadratic in t'', although the algebra is tedious if done by hand, so is best done with Maple.

$$S_{cl} = \int_0^t L\, dt'' \tag{33}$$

$$= \frac{1}{3}\frac{f^2t^3}{m} + \left(\frac{x-x'}{t} - \frac{1}{2}\frac{ft}{m}\right) ft^2 + \frac{1}{2}m\left(\frac{x-x'}{t} - \frac{1}{2}\frac{ft}{m}\right)^2 t + fxt \tag{34}$$

$$= -\frac{f^2t^3}{24m} + \frac{1}{2}ft\left(x+x'\right) + \frac{m\left(x-x'\right)^2}{2t} \tag{35}$$

From 21, this gives a propagator of

$$U\left(x,t;x'\right) = \sqrt{\frac{m}{2\pi\hbar it}}\exp\left[\frac{i}{\hbar}\left(-\frac{f^2t^3}{24m} + \frac{1}{2}ft\left(x+x'\right) + \frac{m\left(x-x'\right)^2}{2t}\right)\right] \tag{36}$$

This agrees with Shankar's result in his equation 5.4.31.

As another example, consider the harmonic oscillator, where the potential is

$$V = \frac{1}{2}m\omega^2x^2 \tag{37}$$

This potential is also of the form 2, so the propagator must have the form 20. This time, however, since $c \neq 0$, the function $A\left(t\right)$ will probably not have the form used in 21. The best we can say therefore is that

$$U\left(x,t;x',t'\right) = A\left(t\right)e^{iS_{cl}/\hbar} \tag{38}$$

where $A\left(t\right)$ has the form (from 19):

$$A\left(t\right) = \int_0^0 \exp\left[\frac{i}{\hbar}\int_0^t\left(\frac{m\dot{y}^2}{2} - \frac{1}{2}m\omega^2y^2\right)dt''\right]\mathfrak{D}\left[y\left(t''\right)\right] \tag{39}$$

We worked out the classical action for the harmonic oscillator earlier and found

$$S_{cl} = \frac{m\omega}{2\sin\omega t}\left[\left(x'^2 + x^2\right)\cos\omega t - 2x'x\right] \tag{40}$$

where the particle is at x' at $t'' = 0$ and at x at $t'' = t$. The propagator is therefore

$$U\left(x,t;x'\right) = A\left(t\right)\exp\left[\frac{im\omega}{2\hbar\sin\omega t}\left(\left(x'^2 + x^2\right)\cos\omega t - 2x'x\right)\right] \tag{41}$$

with $A\left(t\right)$ given by 39.

COMMENTS

Name: Alex

Error in equation 0.18 I believe the RHS should be equal to m/2, not m. I think this is also incorrect in Shankar.

Time: October 25, 2017 at 11:23 pm

=========

Fixed now. Thanks.

PINGBACKS

Pingback: Harmonic oscillator energies and eigenfunctions derived from the propagator

HARMONIC OSCILLATOR ENERGIES AND EIGENFUNCTIONS DERIVED FROM THE PROPAGATOR

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Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 8. Section 8.6, Exercise 8.6.3.

Post date: 14 Feb 2017

Given the propagator for the harmonic oscillator, it is possible to work backwards and deduce the eigenvalues and eigenfunctions of the Hamiltonian, although this isn't the easiest way to find them. We've seen that the propagator for the oscillator is

$$U\left(x,t;x'\right)=A\left(t\right)\exp\left[\frac{im\omega}{2\hbar\sin\omega t}\left(\left(x'^{2}+x^{2}\right)\cos\omega t-2x'x\right)\right] \tag{1}$$

where $A\left(t\right)$ is some function of time which is found by doing a path integral. Shankar cheats a bit by just telling us what A is:

$$A\left(t\right)=\sqrt{\frac{m\omega}{2\pi i\hbar\sin\omega t}} \tag{2}$$

To deduce (some of) the energy levels, we can compare the propagator with its more traditional form

$$U\left(t\right)=\sum_{n}e^{-iE_{n}t/\hbar}\left|E_{n}\right\rangle\left\langle E_{n}\right| \tag{3}$$

where E_n is the nth energy level. In position space this is

$$U\left(t\right)=\sum_{n}\psi_{n}^{*}\left(x\right)\psi_{n}\left(x\right)e^{-iE_{n}t/\hbar} \tag{4}$$

We can try finding the energy levels as follows. We take $x=x'=t'=0$, which is equivalent to taking the end time t to be a multiple of a complete period of the oscillator, so that the particle has returned to its starting point. In that case, 1 becomes

$$U\left(x,t;x'\right)=A\left(t\right)=\sqrt{\frac{m\omega}{2\pi i\hbar\sin\omega t}} \tag{5}$$

If we can expand this quantity in powers of $e^{-i\omega t}$, we can compare it with the series 4 and read off the energies from the exponents in the series. To do this, we write

$$A(t) = \sqrt{\frac{m\omega}{\pi\hbar\left(e^{i\omega t} - e^{-i\omega t}\right)}} \tag{6}$$

$$= \sqrt{\frac{m\omega}{\pi\hbar}} e^{-i\omega t/2} \frac{1}{\sqrt{1 - e^{-2i\omega t}}} \tag{7}$$

To save writing, we'll define the symbol

$$\eta \equiv e^{-i\omega t} \tag{8}$$

so that

$$A(t) = \sqrt{\frac{m\omega}{\pi\hbar}} \eta^{1/2} \frac{1}{\sqrt{1 - \eta^2}} \tag{9}$$

We can now expand the last factor using the binomial expansion to get

$$A(t) = \sqrt{\frac{m\omega}{\pi\hbar}} \eta^{1/2} \left[1 + \frac{1}{2}\eta^2 + \frac{3}{8}\eta^4 + \ldots\right] \tag{10}$$

In terms of the original variables, we get

$$A(t) = \sqrt{\frac{m\omega}{\pi\hbar}} \left[e^{-i\omega t/2} + \frac{1}{2} e^{-5i\omega t/2} + \frac{3}{8} e^{-9i\omega t/2} + \ldots\right] \tag{11}$$

Comparing with 4, we find energy levels of

$$E = \frac{\hbar\omega}{2}, \frac{5\hbar\omega}{2}, \frac{9\hbar\omega}{2}, \ldots \tag{12}$$

These correspond to $E_0, E_2, E_4, \ldots$. The odd energy levels $\left(\frac{3\hbar\omega}{2}, \frac{7\hbar\omega}{2}, \ldots\right)$ are missing because the corresponding wave functions $\psi_n(x)$ are odd functions of x and are therefore zero at $x = 0$, so the corresponding terms in 4 vanish. The numerical coefficients in 11 give us $|\psi_n(0)|^2$ for $n = 0, 2, 4, \ldots$.

To get the other energies, as well as the eigenfunctions, from a comparison of 1 and 4 is possible, but quite messy, even for the lower energies. To do it, we take $t' = 0$ as before, but now we take $x = x' \neq 0$. That is, we start the oscillator off at some location $x' \neq 0$ and then look at it exactly one period later, when it has returned to the same position. The propagator 1 now becomes

$$U\left(x,t;x'\right) = \sqrt{\frac{m\omega}{2\pi i\hbar\sin\omega t}}\exp\left[\frac{im\omega}{2\hbar\sin\omega t}\left(2x^2\left(\cos\omega t-1\right)\right)\right] \tag{13}$$

$$= \sqrt{\frac{m\omega}{\pi\hbar\left(e^{i\omega t}-e^{-i\omega t}\right)}}\exp\left[-\frac{m\omega}{\hbar\left(e^{i\omega t}-e^{-i\omega t}\right)}\left(x^2\left(\left(e^{i\omega t}+e^{-i\omega t}\right)-2\right)\right)\right] \tag{14}$$

$$= \sqrt{\frac{m\omega}{\pi\hbar}}\eta^{1/2}\frac{1}{\sqrt{1-\eta^2}}\exp\left[-\frac{m\omega x^2}{\hbar}\left(\frac{\frac{1}{\eta}+\eta-2}{\frac{1}{\eta}-\eta}\right)\right] \tag{15}$$

$$= \sqrt{\frac{m\omega}{\pi\hbar}}\eta^{1/2}\frac{1}{\sqrt{1-\eta^2}}\exp\left[-\frac{m\omega x^2}{\hbar}\left(\frac{1+\eta^2-2\eta}{1-\eta^2}\right)\right] \tag{16}$$

We now need to expand this in a power series in η, which gets very messy so is best handled with software like Maple. Shankar asks only for the first two terms in the series (the terms corresponding to $\eta^{1/2}$ and $\eta^{3/2}$) but even doing this by hand can get very tedious. The result from Maple is, for the first two terms:

$$\eta^{1/2} \to \sqrt{\frac{m\omega}{\pi\hbar}}e^{-m\omega x^2/\hbar}\eta^{1/2} = \sqrt{\frac{m\omega}{\pi\hbar}}e^{-m\omega x^2/\hbar}e^{-i\omega t/2} \tag{17}$$

$$\eta^{3/2} \to \sqrt{\frac{m\omega}{\pi\hbar}}\frac{2m\omega}{\hbar}e^{-m\omega x^2/\hbar}x^2\eta^{3/2} = \sqrt{\frac{m\omega}{\pi\hbar}}\frac{2m\omega}{\hbar}e^{-m\omega x^2/\hbar}x^2e^{-3i\omega t/2} \tag{18}$$

Comparing this with 4, we can read off:

$$E_0 = \frac{\hbar\omega}{2} \tag{19}$$

$$\left|\psi_0\left(x\right)\right|^2 = \sqrt{\frac{m\omega}{\pi\hbar}}e^{-m\omega x^2/\hbar} \tag{20}$$

$$E_1 = \frac{3\hbar\omega}{2} \tag{21}$$

$$\left|\psi_1\left(x\right)\right|^2 = \sqrt{\frac{m\omega}{\pi\hbar}}\frac{2m\omega}{\hbar}e^{-m\omega x^2/\hbar}x^2 \tag{22}$$

To check this, we recall the eigenfunctions we worked out earlier, using Hermite polynomials

$$\psi_n(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\frac{1}{\sqrt{2^n n!}}H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right)e^{-m\omega x^2/2\hbar} \tag{23}$$

The first two Hermite polynomials are

$$H_0\left(\sqrt{\frac{m\omega}{\hbar}}x\right) = 1 \tag{24}$$

$$H_1\left(\sqrt{\frac{m\omega}{\hbar}}x\right) = 2\sqrt{\frac{m\omega}{\hbar}}x \tag{25}$$

Plugging these into 23 and comparing with 20 and 22 shows we got the right answer.

PATH INTEGRAL TO SCHRÖDINGER EQUATION FOR A VECTOR POTENTIAL

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Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 8. Section 8.6, Exercise 8.6.4.

Post date: 19 Feb 2017

When we showed that the path integral approach is equivalent to the Schrödinger equation, we did so for a scalar potential V, so that the Lagrangian is the usual $L = T - V$, and we can use that to calculate the action over an infinitestimal time interval ε, during which time the particle moves from x' to x. In the calculation, we chose the value of V at the midpoint of this interval, that is $V\left(\frac{x+x'}{2}\right)$. In fact, in this derivation it didn't matter where in the interval $[x', x]$ we chose to evaluate V, since we took only terms up to first order in ε, and moving the point at which we evaluate V introduced terms only of order ε^2 or higher.

Things get a bit more complicated if we consider a system such as the electromagnetic force, where the Lagrangian is no longer just $T - V$, but becomes

$$L = \frac{1}{2}m\mathbf{v}\cdot\mathbf{v} - q\phi + \frac{q}{c}\mathbf{v}\cdot\mathbf{A} \tag{1}$$

To examine the effect this has on the demonstration that the path integral approach is equivalent to the Schrödinger equation, we'll consider only one dimension, and leave out the electrostatic potential ϕ since it's just a scalar potential and we already know that such potentials do indeed convert to the Schrödinger equation. Thus the Lagrangian we'll consider is

$$L = \frac{1}{2}mv^2 + \frac{q}{c}vA \tag{2}$$

Over the infinitesimal time interval ε we have

$$v = \frac{x - x'}{\varepsilon} \tag{3}$$

The propagator over this time interval is

$$U\left(x,\varepsilon;x',0\right)=\sqrt{\frac{m}{2\pi\hbar\varepsilon i}}\exp\left[\frac{i}{\hbar}\left(\frac{1}{2}m\frac{\left(x-x'\right)^2}{\varepsilon}+\varepsilon\frac{q}{c}\frac{x-x'}{\varepsilon}A\left(x+\alpha\left(x-x'\right)\right)\right)\right] \tag{4}$$

$$=\sqrt{\frac{m}{2\pi\hbar\varepsilon i}}\exp\left[\frac{i}{\hbar}\left(\frac{1}{2}m\frac{\eta^2}{\varepsilon}-\frac{q}{c}\eta A\left(x+\alpha\eta\right)\right)\right] \tag{5}$$

$$=\sqrt{\frac{m}{2\pi\hbar\varepsilon i}}\exp\left(\frac{im\eta^2}{2\hbar\varepsilon}\right)\exp\left[-\frac{iq}{\hbar c}\eta A\left(x+\alpha\eta\right)\right] \tag{6}$$

where α is a parameter that we can vary between 0 and 1 in order to vary the point along the path from x' to x at which we evaluate the vector potential A. Also,

$$\eta\equiv x'-x \tag{7}$$

Using the same argument as before, we require

$$|\eta|\lesssim\sqrt{\frac{2\hbar\varepsilon\pi}{m}} \tag{8}$$

so calculations to first order in ε must include terms up to second order in η.

Once we have $U\left(x,\varepsilon;x',0\right)$, we can find $\psi\left(x,\varepsilon\right)$ from

$$\psi\left(x,\varepsilon\right)=\int_{-\infty}^{\infty}U\left(x,\varepsilon;x',0\right)\psi\left(x',0\right)dx' \tag{9}$$

To find U to first order in ε, we need to expand the second exponential in 6 out to terms in η^2, so we first look at the argument of the exponential:

$$-\frac{iq}{\hbar c}\eta A\left(x+\alpha\eta\right)=-\frac{iq}{\hbar c}\left(\eta A\left(x\right)+\alpha\eta^2\frac{\partial A}{\partial x}+\ldots\right) \tag{10}$$

where the derivative is evaluated at the endpoint x and is constant in the integral. The second exponential in 6 now becomes, to second order in η:

$$\exp\left[-\frac{iq}{\hbar c}\eta A\left(x+\alpha\eta\right)\right]=1-\frac{iq}{\hbar c}\left(\eta A\left(x\right)+\alpha\eta^2\frac{\partial A}{\partial x}\right)-\left(\frac{q}{\hbar c}\right)^2\frac{\eta^2A^2\left(x\right)}{2} \tag{11}$$

We also need the expansion of the wave function in 9 up to second order in η:

$$\psi\left(x+\eta,0\right)=\psi\left(x,0\right)+\eta\frac{\partial\psi}{\partial x}+\frac{\eta^2}{2}\frac{\partial^2\psi}{\partial x^2} \tag{12}$$

Again, both derivatives are evaluated at the endpoint x and are constants in the integral.

We now need to do the integral 9, which consists of several standard Gaussian integrals. From 7, $dx' = d\eta$, so

$$\int_{-\infty}^{\infty} U\left(x,\varepsilon;x',0\right)\psi\left(x',0\right)dx' = \sqrt{\frac{m}{2\pi\hbar\varepsilon i}}\psi\left(x,0\right)\int_{-\infty}^{\infty}\exp\left(\frac{im\eta^2}{2\hbar\varepsilon}\right)d\eta + \tag{13}$$

$$\sqrt{\frac{m}{2\pi\hbar\varepsilon i}}\left(\frac{\partial\psi}{\partial x} - \frac{iq}{\hbar c}A\left(x\right)\psi\left(x,0\right)\right)\int_{-\infty}^{\infty}\exp\left(\frac{im\eta^2}{2\hbar\varepsilon}\right)\eta\, d\eta + \tag{14}$$

$$\sqrt{\frac{m}{2\pi\hbar\varepsilon i}}\left[\frac{1}{2}\frac{\partial^2\psi}{\partial x^2} - \frac{iq}{\hbar c}A\left(x\right)\frac{\partial\psi}{\partial x} + \right. \tag{15}$$

$$\left.\psi\left(x,0\right)\left(-\frac{iq\alpha}{\hbar c}\frac{\partial A}{\partial x} - \frac{1}{2}\left(\frac{qA\left(x\right)}{\hbar c}\right)^2\right)\right]\times \tag{16}$$

$$\int_{-\infty}^{\infty}\exp\left(\frac{im\eta^2}{2\hbar\varepsilon}\right)\eta^2 d\eta \tag{17}$$

We can now do the integrals:

$$\int_{-\infty}^{\infty}\exp\left(\frac{im\eta^2}{2\hbar\varepsilon}\right)d\eta = \sqrt{\frac{2\pi\hbar\varepsilon i}{m}} \tag{18}$$

$$\int_{-\infty}^{\infty}\exp\left(\frac{im\eta^2}{2\hbar\varepsilon}\right)\eta\, d\eta = 0 \tag{19}$$

$$\int_{-\infty}^{\infty}\exp\left(\frac{im\eta^2}{2\hbar\varepsilon}\right)\eta^2 d\eta = -\frac{\hbar\varepsilon}{im}\sqrt{\frac{2\pi\hbar\varepsilon i}{m}} \tag{20}$$

Plugging these in we get

$$\psi\left(x,\varepsilon\right) = \psi\left(x,0\right) - \frac{\hbar\varepsilon}{im}\left[\frac{1}{2}\frac{\partial^2\psi}{\partial x^2} - \frac{iq}{\hbar c}A\left(x\right)\frac{\partial\psi}{\partial x} + \psi\left(x,0\right)\left(-\frac{iq\alpha}{\hbar c}\frac{\partial A}{\partial x} - \frac{1}{2}\left(\frac{qA\left(x\right)}{\hbar c}\right)^2\right)\right] \tag{21}$$

$$= \psi\left(x,0\right) + \frac{\varepsilon}{i\hbar}\left[-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + \frac{i\hbar q}{mc}A\left(x\right)\frac{\partial\psi}{\partial x} + \psi\left(x,0\right)\left(\frac{i\hbar q\alpha}{mc}\frac{\partial A}{\partial x} + \frac{1}{2m}\left(\frac{qA\left(x\right)}{c}\right)^2\right)\right] \tag{22}$$

We can compare this with the quantum version of the Hamiltonian for the vector potential part of the electromagnetic force. The classical Hamiltonian is

$$H = \frac{|\mathbf{p} - q\mathbf{A}/c|^2}{2m} \tag{23}$$

Because $\mathbf{A}$ depends on x, it doesn't commute with $\mathbf{p}$ so to get the quantum version we need to symmetrize when we expand the square. The one dimensional version is

$$H = \frac{P^2}{2m} - \frac{q}{2mc}PA - \frac{q}{2mc}AP + \frac{q^2A^2}{2mc^2} \tag{24}$$

In the coordinate basis, we have, using $P = -i\hbar\partial/\partial x$

$$H\psi = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + \frac{i\hbar q}{2mc}\left(\frac{\partial(A\psi)}{\partial x} + A\frac{\partial\psi}{\partial x}\right) + \frac{q^2A^2}{2mc^2}\psi \tag{25}$$

$$= -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + \frac{i\hbar q}{2mc}\left(2A\frac{\partial\psi}{\partial x} + \psi\frac{\partial A}{\partial x}\right) + \frac{q^2A^2}{2mc^2}\psi \tag{26}$$

$$= -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + \frac{i\hbar q}{mc}\left(A\frac{\partial\psi}{\partial x} + \frac{1}{2}\psi\frac{\partial A}{\partial x}\right) + \frac{q^2A^2}{2mc^2}\psi \tag{27}$$

Returning to the result we got from the path integral, upon rearranging 22 we get

$$i\hbar\frac{\psi(x,\varepsilon) - \psi(x,0)}{\varepsilon} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + \frac{i\hbar q}{mc}\left(A(x)\frac{\partial\psi}{\partial x} + \alpha\psi(x,0)\frac{\partial A}{\partial x}\right) + \frac{\psi(x,0)}{2m}\left(\frac{qA(x)}{c}\right)^2 \tag{28}$$

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + \frac{i\hbar q}{mc}\left(A(x)\frac{\partial\psi}{\partial x} + \alpha\psi\frac{\partial A}{\partial x}\right) + \frac{\psi}{2m}\left(\frac{qA(x)}{c}\right)^2 \tag{29}$$

where in the last line we took the limit as $\varepsilon \to 0$ on the LHS to get Schrödinger's equation in the form

$$i\hbar\frac{\partial\psi}{\partial t} = H\psi \tag{30}$$

Comparing the RHS of 29 with 27, we see that they are equal provided we take $\alpha = \frac{1}{2}$. Thus in this case, we really do need to evaluate the vector potential A at the midpoint of the path.

UNCERTAINTY PRINCIPLE - A STRONGER FORM

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 9.

Post date: 25 May 2017

[If some equations are too small to read easily, use your browser's magnifying option (Ctrl + on Chrome, probably something similar on other browsers).]

Shankar's derivation of the general uncertainty principle relating the variances of two Hermitian operators actually gives a different result from that in Griffiths. To follow this post, you should first review the earlier post. To keep things consistent I'll use the original Griffiths notation up to equation 11, which is a summary of the earlier post.

Shankar's derivation is the same as Griffiths's up to equation (13) in the earlier post. To summarize, we have two operators $\hat{A}$ and $\hat{B}$ and calculate their variances as

$$\sigma_A^2 = \left\langle \Psi | (\hat{A} - \langle A \rangle)^2 \Psi \right\rangle \tag{0.1}$$

$$= \left\langle \left(\hat{A} - \langle A \rangle\right) \Psi | \left(\hat{A} - \langle A \rangle\right) \Psi \right\rangle \tag{0.2}$$

$$\equiv \langle f | f \rangle \tag{0.3}$$

where the function f is defined by this equation.

Similarly, for $\hat{B}$:

$$\sigma_B^2 = \left\langle \Psi | (\hat{B} - \langle B \rangle)^2 \Psi \right\rangle \tag{0.4}$$

$$= \left\langle \left(\hat{B} - \langle B \rangle\right) \Psi | \left(\hat{B} - \langle B \rangle\right) \Psi \right\rangle \tag{0.5}$$

$$\equiv \langle g | g \rangle \tag{0.6}$$

We now invoke the Schwarz inequality to say

$$\sigma_A^2 \sigma_B^2 = \langle f | f \rangle \langle g | g \rangle \tag{0.7}$$

$$\geq |\langle f | g \rangle|^2 \tag{0.8}$$

At this point, Griffiths continues by saying that

$$|\langle f | g \rangle|^2 \geq (\Im \langle f | g \rangle)^2 \tag{0.9}$$

That is, he throws away the real part of $\langle f|g\rangle$ to get another inequality. Shankar retains the full complex number and thus states that

$$|\langle f|g\rangle|^2 = \left|\left\langle \left(\hat{A}-\langle A\rangle\right)\Psi\right| \left(\hat{B}-\langle B\rangle\right)\Psi\right\rangle\Big|^2 \tag{0.10}$$

$$= \left|\left\langle \Psi\right| \left(\hat{A}-\langle A\rangle\right)\left(\hat{B}-\langle B\rangle\right)\left|\Psi\right\rangle\right|^2 \tag{0.11}$$

Defining the operators

$$\hat{\Omega} \equiv \hat{A}-\langle A\rangle \tag{0.12}$$

$$\hat{\Lambda} \equiv \hat{B}-\langle B\rangle \tag{0.13}$$

we have

$$|\langle f|g\rangle|^2 = \left|\left\langle \Psi\right|\hat{\Omega}\hat{\Lambda}\left|\Psi\right\rangle\right|^2 \tag{0.14}$$

$$= \frac{1}{4}\left|\left\langle \Psi\right|\left[\hat{\Omega},\hat{\Lambda}\right]_+ + \left[\hat{\Omega},\hat{\Lambda}\right]\left|\Psi\right\rangle\right|^2 \tag{0.15}$$

where

$$\left[\hat{\Omega},\hat{\Lambda}\right]_+ \equiv \hat{\Omega}\hat{\Lambda}+\hat{\Lambda}\hat{\Omega} \tag{0.16}$$

is the anticommutator. For two Hermitian operators, the commutator is the difference between a value and its complex conjugate, so is always pure imaginary (and thus the anticommutator is always real), so we can write this as

$$\left[\hat{\Omega},\hat{\Lambda}\right] = i\Gamma \tag{0.17}$$

for some Hermitian operator Γ. Using the triangle inequality, we thus arrive at

$$\sigma_A^2\sigma_B^2 \geq |\langle f|g\rangle|^2 \geq \frac{1}{4}\left\langle \Psi\right|\left[\hat{\Omega},\hat{\Lambda}\right]_+\left|\Psi\right\rangle^2 + \frac{1}{4}\langle\Psi|\Gamma|\Psi\rangle^2 \tag{0.18}$$

Comparing this with Griffiths's result, he had

$$\sigma_A^2\sigma_B^2 \geq \left(\frac{1}{2i}\langle[\hat{A},\hat{B}]\rangle\right)^2 = \frac{1}{4}\langle\Psi|\Gamma|\Psi\rangle^2 \tag{0.19}$$

That is, Griffiths's uncertainty principle is actually weaker than Shankar's as he includes only the last term in 0.18. For canonically conjugate operators (such as X and P) the commutator is always

$$[X,P] = i\hbar \tag{0.20}$$

so the last term in 0.18 is always $\hbar^2/4$ for any wave function Ψ. The first term in 0.18, which involves the anticommutator, will, in general, depend on the wave function Ψ, but it is always positive (or zero), so we can still state that, for such operators

$$\sigma_A^2 \sigma_B^2 \geq \frac{\hbar^2}{4} \tag{0.21}$$

UNCERTAINTIES IN THE HARMONIC OSCILLATOR AND HYDROGEN ATOM

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 9, Exercises 9.4.1 - 9.4.2.

Post date: 21 Feb 2017

Here we'll look at a couple of calculations relevant to the application of the uncertainty principle to the hydrogen atom. When calculating uncertainties, we need to find the average values of various quantities. First, we'll look at an average in the case of the harmonic oscillator.

The harmonic oscillator eigenstates are

$$\psi_n(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right) e^{-m\omega x^2/2\hbar} \tag{1}$$

where H_n is the nth Hermite polynomial. For $n = 1$, we have

$$H_1\left(\sqrt{\frac{m\omega}{\hbar}}x\right) = 2\sqrt{\frac{m\omega}{\hbar}}x \tag{2}$$

so

$$\psi_1(x) = \frac{\sqrt{2}}{\pi^{1/4}} \left(\frac{m\omega}{\hbar}\right)^{3/4} x\, e^{-m\omega x^2/2\hbar} \tag{3}$$

For this state, we can calculate the average

$$\left\langle \frac{1}{X^2} \right\rangle = \int_{-\infty}^{\infty} \psi_1^2(x) \frac{1}{x^2} dx \tag{4}$$

$$= \frac{2}{\sqrt{\pi}} \left(\frac{m\omega}{\hbar}\right)^{3/2} \int_{-\infty}^{\infty} e^{-m\omega x^2/\hbar} dx \tag{5}$$

$$= \frac{2}{\sqrt{\pi}} \left(\frac{m\omega}{\hbar}\right)^{3/2} \sqrt{\frac{\pi\hbar}{m\omega}} \tag{6}$$

$$= \frac{2m\omega}{\hbar} \tag{7}$$

where we evaluated the Gaussian integral in the second line.

We can compare this to $1/\left\langle X^2 \right\rangle$ as follows:

$$\left\langle X^2 \right\rangle = \int_{-\infty}^{\infty} \psi_1^2(x) x^2 dx \tag{8}$$

$$= \frac{2}{\sqrt{\pi}} \left(\frac{m\omega}{\hbar}\right)^{3/2} \int_{-\infty}^{\infty} e^{-m\omega x^2/\hbar} x^4 dx \tag{9}$$

$$= \frac{2}{\sqrt{\pi}} \left(\frac{m\omega}{\hbar}\right)^{3/2} \frac{3\sqrt{\pi}}{4} \left(\frac{\hbar}{m\omega}\right)^{5/2} \tag{10}$$

$$= \frac{3}{2}\frac{\hbar}{m\omega} \tag{11}$$

$$\frac{1}{\langle X^2 \rangle} = \frac{2}{3}\frac{m\omega}{\hbar} \tag{12}$$

Thus $\left\langle \frac{1}{X^2} \right\rangle$ and $\frac{1}{\langle X^2 \rangle}$ have the same order of magnitude, although they are not equal.

In three dimensions, we consider the ground state of hydrogen

$$\psi_{100}(r) = \frac{1}{\sqrt{\pi} a_0^{3/2}} e^{-r/a_0} \tag{13}$$

where a_0 is the Bohr radius

$$a_0 \equiv \frac{\hbar^2}{me^2} \tag{14}$$

with m and e being the mass and charge of the electron. The wave function is normalized as we can see by doing the integral (in 3 dimensions):

$$\int \psi_{100}^2(r) d^3\mathbf{r} \;\; = \;\; \frac{4\pi}{\pi a_0^3} \int_0^{\infty} e^{-2r/a_0} r^2 dr \tag{15}$$

We can use the formula (given in Shankar's Appendix 2)

$$\int_0^{\infty} e^{-r/\alpha} r^n dr = \frac{n!}{\alpha^{n+1}} \tag{16}$$

We get

$$\int \psi_{100}^2(r) d^3\mathbf{r} = \frac{4\pi}{\pi a_0^3} \frac{2!}{2^3} a_0^3 = 1 \tag{17}$$

as required.

For a spherically symmetric wave function centred at $r = 0$,

$$(\Delta X)^2 = \left\langle X^2 \right\rangle - \langle X \rangle^2 = \left\langle X^2 \right\rangle \tag{18}$$

with identical relations for Y and Z. Since

$$r^2 = x^2 + y^2 + z^2 \tag{19}$$

$$\left\langle r^2 \right\rangle = \left\langle x^2 \right\rangle + \left\langle y^2 \right\rangle + \left\langle z^2 \right\rangle = 3\left\langle X^2 \right\rangle \tag{20}$$

$$\left\langle X^2 \right\rangle = \frac{1}{3}\left\langle r^2 \right\rangle \tag{21}$$

Thus

$$\left\langle X^2 \right\rangle = \frac{1}{3}\int \psi_{100}^2(r) r^2 d^3\mathbf{r} \tag{22}$$

$$= \frac{4\pi}{3\pi a_0^3}\int_0^\infty e^{-2r/a_0} r^4 dr \tag{23}$$

$$= \frac{4}{3a_0^3}\frac{4!}{2^5}a_0^5 \tag{24}$$

$$= a_0^2 \tag{25}$$

$$\Delta X = a_0 = \frac{\hbar^2}{me^2} \tag{26}$$

We can also find

$$\left\langle \frac{1}{r} \right\rangle = \int \psi_{100}^2(r)\frac{1}{r} d^3\mathbf{r} \tag{27}$$

$$= \frac{4\pi}{\pi a_0^3}\int_0^\infty e^{-2r/a_0} r\, dr \tag{28}$$

$$= \frac{4}{a_0^3}\frac{a_0^2}{4} \tag{29}$$

$$= \frac{1}{a_0} \tag{30}$$

$$\langle r \rangle = \int \psi_{100}^2(r) r\, d^3\mathbf{r} \tag{31}$$

$$= \frac{4\pi}{\pi a_0^3}\int_0^\infty e^{-2r/a_0} r^3 dr \tag{32}$$

$$= \frac{4}{a_0^3}\frac{6a_0^4}{16} \tag{33}$$

$$= \frac{3}{2}a_0 \tag{34}$$

Thus both $\left\langle \frac{1}{r} \right\rangle$ and $\frac{1}{\langle r \rangle}$ are of the same order of magnitude as $1/a_0 = me^2/\hbar^2$.

PINGBACKS

Pingback: Uncertainty principle and an estimate of the ground state energy of hydrogen

UNCERTAINTY PRINCIPLE AND AN ESTIMATE OF THE GROUND STATE ENERGY OF HYDROGEN

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Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 9, Exercise 9.4.3.

Post date: 23 Feb 2017

The uncertainty principle can be used to get an estimate of the ground state energy in some systems. In his section 9.4, Shankar shows how this is done for the hydrogen atom, treating the system as a proper 3-d system.

A somewhat simpler analysis can be done by treating the hydrogen atom as a one-dimensional system. The Hamiltonian is

$$H = \frac{P^2}{2m} - \frac{e^2}{(R^2)^{1/2}} \tag{1}$$

where m and e are the mass and charge of the electron. The operators P and R stand for the 3-d momentum and position:

$$\begin{aligned} P^2 &= P_x^2 + P_y^2 + P_z^2 && (2)\\ R^2 &= X^2 + Y^2 + Z^2 && (3) \end{aligned}$$

If we ignore the expansions of P^2 and R^2 and treat the Hamiltonian as a function of the operators P and R on their own, we can use the uncertainty principle to get a bound on the ground state energy. By analogy with one-dimensional position and momentum, we assume that the uncertainties are related by

$$\Delta P \cdot \Delta R \geq \frac{\hbar}{2} \tag{4}$$

By using coordinates such that the hydrogen atom is centred at the origin, and from the spherical symmetry of the ground state, we have

$$\begin{aligned} (\Delta P)^2 &= \left\langle P^2 \right\rangle - \langle P \rangle^2 = \left\langle P^2 \right\rangle && (5)\\ (\Delta R)^2 &= \left\langle R^2 \right\rangle - \langle R \rangle^2 = \left\langle R^2 \right\rangle && (6) \end{aligned}$$

We can then write 1 as

$$\langle H\rangle = \frac{\langle P^2\rangle}{2m} - e^2\left\langle \frac{1}{(R^2)^{1/2}}\right\rangle \tag{7}$$

$$\simeq \frac{\langle P^2\rangle}{2m} - \frac{e^2}{\left\langle\sqrt{\langle R^2\rangle}\right\rangle} \tag{8}$$

where in the last line we used an argument similar to that considered earlier, in which we showed that, for a one-dimensional system,

$$\left\langle \frac{1}{X^2}\right\rangle \simeq \frac{1}{\langle X^2\rangle} \tag{9}$$

where the $\simeq$ sign means 'same order of magnitude'. We can now write the mean of the Hamiltonian in terms of the uncertainties:

$$\langle H\rangle \simeq \frac{(\Delta P)^2}{2m} - \frac{e^2}{\Delta R} \tag{10}$$

$$\gtrsim \frac{\hbar^2}{8m(\Delta R)^2} - \frac{e^2}{\Delta R} \tag{11}$$

We can now minimize $\langle H\rangle$:

$$\frac{\partial\langle H\rangle}{\partial(\Delta R)} = -\frac{\hbar^2}{4m(\Delta R)^3} + \frac{e^2}{(\Delta R)^2} = 0 \tag{12}$$

$$\Delta R = \frac{\hbar^2}{4me^2} \tag{13}$$

This gives an estimate for the ground state energy of

$$\langle H\rangle_{g.s.} \simeq -\frac{2me^4}{\hbar^2} \tag{14}$$

The actual value is

$$E_0 = -\frac{me^4}{2\hbar^2} \tag{15}$$

so our estimate is too large (in magnitude) by a factor of 4. For comparison, the estimate worked out by Shankar for the 3-d case is

$$\langle H\rangle \gtrsim -\frac{2me^4}{9\hbar^2} \tag{16}$$

This estimate is too small by around a factor of 2.

DIRECT PRODUCT OF TWO VECTOR SPACES

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Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 10, Exercise 10.1.1.

Post date: 26 Feb 2017

Although we've studied quantum systems of more than one particle before (for example, systems of fermions and bosons) as covered by Griffiths's book, the wave functions associated with such particles were just given as products of single-particle wave functions (or linear combinations of these products). We didn't examine the linear algebra behind these functions. In his chapter 10, Shankar begins by describing the algebra of a direct product vector space, so we'll review this here.

The physics begins with an extension of the postulate of quantum mechanics that, for a single particle, the position and momentum obey the commutation relation

$$[X, P] = i\hbar \tag{1}$$

To extend this to multi-particle systems, we propose

$$\begin{aligned} [X_i, P_j] &= i\hbar\delta_{ij} && (2)\\ [X_i, X_j] &= [P_i, P_j] = 0 && (3) \end{aligned}$$

where the subscripts refer to the particle we're considering.

These postulates are translations of the classical Poisson brackets from classical mechanics, following the prescription that to obtain the quantum commutator, we multiply the classical Poisson bracket by $i\hbar$. The physics in these relations is that properties such as position or momentum of different particles are simultaneously observable, although the position and momentum of a single particle are still governed by the uncertainty principle.

We'll now restrict our attention to a two-particle system. In such a system, the eigenstate of the position operators is written as $|x_1 x_2\rangle$ and satisfies the eigenvalue equation

$$X_i |x_1 x_2\rangle = x_i |x_1 x_2\rangle \tag{4}$$

Operators referring to particle i effectively ignore any quantities associated with the other particle.

So what exactly are these states $|x_1 x_2\rangle$? They are a set of vectors that span a Hilbert space that describes the state of two particles. Note that we can use any two commuting operators $\mathbf{\Omega}_1(X_1, P_1)$ and $\mathbf{\Omega}_2(X_2, P_2)$ to create a set of eigenkets $|\omega_1 \omega_2\rangle$ which also span the space. Any operator that is a function of the position and momentum of only one of the particles always commutes with a similar operator that is a function of only the other particle, since the position and momentum operators of which it is a function commute with those of the other operator. That is

$$[\mathbf{\Omega}(X_1, P_1), \mathbf{\Lambda}(X_2, P_2)] = 0 \tag{5}$$

The space spanned by $|x_1 x_2\rangle$ can also be written as a *direct product* of two one-particle spaces. This space is written as $\mathbb{V}_{1\otimes 2}$ where the symbol $\otimes$ is the direct product symbol (it's also the logo of the X-Men, but we won't pursue that). The direct product is composed of the two single-particle spaces $\mathbb{V}_1$ (spanned by $|x_1\rangle$) and $\mathbb{V}_2$ (spanned by $|x_2\rangle$). The notation gets quite cumbersome at this point, so let's spell it out carefully. For an operator $\mathbf{\Omega}$, we can specify which *particle* it acts on by a subscript, and which *space* it acts on by a superscript. Thus $X_1^{(1)}$ is the position operator for particle 1, which operates on the vector space $\mathbb{V}_1$. It might seem redundant at this point to specify both the particle and the space, since it would seem that these are always the same. However, be patient...

From the two one-particle spaces, we can form the two-particle space by taking the direct product of the two one-particle states. Thus the state in which particle 1 is in state $|x_1\rangle$ and particle 2 is in state $|x_2\rangle$ is written as

$$|x_1 x_2\rangle = |x_1\rangle \otimes |x_2\rangle \tag{6}$$

It is important to note that this object is composed of two vectors from *different* vector spaces. The inner and outer products we've dealt with up to now, for things like finding the probability that a state has a particular value and so on, that is, objects like $\langle\psi_1|\psi_2\rangle$ and $|\psi_1\rangle\langle\psi_2|$, are composed of two vectors from the *same* vector space, so no direct product is needed.

If we recall the direct sum of two vector spaces

$$\mathbb{V}_{1\oplus 2} = \mathbb{V}_1 \oplus \mathbb{V}_2 \tag{7}$$

in that case, the dimension of $\mathbb{V}_{1\oplus 2}$ is the sum of the dimensions of $\mathbb{V}_1$ and $\mathbb{V}_2$. For a direct product we see from 6 that for each vector $|x_1\rangle$ there is one basis vector for each vector $|x_2\rangle$. Thus the number of basis vectors is the *product* of the number of basis vectors in each of the two one-particle spaces. In other words, the dimension of a direct product is the product of the dimensions of the two vector spaces of which it is composed. [In the case here, both the spaces $\mathbb{V}_1$ and $\mathbb{V}_2$ have infinite dimension, so the

dimension of $\mathbb{V}_{1\otimes 2}$ is in effect, 'doubly infinite'. In a case where $\mathbb{V}_1$ and $\mathbb{V}_2$ have finite dimension, we can then just multiply these dimensions to get the dimension of $\mathbb{V}_{1\otimes 2}$.]

As $\mathbb{V}_{1\otimes 2}$ is a vector space with basis vectors $|x_1\rangle \otimes |x_2\rangle$, any linear combination of the basis vectors is also a vector in the space $\mathbb{V}_{1\otimes 2}$. Thus the vector

$$|\psi\rangle = |x_1\rangle \otimes |x_2\rangle + |y_1\rangle \otimes |y_2\rangle \tag{8}$$

is in $\mathbb{V}_{1\otimes 2}$, although it can't be written as a direct product of the two one-particle spaces $\mathbb{V}_1$ and $\mathbb{V}_2$.

Having defined the direct product space, we now need to consider operators in this space. Although Shankar states that it 'is intuitively clear' that a single particle operator such as $X_1^{(1)}$ must have a corresponding operator in the product space that has the same effect has $X_1^{(1)}$ has on the single particle state, it seems to me to be more of a postulate. In any case, it is proposed that if

$$X_1^{(1)} |x_1\rangle = x_1 |x_1\rangle \tag{9}$$

then in the product space there must be an operator $X_1^{(1)\otimes(2)}$ that operates only on particle 1, with the same effect, that is

$$X_1^{(1)\otimes(2)} |x_1\rangle \otimes |x_2\rangle = x_1 |x_1\rangle \otimes |x_2\rangle \tag{10}$$

The notation can be explained as follows. The subscript 1 in $X_1^{(1)\otimes(2)}$ means that the operator operates on particle 1, while the superscript $(1)\otimes(2)$ means that the operator operates in the product space $\mathbb{V}_{1\otimes 2}$. In effect, the operator $X_1^{(1)\otimes(2)}$ is the product of two one-particle operators $X_1^{(1)}$, which operates on space $\mathbb{V}_1$ and an identity operator $I_2^{(2)}$ which operates on space $\mathbb{V}_2$. That is, we can write

$$\begin{aligned} X_1^{(1)\otimes(2)} &= X_1^{(1)} \otimes I_2^{(2)} && (11)\\ X_1^{(1)\otimes(2)} |x_1\rangle \otimes |x_2\rangle &= \left|X_1^{(1)} x_1\right\rangle \otimes \left|I_2^{(2)} x_2\right\rangle && (12)\\ &= x_1 |x_1\rangle \otimes |x_2\rangle && (13) \end{aligned}$$

Generally, if we have two one-particle operators $\Gamma_1^{(1)}$ and $\Lambda_2^{(2)}$, each of which operates on a different one-particle state, then we can form a direct product operator with the property

$$\left(\Gamma_1^{(1)} \otimes \Lambda_2^{(2)}\right) |\omega_1\rangle \otimes |\omega_2\rangle = \left|\Gamma_1^{(1)} \omega_1\right\rangle \otimes \left|\Lambda_2^{(2)} \omega_2\right\rangle \tag{14}$$

That is, a single-particle operator that operates on space i that forms part of a direct product operator operates only on the factor of a direct product vector that corresponds to the one-particle space. Given this property, it's fairly easy to derive a few properties of direct product operators.

$$\left[\Omega_1^{(1)} \otimes I^{(2)}, I^{(1)} \otimes \Lambda_2^{(2)}\right] |\omega_1\rangle \otimes |\omega_2\rangle = \Omega_1^{(1)} \otimes I^{(2)} I^{(1)} \otimes \Lambda_2^{(2)} |\omega_1\rangle \otimes |\omega_2\rangle - \tag{15}$$

$$I^{(1)} \otimes \Lambda_2^{(2)} \Omega_1^{(1)} \otimes I^{(2)} |\omega_1\rangle \otimes |\omega_2\rangle \tag{16}$$

$$= \Omega_1^{(1)} \otimes I^{(2)} \left| I^{(1)} \omega_1 \right\rangle \otimes \left| \Lambda_2^{(2)} \omega_2 \right\rangle - \tag{17}$$

$$I^{(1)} \otimes \Lambda_2^{(2)} \left| \Omega_1^{(1)} \omega_1 \right\rangle \otimes \left| I^{(2)} \omega_2 \right\rangle \tag{18}$$

$$= \left| \Omega_1^{(1)} \omega_1 \right\rangle \otimes \left| I^{(2)} \Lambda_2^{(2)} \omega_2 \right\rangle - \tag{19}$$

$$\left| I^{(1)} \Omega_1^{(1)} \omega_1 \right\rangle \otimes \left| \Lambda_2^{(2)} \omega_2 \right\rangle \tag{20}$$

$$= \left| \Omega_1^{(1)} \omega_1 \right\rangle \otimes \left| \Lambda_2^{(2)} \omega_2 \right\rangle - \left| \Omega_1^{(1)} \omega_1 \right\rangle \otimes \left| \Lambda_2^{(2)} \omega_2 \right\rangle \tag{21}$$

$$= 0 \tag{22}$$

This derivation shows that the identity operators effectively cancel out and we're left with the earlier commutator 5 between two operators that operate on different spaces.

The next derivation involves the successive operation of two direct product operators.

$$\left(\Omega_1^{(1)} \otimes \Gamma_2^{(2)}\right)\left(\theta_1^{(1)} \otimes \Lambda_2^{(2)}\right)|\omega_1\rangle \otimes |\omega_2\rangle = \left(\Omega_1^{(1)} \otimes \Gamma_2^{(2)}\right)\left|\theta_1^{(1)}\omega_1\right\rangle \otimes \left|\Lambda_2^{(2)}\omega_2\right\rangle \tag{23}$$

$$= \left|\Omega_1^{(1)}\theta_1^{(1)}\omega_1\right\rangle \otimes \left|\Gamma_2^{(2)}\Lambda_2^{(2)}\omega_2\right\rangle \tag{24}$$

$$= \left(\Omega_1^{(1)}\theta_1^{(1)}\right) \otimes \left(\Gamma_2^{(2)}\Lambda_2^{(2)}\right)|\omega_1\rangle \otimes |\omega_2\rangle \tag{25}$$

$$= \left\{(\Omega\theta)^{(1)} \otimes (\Gamma\Lambda)^{(2)}\right\}|\omega_1\rangle \otimes |\omega_2\rangle \tag{26}$$

$$\left(\Omega_1^{(1)} \otimes \Gamma_2^{(2)}\right)\left(\theta_1^{(1)} \otimes \Lambda_2^{(2)}\right) = (\Omega\theta)^{(1)} \otimes (\Gamma\Lambda)^{(2)} \tag{27}$$

Next, another commutator identity. Given

$$\left[\Omega_1^{(1)}, \Lambda_1^{(1)}\right] = \Gamma_1^{(1)} \tag{28}$$

we have

$$\left[\Omega_1^{(1)\otimes(2)}, \Lambda_1^{(1)\otimes(2)}\right]|\omega_1\rangle \otimes |\omega_2\rangle = \left[\Omega_1^{(1)} \otimes I^{(2)}, \Lambda_1^{(1)} \otimes I^{(2)}\right]|\omega_1\rangle \otimes |\omega_2\rangle \tag{29}$$

$$= \left|\left[\Omega_1^{(1)}, \Lambda_1^{(1)}\right]\omega_1\right\rangle \otimes \left|I^{(2)}\omega_2\right\rangle \tag{30}$$

$$= \left|\Gamma_1^{(1)}\omega_1\right\rangle \otimes \left|I^{(2)}\omega_2\right\rangle \tag{31}$$

$$= \Gamma_1^{(1)} \otimes I^{(2)}|\omega_1\rangle \otimes |\omega_2\rangle \tag{32}$$

$$\left[\Omega_1^{(1)\otimes(2)}, \Lambda_1^{(1)\otimes(2)}\right] = \Gamma_1^{(1)} \otimes I^{(2)} \tag{33}$$

Finally, the square of the sum of two operators:

$$\left(\Omega_1^{(1)\otimes(2)}+\Omega_2^{(1)\otimes(2)}\right)^2|\omega_1\rangle\otimes|\omega_2\rangle=\left(\Omega_1^{(1)}\otimes I^{(2)}+I^{(1)}\otimes\Omega_2^{(2)}\right)^2|\omega_1\rangle\otimes|\omega_2\rangle \tag{34}$$

$$=\left(\Omega_1^{(1)}\otimes I^{(2)}\right)^2|\omega_1\rangle\otimes|\omega_2\rangle+ \tag{35}$$

$$\Omega_1^{(1)}\otimes I^{(2)}I^{(1)}\otimes\Omega_2^{(2)}|\omega_1\rangle\otimes|\omega_2\rangle+ \tag{36}$$

$$I^{(1)}\otimes\Omega_2^{(2)}\Omega_1^{(1)}\otimes I^{(2)}|\omega_1\rangle\otimes|\omega_2\rangle+ \tag{37}$$

$$\left(I^{(1)}\otimes\Omega_2^{(2)}\right)^2|\omega_1\rangle\otimes|\omega_2\rangle \tag{38}$$

$$=\left|\left(\Omega_1^2\right)^{(1)}\omega_1\right\rangle\otimes\left|I^{(2)}\omega_2\right\rangle+ \tag{39}$$

$$\left|\Omega_1^{(1)}\omega_1\right\rangle\otimes\left|\Omega_2^{(2)}\omega_2\right\rangle+ \tag{40}$$

$$\left|\Omega_1^{(1)}\omega_1\right\rangle\otimes\left|\Omega_2^{(2)}\omega_2\right\rangle+ \tag{41}$$

$$\left|I^{(1)}\omega_1\right\rangle\otimes\left|\left(\Omega_2^2\right)^{(2)}\omega_2\right\rangle \tag{42}$$

$$=\left(\left(\Omega_1^2\right)^{(1)}\otimes I^{(2)}+2\Omega_1^{(1)}\otimes\Omega_2^{(2)}+I^{(1)}\otimes\left(\Omega_2^2\right)^{(2)}\right)|\omega_1\rangle\otimes|\omega_2\rangle \tag{43}$$

$$\left(\Omega_1^{(1)\otimes(2)}+\Omega_2^{(1)\otimes(2)}\right)^2=\left(\Omega_1^2\right)^{(1)}\otimes I^{(2)}+2\Omega_1^{(1)}\otimes\Omega_2^{(2)}+I^{(1)}\otimes\left(\Omega_2^2\right)^{(2)} \tag{44}$$

In this derivation, we used the fact that the identity operator leaves its operand unchanged, and thus that $\left(I^2\right)^{(i)}=I^{(i)}$ for either space i.

PINGBACKS

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DIRECT PRODUCT OF VECTOR SPACES: 2-DIM EXAMPLES

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Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 10, Exercise 10.1.2.

Post date: 27 Feb 2017

To help with understanding the direct product of two vector spaces, some examples with a couple of 2-d vector spaces are useful. Suppose the one-particle Hilbert space is two-dimensional, with basis vectors $|+\rangle$ and $|-\rangle$. Now suppose we have two such particles, each in its own 2-d space, $\mathbb{V}_1$ for particle 1 and $\mathbb{V}_2$ for particle 2. We can define a couple of operators by their matrix elements in these two spaces. We define

$$\sigma_1^{(1)} \equiv \begin{bmatrix} a & b \\ c & d \end{bmatrix} \tag{1}$$

$$\sigma_2^{(2)} \equiv \begin{bmatrix} e & f \\ g & h \end{bmatrix} \tag{2}$$

where the first column and row refer to basis vector $|+\rangle$ and the second column and row to $|-\rangle$. Recall that the subscript on each σ refers to the particle and the superscript refers to the vector space. Thus $\sigma_1^{(1)}$ is an operator in space $\mathbb{V}_1$ for particle 1.

Now consider the direct product space $\mathbb{V}_1 \otimes \mathbb{V}_2$, which is spanned by the four basis vectors formed by direct products of the two basis vectors in each of the one-particle spaces, that is by $|+\rangle \otimes |+\rangle$, $|+\rangle \otimes |-\rangle$, $|-\rangle \otimes |+\rangle$ and $|-\rangle \otimes |-\rangle$. Each of the σ operators has a corresponding version in the product space, which is formed by taking the direct product of the one-particle version for one of the particles with the identity operator for the other particle. That is

$$\sigma_1^{(1)\otimes(2)} = \sigma_1^{(1)} \otimes I^{(2)} \tag{3}$$

$$\sigma_2^{(1)\otimes(2)} = I^{(1)} \otimes \sigma_2^{(2)} \tag{4}$$

To get the matrix elements in the product space, we need the form of the identity operators in the one-particle spaces. They are, as usual

$$I^{(1)} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \tag{5}$$

$$I^{(2)} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \tag{6}$$

I've written the two identity operators as separate equations since although they have the same numerical form as a matrix, the two operators operate on different spaces, so they are technically different operators. To get the matrix elements of $\sigma_1^{(1)\otimes(2)}$ we can expand the direct product (Shankar suggests using the 'method of images', although I have no idea what this is. I doubt that it's the same method of images used in electrostatics, and Google draws a blank for any other kind of method of images.) In any case, we can form the product by taking the corresponding matrix elements. For example

$$\left\langle ++\left|\sigma_1^{(1)\otimes(2)}\right|++\right\rangle = \left(\langle +|\otimes\langle +|\right)\sigma_1^{(1)}\otimes I^{(2)}\left(|+\rangle\otimes|+\rangle\right) \tag{7}$$

$$= \left\langle +\left|\sigma_1^{(1)}\right|+\right\rangle\left\langle +\left|I^{(2)}\right|+\right\rangle \tag{8}$$

$$= a\times 1 = a \tag{9}$$

When working out the RHS of the first line, remember that operators with a superscript (1) operate only on bras and kets from the space $\mathbb{V}_1$ and operators with a superscript (2) operate only on bras and kets from the space $\mathbb{V}_2$. Applying the same technique for the remaining elements gives

$$\sigma_1^{(1)\otimes(2)} = \sigma_1^{(1)}\otimes I^{(2)} = \begin{bmatrix} a & 0 & b & 0 \\ 0 & a & 0 & b \\ c & 0 & d & 0 \\ 0 & c & 0 & d \end{bmatrix} \tag{10}$$

Another less tedious way of getting this result is to note that we can form the direct product by taking each element in the first matrix $\sigma_1^{(1)}$ from 1 and multiply it into the second matrix $I^{(2)}$ from 6. Thus the top 2×2 elements in $\sigma_1^{(1)\otimes(2)}$ are obtained by taking the element $\left\langle +\left|\sigma_1^{(1)}\right|+\right\rangle = a$ from 1 and multiplying it into the matrix $I^{(2)}$ from 6. That is, the upper left 2×2 block is formed from

$$aI_{2\times 2}^{(2)} = \begin{bmatrix} a & 0 \\ 0 & a \end{bmatrix} \tag{11}$$

and so on for the other three 2×2 blocks in the complete matrix. Note that it's important to get things in the right order, as the direct product is not commutative.

To get the other direct product, we can apply the same technique:

$$\sigma_2^{(1)\otimes(2)} = I^{(1)} \otimes \sigma_2^{(2)} = \begin{bmatrix} e & f & 0 & 0 \\ g & h & 0 & 0 \\ 0 & 0 & e & f \\ 0 & 0 & g & h \end{bmatrix} \tag{12}$$

Again, note that

$$I^{(1)} \otimes \sigma_2^{(2)} \neq \sigma_2^{(2)} \otimes I^{(1)} = \begin{bmatrix} e & 0 & f & 0 \\ 0 & e & 0 & f \\ g & 0 & h & 0 \\ 0 & g & 0 & h \end{bmatrix} \tag{13}$$

Finally, we can work out the direct product version of the product of two one-particle operators. That is, we want

$$(\sigma_1\sigma_2)^{(1)\otimes(2)} = \sigma_1^{(1)} \otimes \sigma_2^{(2)} \tag{14}$$

We can do this in two ways. First, we can apply the same recipe as in the previous example. We take each element of $\sigma_1^{(1)}$ and multiply it into the full matrix $\sigma_2^{(2)}$:

$$\sigma_1^{(1)} \otimes \sigma_2^{(2)} \quad = \quad \begin{bmatrix} ae & af & be & bf \\ ag & ah & bg & bh \\ ce & cf & de & df \\ cg & ch & dg & dh \end{bmatrix} \tag{15}$$

Second, we can take the matrix product of $\sigma_1^{(1)\otimes(2)}$ from 10 with $\sigma_2^{(1)\otimes(2)}$ from 12:

$$(\sigma_1\sigma_2)^{(1)\otimes(2)} = \begin{bmatrix} a & 0 & b & 0 \\ 0 & a & 0 & b \\ c & 0 & d & 0 \\ 0 & c & 0 & d \end{bmatrix} \begin{bmatrix} e & f & 0 & 0 \\ g & h & 0 & 0 \\ 0 & 0 & e & f \\ 0 & 0 & g & h \end{bmatrix} \tag{16}$$

$$= \begin{bmatrix} ae & af & be & bf \\ ag & ah & bg & bh \\ ce & cf & de & df \\ cg & ch & dg & dh \end{bmatrix} \tag{17}$$

DECOUPLING THE TWO-PARTICLE HAMILTONIAN

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Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 10, Exercise 10.1.3.

Post date: 2 Mar 2017

Shankar shows that, for a two-particle system, the state vector $|\psi\rangle$ is an element of the direct product space $\mathbb{V}_{1\otimes 2}$. Its evolution in time is determined by the Schrödinger equation, as usual, so that

$$i\hbar\left|\dot{\psi}\right\rangle = H\left|\psi\right\rangle = \left[\frac{P_1^2}{2m_1} + \frac{P_2^2}{2m_2} + V\left(X_1, X_2\right)\right]\left|\psi\right\rangle \tag{1}$$

The method by which this equation can be solved (if it *can* be solved, that is) depends on the form of the potential V. If the two particles interact only with some external potential, and not with each other, then V is composed of a sum of terms, each of which depends only on X_1 or X_2, but not on both. In such cases, we can split H into two parts, one of which (H_1) depends only on operators pertaining to particle 1 and the other (H_2) on operators pertaining to particle 2. If the eigenvalues (allowed energies) of particle i are given by E_i, then the stationary states are direct products of the corresponding single particle eigenstates. That is, in general

$$H\left|E\right\rangle = \left(H_1 + H_2\right)\left|E_1\right\rangle \otimes \left|E_2\right\rangle = \left(E_1 + E_2\right)\left|E_1\right\rangle \otimes \left|E_2\right\rangle = E\left|E\right\rangle \tag{2}$$

Thus the two-particle state $|E\rangle = |E_1\rangle \otimes |E_2\rangle$. Since a stationary state $|E_i\rangle$ evolves in time according to

$$\left|\psi_i\left(t\right)\right\rangle = \left|E_i\right\rangle e^{-iE_i t/\hbar} \tag{3}$$

the compound two-particle state evolves according to

$$\left|\psi\left(t\right)\right\rangle = e^{-iE_1 t/\hbar}\left|E_1\right\rangle \otimes e^{-iE_2 t/\hbar}\left|E_2\right\rangle \tag{4}$$

$$= e^{-i(E_1+E_2)t/\hbar}\left|E\right\rangle \tag{5}$$

$$= e^{-iEt/\hbar}\left|E\right\rangle \tag{6}$$

In this case, the two particles are essentially independent of each other, and the compound state is just the product of the two separate one-particle states.

If H is not separable, which will occur if V contains terms involving both X_1 and X_2 in the same term, we cannot, in general, reduce the system to the product of two one-particle systems. There are a couple of instances, however, where such a reduction can be done.

The first instance is if the potential is a function of $x_2 - x_1$ only, in other words, that the interaction between the particles depends only on the distance between them. Shankar shows that in this case we can transform the system to that of a reduced mass $\mu = m_1 m_2 / (m_1 + m_2)$ and a centre of mass $M = m_1 + m_2$. We've already seen this problem solved by means of separation of variables. The result is that the state vector is the product of a vector for a free particle of mass M and of a vector of a particle with reduced mass μ moving in the potential V.

Another case where we can decouple the Hamiltonian is in a system of harmonic oscillators. We've already seen this system solved for two masses in classical mechanics using diagonalization of the matrix describing the equations of motion. The classical Hamiltonian is

$$H = \frac{p_1^2}{2m} + \frac{p_2^2}{2m} + \frac{m\omega^2}{2}\left[x_1^2 + x_2^2 + (x_1 - x_2)^2\right] \tag{7}$$

The earlier solution involved introducing normal coordinates

$$x_I = \frac{1}{\sqrt{2}}(x_1 + x_2) \tag{8}$$

$$x_{II} = \frac{1}{\sqrt{2}}(x_1 - x_2) \tag{9}$$

and corresponding momenta

$$p_I = \frac{1}{\sqrt{2}}(p_1 + p_2) \tag{10}$$

$$p_{II} = \frac{1}{\sqrt{2}}(p_1 - p_2) \tag{11}$$

These normal coordinates are canonical as we can verify by calculating the Poisson brackets. For example

$$\{x_I, p_I\} = \sum_i \left(\frac{\partial x_I}{\partial x_i}\frac{\partial p_I}{\partial p_i} - \frac{\partial x_I}{\partial p_i}\frac{\partial p_I}{\partial x_i} \right) \tag{12}$$

$$= 1 \tag{13}$$

$$\{x_I, x_{II}\} = \sum_i \left(\frac{\partial x_I}{\partial x_i}\frac{\partial x_{II}}{\partial p_i} - \frac{\partial x_I}{\partial p_i}\frac{\partial x_{II}}{\partial x_i} \right) \tag{14}$$

$$= 0 \tag{15}$$

and so on, with the general result

$$\{x_i, p_j\} = \delta_{ij} \tag{16}$$

$$\{x_i, x_j\} = \{p_i, p_j\} = 0 \tag{17}$$

We can invert the transformation to get

$$x_1 = \frac{1}{\sqrt{2}}(x_I + x_{II}) \tag{18}$$

$$x_2 = \frac{1}{\sqrt{2}}(x_I - x_{II}) \tag{19}$$

and

$$p_1 = \frac{1}{\sqrt{2}}(p_I + p_{II}) \tag{20}$$

$$p_2 = \frac{1}{\sqrt{2}}(p_I - p_{II}) \tag{21}$$

Inserting these into 7 we get

$$H = \frac{1}{4m}\left[(p_I + p_{II})^2 + (p_I - p_{II})^2 \right] + \tag{22}$$

$$\frac{m\omega^2}{4}\left[(x_I + x_{II})^2 + (x_I - x_{II})^2 + 4x_{II}^2 \right] \tag{23}$$

$$= \frac{p_I^2}{2m} + \frac{p_{II}^2}{2m} + \frac{m\omega^2}{2}\left(x_I^2 + \frac{3}{2}x_{II}^2 \right) \tag{24}$$

We can now subsitute the usual quantum mechanical operators to get the quantum Hamiltonian:

$$H = -\frac{\hbar^2}{2m}\left(P_I^2 + P_{II}^2 \right) + \frac{m\omega^2}{2}\left(X_I^2 + \frac{3}{2}X_{II}^2 \right) \tag{25}$$

In the coordinate basis, this is

$$H = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x_I^2} + \frac{\partial^2}{\partial x_{II}^2}\right) + \frac{m\omega^2}{2}\left(x_I^2 + \frac{3}{2}x_{II}^2\right) \tag{26}$$

The Hamiltonian is now decoupled and can be solved by separation of variables.

We could have arrived at this result by starting with 7 and promoting x_i and p_i to quantum operators directly, then made the substitution to normal coordinates. We would then start with

$$H = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2}\right) + \frac{m\omega^2}{2}\left[x_1^2 + x_2^2 + (x_1 - x_2)^2\right] \tag{27}$$

The potential term on the right transforms the same way as before, so we get

$$\frac{m\omega^2}{2}\left[x_1^2 + x_2^2 + (x_1 - x_2)^2\right] \rightarrow \frac{m\omega^2}{2}\left(x_I^2 + \frac{3}{2}x_{II}^2\right) \tag{28}$$

To transform the two derivatives, we need to use the chain rule a couple of times. To get the first derivatives:

$$\begin{aligned}
\frac{\partial\psi}{\partial x_1} &= \frac{\partial\psi}{\partial x_I}\frac{\partial x_I}{\partial x_1} + \frac{\partial\psi}{\partial x_{II}}\frac{\partial x_{II}}{\partial x_1} && (29)\\
&= \frac{1}{\sqrt{2}}\left(\frac{\partial\psi}{\partial x_I} + \frac{\partial\psi}{\partial x_{II}}\right) && (30)\\
\frac{\partial\psi}{\partial x_2} &= \frac{\partial\psi}{\partial x_I}\frac{\partial x_I}{\partial x_2} + \frac{\partial\psi}{\partial x_{II}}\frac{\partial x_{II}}{\partial x_2} && (31)\\
&= \frac{1}{\sqrt{2}}\left(\frac{\partial\psi}{\partial x_I} - \frac{\partial\psi}{\partial x_{II}}\right) && (32)
\end{aligned}$$

Now the second derivatives:

$$\frac{\partial^2\psi}{\partial x_1^2} = \frac{\partial}{\partial x_I}\left(\frac{\partial\psi}{\partial x_1}\right)\frac{\partial x_I}{\partial x_1} + \frac{\partial}{\partial x_{II}}\left(\frac{\partial\psi}{\partial x_1}\right)\frac{\partial x_{II}}{\partial x_1} \tag{33}$$

$$= \frac{1}{2}\left[\frac{\partial}{\partial x_I}\left(\frac{\partial\psi}{\partial x_I} + \frac{\partial\psi}{\partial x_{II}}\right) + \frac{\partial}{\partial x_{II}}\left(\frac{\partial\psi}{\partial x_I} + \frac{\partial\psi}{\partial x_{II}}\right)\right] \tag{34}$$

$$= \frac{1}{2}\left[\frac{\partial^2\psi}{\partial x_I^2} + 2\frac{\partial^2\psi}{\partial x_I \partial x_{II}} + \frac{\partial^2\psi}{\partial x_{II}^2}\right] \tag{35}$$

$$\frac{\partial^2\psi}{\partial x_2^2} = \frac{\partial}{\partial x_I}\left(\frac{\partial\psi}{\partial x_2}\right)\frac{\partial x_I}{\partial x_1} + \frac{\partial}{\partial x_{II}}\left(\frac{\partial\psi}{\partial x_2}\right)\frac{\partial x_{II}}{\partial x_1} \tag{36}$$

$$= \frac{1}{2}\left[\frac{\partial}{\partial x_I}\left(\frac{\partial\psi}{\partial x_I} - \frac{\partial\psi}{\partial x_{II}}\right) - \frac{\partial}{\partial x_{II}}\left(\frac{\partial\psi}{\partial x_I} - \frac{\partial\psi}{\partial x_{II}}\right)\right] \tag{37}$$

$$= \frac{1}{2}\left[\frac{\partial^2\psi}{\partial x_I^2} - 2\frac{\partial^2\psi}{\partial x_I \partial x_{II}} + \frac{\partial^2\psi}{\partial x_{II}^2}\right] \tag{38}$$

Combining the two derivatives, we get

$$\frac{\partial^2\psi}{\partial x_1^2} + \frac{\partial^2\psi}{\partial x_2^2} = \frac{\partial^2\psi}{\partial x_I^2} + \frac{\partial^2\psi}{\partial x_{II}^2} \tag{39}$$

Inserting this, together with 28, into 27 we get 26 again.

HARMONIC OSCILLATOR IN 2-D AND 3-D, AND IN POLAR AND SPHERICAL COORDINATES

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Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 10, Exercises 10.2.2 - 10.2.3.

Post date: 4 Mar 2017

We've seen that the 3-d isotropic harmonic oscillator can be solved in rectangular coordinates using separation of variables. The Hamiltonian is

$$H = \frac{p_x^2 + p_y^2 + p_z^2}{2m} + \frac{m\omega^2}{2}\left(x^2 + y^2 + z^2\right) \tag{1}$$

The solution to the Schrödinger equation is just the product of three one-dimensional oscillator eigenfunctions, one for each coordinate. That is

$$\psi_n(x, y, z) = \psi_{n_x}(x)\,\psi_{n_y}(y)\,\psi_{n_z}(z) \tag{2}$$

Each one-dimensional eigenfunction can be expressed in terms of Hermite polynomials as

$$\psi_{n_x}(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^{n_x} n_x!}} H_{n_x}\left(\sqrt{\frac{m\omega}{\hbar}}x\right) e^{-m\omega x^2/2\hbar} \tag{3}$$

with the functions for y and z obtained by replacing x by y or z and n_x by n_y or n_z. We also saw earlier that in the 3-d oscillator, the total energy for state $\psi_n(x, y, z)$ is given in terms of the quantum numbers of the three 1-d oscillators as

$$E_n = \hbar\omega\left(n + \frac{3}{2}\right) = \hbar\omega\left(n_x + n_y + n_z + \frac{3}{2}\right) \tag{4}$$

and that the degeneracy of level n is $\frac{1}{2}(n+1)(n+2)$.

Since the Hermite polynomial H_{n_x} has parity $(-1)^{n_x}$ (that is, odd (even) polynomials are odd (even) functions), the 3-d wave function ψ_n has parity $(-1)^{n_x}(-1)^{n_y}(-1)^{n_z} = (-1)^n$.

We can write the one $n = 0$ state and three $n = 1$ states in spherical coordinates using the standard transformation

$$x = r\sin\theta\cos\phi \quad (5)$$
$$y = r\sin\theta\sin\phi \quad (6)$$
$$z = r\cos\phi \quad (7)$$

Using the notation $\psi_n = \psi_{n_x n_y n_z} = \psi_{n_x}\psi_{n_y}\psi_{n_z}$, we have, using $H_0(y) = 1$ and $H_1(y) = 2y$:

$$\psi_{000} = \left(\frac{m\omega}{\pi\hbar}\right)^{3/4} e^{-m\omega r^2/2\hbar} \quad (8)$$
$$\psi_{100} = \sqrt{\frac{2m\omega}{\hbar}}\left(\frac{m\omega}{\pi\hbar}\right)^{3/4} e^{-m\omega r^2/2\hbar} r\sin\theta\cos\phi \quad (9)$$
$$\psi_{010} = \sqrt{\frac{2m\omega}{\hbar}}\left(\frac{m\omega}{\pi\hbar}\right)^{3/4} e^{-m\omega r^2/2\hbar} r\sin\theta\sin\phi \quad (10)$$
$$\psi_{001} = \sqrt{\frac{2m\omega}{\hbar}}\left(\frac{m\omega}{\pi\hbar}\right)^{3/4} e^{-m\omega r^2/2\hbar} r\cos\theta \quad (11)$$

We can check that these are the correct spherical versions of the eigenfunctions by using the Schrödinger equation in spherical coordinates, which is

$$H\psi = \left[-\frac{\hbar^2\nabla^2}{2m} + \frac{m\omega^2}{2}r^2\right]\psi = E\psi \quad (12)$$

The spherical laplacian operator is

$$\nabla^2\psi = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2\psi}{\partial\phi^2} \quad (13)$$

You can grind through the derivatives by hand if you like, but I just used Maple to do it, giving the results

$$H\psi_{000} = \frac{3}{2}\hbar\omega\psi_{000} \quad (14)$$
$$H\psi_{100} = \frac{5}{2}\hbar\omega\psi_{100} \quad (15)$$
$$H\psi_{010} = \frac{5}{2}\hbar\omega\psi_{010} \quad (16)$$
$$H\psi_{001} = \frac{5}{2}\hbar\omega\psi_{001} \quad (17)$$

In two dimensions, the analysis is pretty much the same. In the more general case where the masses are equal, but $\omega_x \neq \omega_y$, the Hamiltonian is

$$H = \frac{p_x^2 + p_y^2}{2m} + \frac{m}{2}\left(\omega_x^2 x^2 + \omega_y^2 y^2\right) \tag{18}$$

A solution by separation of variables still works, with the result

$$\psi_n(x,y) = \psi_{n_x}(x)\,\psi_{n_y}(y) \tag{19}$$

The total energy is

$$E_n = E_{n_x} + E_{n_y} = \hbar\omega\left(n_x + \frac{1}{2} + n_y + \frac{1}{2}\right) = \hbar\omega(n+1) \tag{20}$$

For a given energy level $n = n_x + n_y$, there are $n+1$ ways of forming n out of a sum of 2 non-negative integers, so the degeneracy of level n is $n+1$.

The one $n = 0$ state and two $n = 1$ states are

$$\psi_{00} = \left(\frac{m\omega}{\pi\hbar}\right)^{1/2} e^{-m\omega\left(x^2+y^2\right)/2\hbar} \tag{21}$$

$$\psi_{10} = \sqrt{\frac{2m\omega}{\hbar}}\left(\frac{m\omega}{\pi\hbar}\right)^{1/2} e^{-m\omega\left(x^2+y^2\right)/2\hbar} x \tag{22}$$

$$\psi_{01} = \sqrt{\frac{2m\omega}{\hbar}}\left(\frac{m\omega}{\pi\hbar}\right)^{1/2} e^{-m\omega\left(x^2+y^2\right)/2\hbar} y \tag{23}$$

To translate to polar coordinates, we use the transformations

$$x = \rho\cos\phi \tag{24}$$

$$y = \rho\sin\phi \tag{25}$$

so we have

$$\psi_{00} = \left(\frac{m\omega}{\pi\hbar}\right)^{1/2} e^{-m\omega\rho^2/2\hbar} \tag{26}$$

$$\psi_{10} = \sqrt{\frac{2m\omega}{\hbar}}\left(\frac{m\omega}{\pi\hbar}\right)^{1/2} e^{-m\omega\rho^2/2\hbar}\rho\cos\phi \tag{27}$$

$$\psi_{01} = \sqrt{\frac{2m\omega}{\hbar}}\left(\frac{m\omega}{\pi\hbar}\right)^{1/2} e^{-m\omega\rho^2/2\hbar}\rho\sin\phi \tag{28}$$

Again, we can check this by plugging these polar formulas into the polar Schrödinger equation, where the 2-d Laplacian is

$$\nabla^2 = \frac{\partial^2}{\partial \rho^2} + \frac{1}{\rho}\frac{\partial}{\partial \rho} + \frac{1}{\rho^2}\frac{\partial^2}{\partial \phi^2} \tag{29}$$

The results are

$$H\psi_{00} = \hbar\omega\psi_{00} \tag{30}$$
$$H\psi_{10} = 2\hbar\omega\psi_{10} \tag{31}$$
$$H\psi_{01} = 2\hbar\omega\psi_{01} \tag{32}$$

PINGBACKS

Pingback: Harmonic oscillator in 2 dimensions: comparison with rectangular coordinates

Pingback: isotropic harmonic oscillator in 3-d: use of spherical harmonics

IDENTICAL PARTICLES - BOSONS AND FERMIONS REVISITED

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 10, Exercises 10.3.1 - 10.3.3.

Post date: 13 Mar 2017

Although we've looked at the quantum treatment of identical particles as done by Griffiths, it's worth summarizing Shankar's treatment of the topic as it provides a few more insights.

In classical physics, suppose we have two identical particles, where 'identical' here means that all their physical properties such as mass, size, shape, charge and so on are the same. Suppose we do an experiment in which these two particles collide and rebound in some way. Can we tell which particle ends up in which location? We're not allowed to label the particles by writing on them, for example, since then they would no longer be identical. In classical physics, we can determine which particle is which by tracing their histories. For example, if we start with particle 1 at position $\mathbf{r}_1$ and particle 2 at position $\mathbf{r}_2$, then let them collide, and finally measure their locations at some time after the collision, we might find that one particle ends up at position $\mathbf{r}_3$ and the other at position $\mathbf{r}_4$. If we videoed the collision event, we would see the two particles follow well-defined paths before and after the collision, so by observing which particle followed the path that leads from $\mathbf{r}_1$ to the collision and then out again, we can tell whether it ends up at $\mathbf{r}_3$ or $\mathbf{r}_4$. That is, the identification of a particle depends on our ability to watch it as it travels through space.

In quantum mechanics, because of the uncertainty principle, a particle does not have a well-defined trajectory, since in order to define such a trajectory, we would need to specify its position and momentum precisely at each instant of time as it travels. In terms of our collision experiment, if we measured one particle to be at starting position $\mathbf{r}_1$ at time $t = 0$ then we know nothing about its momentum, because we specified the position exactly. Thus we can't tell what trajectory this particle will follow. If we measure the two particles at positions $\mathbf{r}_1$ and $\mathbf{r}_2$ at $t = 0$, and then at $\mathbf{r}_3$ and $\mathbf{r}_4$ at some later time, we have no way of knowing which particle ends up at $\mathbf{r}_3$ and which at $\mathbf{r}_4$. In terms of the state vector, this means that the physics in the state vector must be the same if we exchange the two particles within

the wave function. Since multiplying a state vector ψ by some complex constant α leaves the physics unchanged, this means that we require

$$\psi(a,b) = \alpha\psi(b,a) \tag{1}$$

where a and b represent the two particles.

For a two-particle system, the vector space is spanned by a direct product of the two one-particle vector spaces. Thus the two basis vectors in this vector space that can describe the two particles a and b are $|ab\rangle$ and $|ba\rangle$. If these two particles are identical, then ψ must be some linear combination of these two vectors that satisfies 1. That is

$$\begin{aligned} \psi(b,a) &= \beta|ab\rangle + \gamma|ba\rangle & (2)\\ \psi(a,b) &= \alpha\psi(b,a) & (3)\\ &= \alpha(\beta|ab\rangle + \gamma|ba\rangle) & (4) \end{aligned}$$

However, $\psi(a,b)$ is also just $\psi(b,a)$ with a swapped with b, that is

$$\psi(a,b) = \beta|ba\rangle + \gamma|ab\rangle \tag{5}$$

Since $|ab\rangle$ and $|ba\rangle$ are independent, we can equate their coefficients in the last two equations to get

$$\begin{aligned} \alpha\beta &= \gamma & (6)\\ \alpha\gamma &= \beta & (7) \end{aligned}$$

Inserting the second equation into the first, we get

$$\begin{aligned} \alpha^2\gamma &= \gamma & (8)\\ \alpha^2 &= 1 & (9)\\ \alpha &= \pm 1 & (10) \end{aligned}$$

Thus the two possible state functions 1 are combinations of $|ab\rangle$ and $|ba\rangle$ such that

$$\psi(a,b) = \pm\psi(b,a) \tag{11}$$

The plus sign gives the symmetric state, which can be written as

$$\psi(ab,S) = \frac{1}{\sqrt{2}}(|ab\rangle + |ba\rangle) \tag{12}$$

and the minus sign gives the antisymmetric state

$$\psi(ab, A) = \frac{1}{\sqrt{2}}(|ab\rangle - |ba\rangle) \tag{13}$$

The $\frac{1}{\sqrt{2}}$ factor normalizes the states so that

$$\langle \psi(ab, S) | \psi(ab, S) \rangle = 1 \tag{14}$$
$$\langle \psi(ab, A) | \psi(ab, A) \rangle = 1 \tag{15}$$

This follows because the basis vectors $|ab\rangle$ and $|ba\rangle$ are orthonormal vectors.

Particles with symmetric states are called *bosons* and particles with antisymmetric states are called *fermions*. The *Pauli exclusion principle* for fermions follows directly from 13, since if we set the state variables of the two particles to be the same, that is, $a = b$, then

$$\psi(aa, A) = \frac{1}{\sqrt{2}}(|aa\rangle - |aa\rangle) = 0 \tag{16}$$

The symmetry or antisymmetry rules apply to all the properties of the particle taken as an aggregate. That is, the labels a and b can refer to the particle's location plus its other quantum numbers such as spin, charge, and so on. In order for two fermions to be excluded, the states of the two fermions must be identical in all their quantum numbers, so that two fermions with the same orbital location (as two electrons in the same orbital within an atom, for example) are allowed if their spins are different.

Example 1. Suppose we have 2 identical bosons that are measured to be in states $|\phi\rangle$ and $|\chi\rangle$ where $\langle \phi | \chi \rangle \neq 0$. What is their combined state vector? Since they are bosons, their state vector must be symmetric, so we must have

$$\psi(\phi, \chi) = A|\phi\chi\rangle + B|\chi\phi\rangle \tag{17}$$

Because ψ must be symmetric, we must have $A = B$, so that $\psi(\phi, \chi) = \psi(\chi, \phi)$. The 2-particle states can be written as direct products, so we have

$$\psi(\phi, \chi) = A(|\phi\rangle \otimes |\chi\rangle + |\chi\rangle \otimes |\phi\rangle) \tag{18}$$

To normalize, we have, assuming that $|\phi\rangle$ and $|\chi\rangle$ are normalized:

$$|\psi|^2 = 1 \tag{19}$$
$$= |A|^2 \left(\langle\phi| \otimes \langle\chi| + \langle\chi| \otimes \langle\phi|\right)\left(|\phi\rangle \otimes |\chi\rangle + |\chi\rangle \otimes |\phi\rangle\right) \tag{20}$$
$$= |A|^2 \left(1 + 1 + |\langle\phi|\chi\rangle|^2 + |\langle\chi|\phi\rangle|^2\right) \tag{21}$$
$$A = \frac{\pm 1}{\sqrt{2\left(1 + |\langle\phi|\chi\rangle|^2\right)}} \tag{22}$$

Thus the normalized state vector is (choosing the + sign):

$$\psi(\phi,\chi) \;=\; \frac{1}{\sqrt{2\left(1 + |\langle\phi|\chi\rangle|^2\right)}}\left(|\phi\chi\rangle + |\chi\phi\rangle\right) \tag{23}$$

Notice that this reduces to 12 if $\langle\phi|\chi\rangle = 0$.

For more than 2 particles, we need to form state vectors that are either totally symmetric or totally antisymmetric.

Example 2. Suppose we have 3 identical bosons, and they are measured to be in states 3, 3 and 4. Since two of them are in the same state, there are 3 possible combinations, which we can write as $|334\rangle$, $|343\rangle$ and $|433\rangle$. Assuming these states are orthonormal, the full normalized state vector is

$$\psi(3,3,4) = \frac{1}{\sqrt{3}}\left(|334\rangle + |343\rangle + |433\rangle\right) \tag{24}$$

The $\frac{1}{\sqrt{3}}$ ensures that $|\psi(3,3,4)|^2 = 1$.

Incidentally, for $N \geq 3$ particles, it turns out to be impossible to construct a linear combination of the basis states such that the overall state vector is symmetric with respect to the interchange of some pairs of particles and antisymmetric with respect to the interchange of other pairs. A general proof for all N requires group theory, but for $N = 3$ we can show this by brute force. There are $3! = 6$ basis vectors

$$|123\rangle, |231\rangle, |312\rangle, |132\rangle, |321\rangle, |213\rangle \tag{25}$$

Suppose we require the compound state vector to be symmetric with respect to exchanging 1 and 2. We then must have

$$\psi = A\left(|123\rangle + |213\rangle\right) + B\left(|231\rangle + |132\rangle\right) + C\left(|312\rangle + |321\rangle\right) \tag{26}$$

If we now try to make ψ antisymmetric with respect to exchanging 2 and 3, we must have

$$\psi = D\left(|123\rangle - |132\rangle\right) + E\left(|231\rangle - |321\rangle\right) + F\left(|312\rangle - |213\rangle\right) \tag{27}$$

Comparing the two, we see that

$$A = D = -F \tag{28}$$
$$B = E = -D \tag{29}$$
$$C = F = -E \tag{30}$$

Eliminating A, B, and C we have, combining the 3 equations:

$$D = -E = F \tag{31}$$

But from the first equation, we have $D = -F$, so $F = -F = 0$. From the other equations, this implies that $D = -F = 0$ and $E = -F = 0$, and thus that $A = B = C = 0$. So there is no non-trivial solution that allows both a symmetric and antisymmetric particle exchange within the same state vector.

Example 3. Suppose we have 3 particles and only 3 distinct states that each particle can have. If the particles are distinguishable (not identical) the total number of states is found by considering the possibilities. If all 3 particles are in different states, then there are $3! = 6$ possible overall states. If two particles are in one state and one particle in another, there are $\binom{3}{2} = 3$ ways of choosing the two states, for each of which there are 2 ways of partitioning these two states (that is, which state has 2 particles and which has the other one), and for each of those there are 3 possible configurations, so there are $3 \times 2 \times 3 = 18$ possible configurations. Finally, if all 3 particles are in the same state, there are 3 possibilities. Thus the total for distinguishable particles is $6 + 18 + 3 = 27$.

If the particles are bosons, then if all 3 are in different states, there is only 1 symmetric combination of the 6 basis states. If two particles are in one state and one particle in another, there are $3 \times 2 = 6$ ways of partitioning the states, each of which contributes only one symmetric overall state. Finally, if all 3 particles are in the same state, there are 3 possibilities. Thus the total for bosons is $1 + 6 + 3 = 10$.

For fermions, all three particles must be in different states, so there is only 1 possibility.

PINGBACKS

Pingback: Invariance of symmetric and antisymmetric states; exchange operators

Pingback: Compound systems of fermions and bosons

FERMIONS AND BOSONS IN THE INFINITE SQUARE WELL

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Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 10, Exercise 10.3.4.

Post date: 24 Mar 2017

Suppose we have two identical particles in an infinite square well. The energy levels in a well of width L are

$$E = \frac{(\pi n \hbar)^2}{2mL^2} \tag{1}$$

where $n = 1, 2, 3, \ldots$ The corresponding wave functions are given by

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L} \tag{2}$$

If the total energy of the two particles is $\pi^2\hbar^2/mL^2$, the only possible configuration is for both particles to be in the ground state $n = 1$. This means the particles must be bosons, so the state vector is

$$|x_1, x_2\rangle = \frac{2}{L} \sin \frac{\pi x_1}{L} \sin \frac{\pi x_2}{L} \tag{3}$$

If the total energy is $5\pi^2\hbar^2/2mL^2$, then one particle is in the state $n = 1$ and the other is in $n = 2$. Since the states are different, the particles can be either bosons or fermions. For bosons, the state vector is

$$|x_1, x_2\rangle = \frac{1}{\sqrt{2}} \left[\frac{2}{L} \sin \frac{\pi x_1}{L} \sin \frac{2\pi x_2}{L} + \frac{2}{L} \sin \frac{2\pi x_1}{L} \sin \frac{\pi x_2}{L} \right] \tag{4}$$

$$= \frac{\sqrt{2}}{L} \left[\sin \frac{\pi x_1}{L} \sin \frac{2\pi x_2}{L} + \sin \frac{2\pi x_1}{L} \sin \frac{\pi x_2}{L} \right] \tag{5}$$

For fermions, the state must be antisymmetric, so we have

$$|x_1, x_2\rangle = \frac{\sqrt{2}}{L} \left[\sin \frac{\pi x_1}{L} \sin \frac{2\pi x_2}{L} - \sin \frac{2\pi x_1}{L} \sin \frac{\pi x_2}{L} \right] \tag{6}$$

INVARIANCE OF SYMMETRIC AND ANTISYMMETRIC STATES; EXCHANGE OPERATORS

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Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 10, Exercise 10.3.5.

Post date: 19 Mar 2017

In a system with two particles, the state in the X basis is given by $|x_1, x_2\rangle$ where x_i is the position of particle i. We can define the exchange operator P_{12} as an operator that swaps the two particles, so that

$$P_{12}|x_1, x_2\rangle = |x_2, x_1\rangle \tag{1}$$

To find the eigenvalues and eigenvectors of P_{12} we have

$$P_{12}|\psi(x_1, x_2)\rangle = \alpha|\psi(x_1, x_2)\rangle = \psi(x_2, x_1) \tag{2}$$

where α is the eigenvalue and $|\psi(x_1, x_2)\rangle$ is the eigenvector. Using the same argument as before, we can write

$$|\psi(x_1, x_2)\rangle = \beta|x_1, x_2\rangle + \gamma|x_2, x_1\rangle \tag{3}$$
$$|\psi(x_2, x_1)\rangle = \beta|x_2, x_1\rangle + \gamma|x_1, x_2\rangle \tag{4}$$
$$= \alpha[\beta|x_1, x_2\rangle + \gamma|x_2, x_1\rangle] \tag{5}$$

Equating coefficients in the first and third lines, we arrive at

$$\alpha = \pm 1 \tag{6}$$

which gives the same symmetric and antisymmetric eigenfunctions that we had before:

$$\psi_S(x_1, x_2) = \frac{1}{\sqrt{2}}(|x_1, x_2\rangle + |x_2, x_1\rangle) \tag{7}$$
$$\psi_A(x_1, x_2) = \frac{1}{\sqrt{2}}(|x_1, x_2\rangle - |x_2, x_1\rangle) \tag{8}$$

We can derive a couple of other properties of the exchange operator by noting that if it is applied twice in succession, we get the original state back, so that

$$P_{12}^2 = I \tag{9}$$
$$P_{12} = P_{12}^{-1} \tag{10}$$

Thus the operator is its own inverse.
Consider also the two states $|x_1', x_2'\rangle$ and $|x_1, x_2\rangle$. Then

$$\left\langle x_1', x_2' \left| P_{12}^\dagger P_{12} \right| x_1, x_2 \right\rangle = \langle P_{12} x_1', x_2' | P_{12} x_1, x_2 \rangle \tag{11}$$
$$= \langle x_2', x_1' | x_2, x_1 \rangle \tag{12}$$
$$= \left(\langle x_2' | \otimes \langle x_1' | \right) \left(|x_2\rangle \otimes |x_1\rangle \right) \tag{13}$$
$$= \delta\left(x_2' - x_2\right) \delta\left(x_1' - x_1\right) \tag{14}$$

However, the last line is just equal to the inner product of the original states, that is

$$\langle x_1', x_2' | x_1, x_2 \rangle = \delta\left(x_2 - x_2'\right) \delta\left(x_1 - x_1'\right) = \delta\left(x_2' - x_2\right) \delta\left(x_1' - x_1\right) \tag{15}$$

This means that

$$P_{12}^\dagger P_{12} = I \tag{16}$$
$$P_{12}^\dagger = P_{12}^{-1} = P_{12} \tag{17}$$

Thus P_{12} is both Hermitian and unitary.

Shankar asks us to show that, for a general basis vector $|\omega_1, \omega_2\rangle$, $P_{12} |\omega_1, \omega_2\rangle = |\omega_2, \omega_1\rangle$. One argument could be that, since the X basis spans the space, we can express any other vector such as $|\omega_1, \omega_2\rangle$ as a linear combination of the $|x_1, x_2\rangle$ vectors, so that applying P_{12} to $|\omega_1, \omega_2\rangle$ means applying it to a sum of $|x_1, x_2\rangle$ vectors, which swaps the two particles in every term. I'm not sure if this is a rigorous result. One argument, due to Petra Axolotl, is this:

$$P_{12}|\omega_1\omega_2> \tag{18}$$
$$= \int_{x_1}\int_{x_2} P_{12}|x_1x_2>< x_1x_2|\omega_1\omega_2> \mathrm{d}x_1\mathrm{d}x_2 \tag{19}$$
$$= \int_{x_1}\int_{x_2} P_{12}|x_1x_2>\omega_1(x_1)\omega_2(x_2)\mathrm{d}x_1\mathrm{d}x_2 \tag{20}$$
$$= \int_{x_1}\int_{x_2} P_{12}|x_1x_2>\omega_2(x_2)\omega_1(x_1)\mathrm{d}x_1\mathrm{d}x_2 \tag{21}$$
$$= \int_{x_1}\int_{x_2} |x_2x_1>< x_2x_1|\omega_2\omega_1> \mathrm{d}x_1\mathrm{d}x_2 \tag{22}$$
$$= |\omega_2\omega_1> \tag{23}$$

In any case, if we accept this result it shows that if we start in a state that is totally symmetric (that is, a boson state), this state is an eigenvector of P_{12} with eigenvalue $+1$. Similarly, if we start in an antisymmetric (fermion) state, this state is an eigenvector of P_{12} with eigenvalue -1.

Now we can look at some other properties of P_{12}. Consider

$$P_{12}X_1P_{12}\left|x_1,x_2\right\rangle = P_{12}X_1\left|x_2,x_1\right\rangle \tag{24}$$
$$= x_2P_{12}\left|x_2,x_1\right\rangle \tag{25}$$
$$= x_2\left|x_1,x_2\right\rangle \tag{26}$$
$$= X_2\left|x_1,x_2\right\rangle \tag{27}$$

This follows because the operator X_1 operates on the first particle in the state $|x_2,x_1\rangle$ which on the RHS of the first line is at position x_2. Thus $X_1\left|x_2,x_1\right\rangle = x_2\left|x_2,x_1\right\rangle$, that is, X_1 returns the numerical value of the position of the first particle, which is x_2. This means that in terms of the operators alone

$$P_{12}X_1P_{12} = X_2 \tag{28}$$
$$P_{12}X_2P_{12} = X_1 \tag{29}$$
$$P_{12}P_1P_{12} = P_2 \tag{30}$$
$$P_{12}P_2P_{12} = P_1 \tag{31}$$

In the last two lines, the operator P_i is the momentum of particle i, and the result follows by applying the operators to the momentum basis state $|p_1,p_2\rangle$.

For some general operator which can be expanded in a power series of terms containing powers of X_i and/or P_i, we can use 10 to insert $P_{12}P_{12}$ between every factor of X_i or P_i. For example

$$P_{12}P_1X_2^2X_1P_{12} = P_{12}P_1P_{12}P_{12}X_2P_{12}P_{12}X_2P_{12}P_{12}X_1P_{12} \tag{32}$$

$$= P_2X_1^2X_2 \tag{33}$$

That is, for any operator $\Omega(X_1, P_1; X_2, P_2)$ we have

$$P_{12}\Omega(X_1, P_1; X_2, P_2)P_{12} = \Omega(X_2, P_2; X_1, P_1) \tag{34}$$

The Hamiltonian for a system of two *identical* particles must be symmetric under exchange of the particles, since it represents an observable (the energy), and this observable must remain unchanged if we swap the particles. (In the case of two fermions, the wave function is antisymmetric, but the wave function itself is not an observable. The wave function gets multiplied by -1 if we swap the particles, but the square modulus of the wave function, which contains the physics, remains the same.) Thus we have

$$P_{12}H(X_1, P_1; X_2, P_2)P_{12} = H(X_2, P_2; X_1, P_1) = H(X_1, P_1; X_2, P_2) \tag{35}$$

[Note that this condition doesn't necessarily follow if the two particles are not identical, since exchanging them in this case leads to an observably different system. For example, exchanging the proton and electron in a hydrogen atom leads to a different system.]

The propagator is defined as

$$U(t) = e^{-iHt/\hbar} \tag{36}$$

and the propagator dictates how a state evolves according to

$$|\psi(t)\rangle = U(t)|\psi(0)\rangle \tag{37}$$

Since the only operator on which U depends is H, then U is also invariant, so that

$$P_{12}U(X_1, P_1; X_2, P_2)P_{12} = U(X_2, P_2; X_1, P_1) = U(X_1, P_1; X_2, P_2) \tag{38}$$

Multiplying from the left by P_{12} and subtracting, we get the commutator

$$[U, P_{12}] = 0 \tag{39}$$

For a symmetric state $|\psi_S\rangle$ or antisymmetric state $|\psi_A\rangle$, we have

$$UP_{12}|\psi_S(0)\rangle = U|\psi_S(0)\rangle = |\psi_S(t)\rangle = P_{12}U|\psi_S(0)\rangle \tag{40}$$

$$UP_{12}|\psi_A(0)\rangle = -U|\psi_A(0)\rangle = -|\psi_A(t)\rangle = P_{12}U|\psi_A(0)\rangle \tag{41}$$

This means that states that begin as symmetric or antisymmetric remain symmetric or antisymmetric for all time. In other words, a system that starts in an eigenstate of P_{12} remains in the same eigenstate as time passes.

COMPOUND SYSTEMS OF FERMIONS AND BOSONS

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Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 10, Exercise 10.3.6.

Post date: 17 Mar 2017

In a system of identical particles, we've seen that if the particles are bosons, the state vector is symmetric with respect to the exchange of any two particles (that is, $\psi(a,b) = \psi(b,a)$ where a and b are any two of the particles in the system), while for fermions, the state vector is antisymmetric, meaning that $\psi(a,b) = -\psi(a,b)$. What happens if we have a compound object such as a hydrogen atom that is composed of a collection of fermions and/or bosons?

Suppose we look at the hydrogen atom in particular. It is composed of a proton and an electron, both of which are fermions. The proton and electron are not, of course, identical particles, but now suppose we have *two* hydrogen atoms. The two protons *are* identical fermions, just as are the two electrons. However, when analyzing a system of two hydrogen atoms, the relevant question is what happens to the state vector if we exchange the two atoms. In doing so, we exchange both the two protons and the two electrons. Each exchange multiplies the state vector by -1, so the net effect of exchanging both protons and both electrons is to multiply the state vector by $(-1)^2 = 1$. In other words, a hydrogen atom acts as a boson, even though it is composed of two fermions.

In general, if we have a compound object containing n fermions, then the state vector for a system of two such objects is multiplied by $(-1)^n$ when these two objects are exchanged. That is, a compound object containing an even number of fermions behaves as a boson, while if it contains an odd number of fermions, it behaves as a fermion.

A compound object consisting entirely of bosons will always behave as a boson, no matter how many such bosonic particles it contains, since interchanging all n bosons just multiplies the state vector by $(+1)^n = 1$.

INFINITE SQUARE WELL IN THREE DIMENSIONS

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References: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Problem 4.2.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 10, Exercise 10.2.1.

Post date: 5 Jan 2013.

The three-dimensional particle in a box problem is a fairly straightforward extension of the one dimensional case. The 3-d time-independent Schrödinger equation in rectangular coordinates is

$$-\frac{\hbar^2}{2m}\nabla^2\psi = E\psi \tag{1}$$

Using separation of variables, we can assume that the spatial wave function is the product of three individual functions, each dependent on only one spatial coordinate:

$$\psi(\mathbf{r}) = \xi(x)\eta(y)\zeta(z) \tag{2}$$

Plugging this into the 3-d Schrödinger equation and dividing through by $\xi(x)\eta(y)\zeta(z)$ gives

$$-\frac{\hbar^2}{2m}\left(\frac{\xi_{xx}}{\xi}+\frac{\eta_{yy}}{\eta}+\frac{\zeta_{zz}}{\zeta}\right) = E \tag{3}$$

where a subscript indicates a derivative with respect to that variable, so $\xi_{xx} = d^2\xi/dx^2$ etc.

Since E is a constant (independent of position), and each term in the sum depends on a different independent variable, each term in the sum must itself be a constant. In order to be able to use the analysis from the one-dimensional case, we therefore introduce three constants k_x, k_y and k_z so that

$$\xi_{xx} = -k_x^2\xi \tag{4}$$

$$\eta_{yy} = -k_y^2\eta \tag{5}$$

$$\zeta_{zz} = -k_z^2\zeta \tag{6}$$

From 3 the constants satisify the condition:

$$k_x^2 + k_y^2 + k_z^2 = \frac{2mE}{\hbar^2} \tag{7}$$

From here, we can use the analysis of the infinite square well in one dimension, to get:

$$\xi(x) = \sqrt{\frac{2}{a}} \sin \frac{n_x \pi}{a} x \tag{8}$$

$$\eta(y) = \sqrt{\frac{2}{a}} \sin \frac{n_y \pi}{a} y \tag{9}$$

$$\zeta(z) = \sqrt{\frac{2}{a}} \sin \frac{n_z \pi}{a} z \tag{10}$$

where each of n_x, n_y and n_z can take any positive integer value. From 7, the energies are given by

$$E_i = \frac{\pi^2 \hbar^2}{2ma^2}(n_x^2 + n_y^2 + n_z^2) \tag{11}$$

The various energies can be found by listing the values of n_x, n_y and n_z such that the sums $n_x^2 + n_y^2 + n_z^2$ are listed in ascending order. The degeneracy of each combination of ns can be found by noting that if all three ns are the same, the degeneracy is 1, if two are the same, the degeneracy is 3, and if all three are different, the degeneracy is 6. Thus in the following table, we list only one combination of ns for each degenerate set. The energies are given in units of $\frac{\pi^2\hbar^2}{2ma^2}$

n_x	n_y	n_z	Energy	Degeneracy
1	1	1	$E_1 = 3$	1
2	1	1	$E_2 = 6$	3
2	2	1	$E_3 = 9$	3
3	1	1	$E_4 = 11$	3
2	2	2	$E_5 = 12$	1
3	2	1	$E_6 = 14$	6
3	2	2	$E_7 = 17$	3
4	1	1	$E_8 = 18$	3
3	3	1	$E_9 = 19$	3
4	2	1	$E_{10} = 21$	6
3	3	2	$E_{11} = 22$	3
4	2	2	$E_{12} = 24$	3
4	3	1	$E_{13} = 26$	6
3	3	3	$E_{14} = 27$	4
5	1	1	“	“

The case of E_{14} has a degeneracy of 4, since it can arise from two distinct combinations of ns, as shown. It's an interesting question as to whether this case is unique. Not obvious from a superficial analysis how this could be proved one way or the other.

PINGBACKS

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COMPOUND SYSTEMS OF FERMIONS AND BOSONS

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Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 10, Exercise 10.3.6.

Post date: 17 Mar 2017

In a system of identical particles, we've seen that if the particles are bosons, the state vector is symmetric with respect to the exchange of any two particles (that is, $\psi(a,b) = \psi(b,a)$ where a and b are any two of the particles in the system), while for fermions, the state vector is antisymmetric, meaning that $\psi(a,b) = -\psi(a,b)$. What happens if we have a compound object such as a hydrogen atom that is composed of a collection of fermions and/or bosons?

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A compound object consisting entirely of bosons will always behave as a boson, no matter how many such bosonic particles it contains, since interchanging all n bosons just multiplies the state vector by $(+1)^n = 1$.

CORRESPONDENCE BETWEEN CLASSICAL AND QUANTUM TRANSFORMATIONS

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Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 11.

Post date: 31 Mar 2017

When we consider infinitesimal transformations of some dynamical variable, there is a correspondence between classical and quantum mechanics which we can see as follows. First, we'll summarize the results from classical mechanics. We can define a canonical transformation generated by a variable g as

$$\bar{q}_i = q_i + \varepsilon \frac{\partial g}{\partial p_i} \equiv q_i + \delta q_i \tag{1}$$

$$\bar{p}_i = p_i - \varepsilon \frac{\partial g}{\partial q_i} \equiv p_i + \delta p_i \tag{2}$$

Here, ε is an infintesimal amount and δq_i and δp_i are the infinitesimal amounts by which the coordinates and momenta vary. It follows from these definitions that, for any dynamical variable ω, its variation $\delta\omega$ is given by a Poisson bracket

$$\delta\omega = \omega\left(\bar{q}_i, \bar{p}_i\right) - \omega\left(q_i, p_i\right) = \varepsilon\left\{\omega, g\right\} \tag{3}$$

For the special cases of coordinates and momenta, this is

$$\delta q_i = \varepsilon\left\{q_i, g\right\} \tag{4}$$

$$\delta p_i = \varepsilon\left\{p_i, g\right\} \tag{5}$$

If the generator is the momentum p_j, then

$$\delta q_i = \varepsilon\left\{q_i, p_j\right\} = \varepsilon\delta_{ij} \tag{6}$$

$$\delta p_i = \varepsilon\left\{p_i, p_j\right\} = 0 \tag{7}$$

Thus, in classical mechanics, p_j is the generator of translations in direction j.

If $\omega = H$ (the Hamiltonian) and if $\{H, g\} = 0$, then g is conserved (it doesn't vary with time). Because the transformation 1 and 2 is canonical, it preserves the Poisson brackets so that

$$\left\{\overline{q}_i, \overline{q}_j\right\} = \left\{\overline{p}_i, \overline{p}_j\right\} = 0 \tag{8}$$

$$\left\{\overline{q}_i, \overline{p}_j\right\} = \delta_{ij} \tag{9}$$

What do these things correspond to in quantum mechanics? [I find Shankar's treatment in section 11.2 to be almost tautological, since it merely repeats the derivation given earlier. I'll try to be a bit more general.]

Suppose we have some infinitesimal transformation given by a unitary operator $U(\varepsilon)$. We can then define the changes in X and P by

$$\delta X = U^{\dagger}(\varepsilon) X U(\varepsilon) - X \tag{10}$$

$$\delta P = U^{\dagger}(\varepsilon) P U(\varepsilon) - P \tag{11}$$

Since $U(\varepsilon)$ describes an infinitesimal transformation, we can expand it to first order in ε:

$$U(\varepsilon) = I - \frac{i\varepsilon}{\hbar} G \tag{12}$$

where $G = G^{\dagger}$ is some Hermitian operator known as the generator of the transformation. (We've seen a proof that the translation operator $T(\varepsilon)$ (a special case of $U(\varepsilon)$) is unitary and that its generator is Hermitian earlier, and the current case follows the same reasoning.) Using this form we have from 10 and 11, to order ε:

$$\delta X = \left(I + \frac{i\varepsilon}{\hbar} G\right) X \left(I - \frac{i\varepsilon}{\hbar} G\right) - X \tag{13}$$

$$= -\frac{i\varepsilon}{\hbar}[X, G] \tag{14}$$

$$\delta P = \left(I + \frac{i\varepsilon}{\hbar} G\right) P \left(I - \frac{i\varepsilon}{\hbar} G\right) - P \tag{15}$$

$$= -\frac{i\varepsilon}{\hbar}[P, G] \tag{16}$$

If $G = P$, then

$$\delta X = -\frac{i\varepsilon}{\hbar}[X, P] = \varepsilon I \tag{17}$$

$$\delta P = -\frac{i\varepsilon}{\hbar}[P, P] = 0 \tag{18}$$

Comparing this with 6 and 7 we see that (in one dimension, where the classical coordinate is given by x and momentum by p) there is a correspondence between the classical Poisson bracket and quantum commutator:

$$\{x,p\} \leftrightarrow -\frac{i}{\hbar}[X,P] \tag{19}$$

The momentum operator P in quantum mechanics is thus the generator of translations, just as p generates translations in classical mechanics.

More generally, we can define the variation in some arbitrary dynamical operator Ω in a similar way, using 12 to expand the RHS:

$$\begin{aligned} \delta\Omega &= U^{\dagger}(\varepsilon)\,\Omega U(\varepsilon) - \Omega & (20)\\ &= -\frac{i\varepsilon}{\hbar}[\Omega, G] & (21) \end{aligned}$$

The correspondence with classical mechanics is then

$$\{\omega, g\} \leftrightarrow -\frac{i}{\hbar}[\Omega, G] \tag{22}$$

The general rule is that a quantum commutator is $i\hbar$ times the corresponding classical Poisson bracket.

If $\Omega = H$ and $[H,G] = 0$, then by Ehrenfest's theorem, $\left\langle \dot{G} \right\rangle = 0$ and the average value of G is conserved.

The correspondence is a bit odd in that the generator g in classical mechanics enters as a derivative in 1 and 2 while the generator G in quantum mechanics enters as an operator (no derivatives) in 12.

One other feature is worth noting. A canonical transformation preserves the Poisson brackets 8 in the new coordinate system. In quantum mechanics, it is the commutators that get preserved. For example, using the fact that U is unitary so that $UU^{\dagger} = I$:

$$\begin{aligned} U^{\dagger}[X,P]U &= U^{\dagger}XPU - U^{\dagger}PXU & (23)\\ &= U^{\dagger}XUU^{\dagger}PU - U^{\dagger}PUU^{\dagger}XU & (24)\\ &= \left[U^{\dagger}XU, U^{\dagger}PU\right] & (25) \end{aligned}$$

PINGBACKS

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Pingback: Harmonic oscillator in a magnetic field

TRANSLATION OPERATOR FROM PASSIVE TRANSFORMATIONS

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Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 11.

Post date: 30 Mar 2017

We've seen that the translation operator $T(\varepsilon)$ in quantum mechanics can be derived by considering the translation to be an active transformation, that is, a transformation where the state vectors, rather than the operators, get transformed according to

$$T(\varepsilon)|\psi\rangle = |\psi_\varepsilon\rangle \tag{1}$$

Using this approach, we found that

$$T(\varepsilon) = I - \frac{i\varepsilon}{\hbar}P \tag{2}$$

so that the momentum P is the generator of the transformation.

We can also derive T using a passive transformation, where the state vectors remain the same but the operators are transformed according to

$$\begin{aligned} T^\dagger(\varepsilon)\,XT(\varepsilon) &= X + \varepsilon I & (3)\\ T^\dagger(\varepsilon)\,PT(\varepsilon) &= P & (4) \end{aligned}$$

This is equivalent to an active transformation since

$$\begin{aligned} \left\langle \psi \left| T^\dagger(\varepsilon)\,XT(\varepsilon) \right| \psi \right\rangle &= \langle T(\varepsilon)\,\psi\,|X|\,T(\varepsilon)\,\psi\rangle & (5)\\ &= \langle \psi_\varepsilon\,|X|\,\psi_\varepsilon\rangle & (6)\\ &= x + \varepsilon & (7) \end{aligned}$$

As before we start by taking

$$T(\varepsilon) = I - \frac{i\varepsilon}{\hbar}G \tag{8}$$

where G is some Hermitian operator, so that $G^\dagger = G$. Plugging this into 3 we get, keeping only terms up to order ε:

$$T^{\dagger}(\varepsilon) XT(\varepsilon) = \left(I + \frac{i\varepsilon}{\hbar} G\right) X \left(I - \frac{i\varepsilon}{\hbar} G\right) \tag{9}$$

$$= X + \frac{i\varepsilon}{\hbar} I(GX - XG) \tag{10}$$

$$= X - \frac{i\varepsilon}{\hbar} [X, G] \tag{11}$$

$$= X + \varepsilon I \tag{12}$$

Therefore

$$-\frac{i\varepsilon}{\hbar} [X, G] = \varepsilon I \tag{13}$$

$$[X, G] = i\hbar I \tag{14}$$

Since $[X, P] = i\hbar$ we see that

$$G = P + f(X) \tag{15}$$

The extra $f(X)$ is there because any function of X alone commutes with X, so

$$[X, G] = [X, P] + [X, f(X)] = i\hbar I + 0 \tag{16}$$

We can eliminate $f(X)$ by considering 4.

$$T^{\dagger}(\varepsilon) PT(\varepsilon) = \left(I + \frac{i\varepsilon}{\hbar} G\right) P \left(I - \frac{i\varepsilon}{\hbar} G\right) \tag{17}$$

$$= P + \frac{i\varepsilon}{\hbar} I(GP - PG) \tag{18}$$

$$= P - \frac{i\varepsilon}{\hbar} [P, G] \tag{19}$$

$$= P \tag{20}$$

Thus we must have $[P, G] = 0$, which means that G must be a function of P alone. This means that the most general form for $f(X)$ is $f(X) =$ constant, but there's nothing to be gained by adding some non-zero constant to G, so we can take $f(X) = 0$. Thus we end up with the same form 2 that we got from the active transformation.

Translational invariance is the condition that the Hamiltonian is unaltered by a translation. In the passive representation this is stated by the condition

$$T^{\dagger}(\varepsilon) HT(\varepsilon) = H \tag{21}$$

Since translation is unitary, we can apply a theorem that is valid for any operator Ω which can be expanded in powers of X and P. For any unitary operator U, we have

$$U^{\dagger}\Omega\left(X,P\right)U=\Omega\left(U^{\dagger}XU,U^{\dagger}PU\right) \tag{22}$$

This follows because for a unitary operator $U^{\dagger}U=UU^{\dagger}=I$ so we can insert the product $UU^{\dagger}$ anywhere we like. In particular, we can insert it between each pair of factors in every term of the power series expansion of Ω, for example

$$U^{\dagger}X^{2}P^{2}U=U^{\dagger}XXPPU \tag{23}$$

$$=U^{\dagger}XUU^{\dagger}XUU^{\dagger}PUU^{\dagger}PU \tag{24}$$

$$=\left(U^{\dagger}XU\right)^{2}\left(U^{\dagger}PU\right)^{2} \tag{25}$$

For 21 this means that

$$T^{\dagger}\left(\varepsilon\right)H\left(X,P\right)T\left(\varepsilon\right)=H\left(X+\varepsilon I,P\right)=H\left(X,P\right) \tag{26}$$

As before, this leads to the condition

$$\left[P,H\right]=0 \tag{27}$$

which means that P is conserved, according to Ehrenfest's theorem.

PINGBACKS

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Pingback: Finite transformations: correspondence between classical and quantum

Pingback: Parity transformations

Pingback: Rotational transformations using passive transformations

TRANSLATIONAL INVARIANCE AND CONSERVATION OF MOMENTUM

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Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 11.

Post date: 31 Mar 2017

One consequence of the invariance of the Hamiltonian under translation is that the momentum and Hamiltonian commute:

$$[P, H] = 0 \tag{1}$$

In quantum mechanics, commuting quantities are simultaneously observable, and we can find a basis for the Hilbert space consisting of eigenstates of both P and H. We've seen that Ehrenfest's theorem allows us to conclude that for such a system, the average momentum is conserved so that $\left\langle \dot{P} \right\rangle = 0$. We can go a step further and state that if a system starts out in an eigenstate of P, then it remains in that eigenstate for all time.

First, we need to make a rather subtle observation, which is that

$$[P, H] = 0 \rightarrow [P, U(t)] = 0 \tag{2}$$

That is, if P and H commute, then P also commutes with the propagator $U(t)$. For a time-independent Hamiltonian, the propagator is

$$U(t) = e^{-iHt/\hbar} \tag{3}$$

Since this can be expanded in a power series in the Hamiltonian, condition 2 follows easily enough. What if the Hamiltonian is time-dependent? In this case, the propagator comes out to a time-ordered integral

$$U(t) = T\left\{\exp\left[-\frac{i}{\hbar}\int_0^t H\left(t'\right)dt'\right]\right\} \equiv \lim_{N\to\infty}\prod_{n=0}^{N-1} e^{-i\Delta H(n\Delta)/\hbar} \tag{4}$$

Here the time interval $[0, t]$ is divided into N time slices, each of length $\Delta = t/N$. As explained in the earlier post, the reason we can't just integrate the RHS directly by summing the exponents is that such a procedure works only if the operators in the exponents all commute with each other. If H is time-dependent, its forms at different times may not commute, so we can't get a simple closed form for $U(t)$.

However, if $[P, H(t)] = 0$ for all times, then P commutes with all the exponents on the RHS of 4, so we still get $[P, U(t)] = 0$. Another way of looking at this is by imposing the condition $[P, H(t)] = 0$ we're saying that if $H(t)$ can be expanded in a power series in X and P, it depends only on P, and not on X. This follows from the fact that

$$[X^n, P] = i\hbar n X^{n-1} \tag{5}$$

so that P does not commute with any power of X.

Given that 2 is valid for all Hamiltonians, then if we start in a eigenstate $|p\rangle$ of P, then

$$\begin{aligned} P|p\rangle &= p|p\rangle & (6)\\ PU(t)|p\rangle &= U(t)P|p\rangle & (7)\\ &= U(t)p|p\rangle & (8)\\ &= pU(t)|p\rangle & (9) \end{aligned}$$

Thus $U(t)|p\rangle$ remains an eigenstate of P with the same eigenvalue p for all time. For a single particle moving in one dimension, the state $|p\rangle$ describes a free particle with momentum p (and thus a completely undetermined position).

PINGBACKS

Pingback: Parity transformations

TRANSLATIONAL INVARIANCE IN QUANTUM MECHANICS

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Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 11, Exercises 11.2.1 - 11.2.2.

Post date: 27 Mar 2017

In classical mechanics, we've seen that if a dynamical variable g is used to generate a transformation of the variables q_i and p_i (the coordinates and canonical momenta), then if the Hamiltonian is invariant under this transformation, the quantity g is conserved, meaning that it remains constant over time. We'd like to extend these results to quantum mechanics, but in doing so, there is one large obstacle. In classical mechanics, we can specify the exact position (given by q_i) and the exact momentum (p_i) at every instant in time for every particle. In other words, every particle has a precisely defined trajectory through phase space. Due to the uncertainty principle, we cannot do this in quantum mechanics, since we cannot specify the position and momentum of any particle with arbitrary precision, so we can't define a precise trajectory for any particle.

The way in which this problem is usually handled is to examine the effects of changes in the expectation values of dynamical variables, rather than with their precise values at any given time. In the case of a single particle moving in one dimension, we can apply this idea to investigate how we might invoke translational invariance. Classically, where x is the position variable and p is the momentum, an infinitesimal translation by a distance ε is given by

$$x \rightarrow x+\varepsilon \tag{1}$$
$$p \rightarrow p \tag{2}$$

In quantum mechanics, the equivalent translation is reflected in the expectation values:

$$\langle X\rangle \rightarrow \langle X\rangle+\varepsilon \tag{3}$$
$$\langle P\rangle \rightarrow \langle P\rangle \tag{4}$$

In order to find the expectation values $\langle X\rangle$ and $\langle P\rangle$ we need to use the state vector $|\psi\rangle$. There are two ways of interpreting the transformation. The

first, known as the *active transformation picture*, is to say that translating the position generates a new state vector $|\psi_\varepsilon\rangle$ with the properties

$$\begin{aligned} \langle\psi_\varepsilon|X|\psi_\varepsilon\rangle &= \langle\psi|X|\psi\rangle+\varepsilon \quad (5)\\ \langle\psi_\varepsilon|P|\psi_\varepsilon\rangle &= \langle\psi|P|\psi\rangle \quad (6)\end{aligned}$$

Since $|\psi_\varepsilon\rangle$ is another state vector in the same vector space as $|\psi\rangle$, there must be an operator $T(\varepsilon)$ which we call the translation operator, and which maps one vector onto the other:

$$T(\varepsilon)|\psi\rangle = |\psi_\varepsilon\rangle \quad (7)$$

In terms of the translation operator, the translation becomes

$$\left\langle\psi\left|T^\dagger(\varepsilon)XT(\varepsilon)\right|\psi\right\rangle = \langle\psi|X|\psi\rangle+\varepsilon \quad (8)$$

$$\left\langle\psi\left|T^\dagger(\varepsilon)PT(\varepsilon)\right|\psi\right\rangle = \langle\psi|P|\psi\rangle \quad (9)$$

These relations allow us to define the second interpretation, called the *passive transformation picture*, in which the state vectors do not change, but rather the position and momentum operators change. That is, we can transform the operators according to

$$\begin{aligned} X &\rightarrow T^\dagger(\varepsilon)XT(\varepsilon) = X+\varepsilon I \quad (10)\\ P &\rightarrow T^\dagger(\varepsilon)PT(\varepsilon) = P \quad (11)\end{aligned}$$

We need to find the explicit form for T. To begin, we consider its effect on a position eigenket $|x\rangle$. One possibility is

$$T(\varepsilon)|x\rangle = |x+\varepsilon\rangle \quad (12)$$

However, to be completely general, we should consider the case where T not only shifts x by ε, but also introduces a phase factor. That is, the most general effect of T is

$$T(\varepsilon)|x\rangle = e^{i\varepsilon g(x)/\hbar}|x+\varepsilon\rangle \quad (13)$$

where $g(x)$ is some arbitrary real function of x. Using this form, we have, for some arbitrary state vector $|\psi\rangle$:

$$|\psi_\varepsilon\rangle = T(\varepsilon)|\psi\rangle \tag{14}$$
$$= T(\varepsilon)\int_{-\infty}^{\infty}|x\rangle\langle x|\psi\rangle\,dx \tag{15}$$
$$= \int_{-\infty}^{\infty}e^{i\varepsilon g(x)/\hbar}|x+\varepsilon\rangle\langle x|\psi\rangle\,dx \tag{16}$$
$$= \int_{-\infty}^{\infty}e^{i\varepsilon g(x'-\varepsilon)/\hbar}\left|x'\right\rangle\left\langle x'-\varepsilon\right|\psi\rangle\,dx' \tag{17}$$

To get the last line, we changed the integration variable to $x' = x+\varepsilon$. Multiplying by the bra $\langle x|$ gives, using $\langle x|x'\rangle = \delta(x-x')$:

$$\langle x|T(\varepsilon)|\psi\rangle = \langle x|\psi_\varepsilon\rangle = e^{i\varepsilon g(x-\varepsilon)/\hbar}\langle x-\varepsilon|\psi\rangle \tag{18}$$
$$= e^{i\varepsilon g(x-\varepsilon)/\hbar}\psi(x-\varepsilon) \tag{19}$$

That is, the action of $T(\varepsilon)$ is to move the coordinate axis a distance ε to the right, which means that the new state vector $|\psi_\varepsilon\rangle$ becomes the old state vector at position $x-\varepsilon$. Alternatively, we can leave the coordinate axis alone and shift the wave function a distance ε to the right, so that the new vector at position x is the old vector at position $x-\varepsilon$ (multiplied by a phase factor).

We can now use this result to calculate 8 and 9:

$$\langle\psi_\varepsilon|X|\psi_\varepsilon\rangle = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\langle\psi_\varepsilon|x\rangle\left\langle x\right|X\left|x'\right\rangle\left\langle x'\right|\psi_\varepsilon\rangle\,dx\,dx' \tag{20}$$
$$= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\langle\psi_\varepsilon|x\rangle\,x'\delta\left(x-x'\right)\left\langle x'\right|\psi_\varepsilon\rangle\,dx\,dx' \tag{21}$$
$$= \int_{-\infty}^{\infty}\langle\psi_\varepsilon|x\rangle\,x\langle x|\psi_\varepsilon\rangle\,dx \tag{22}$$
$$= \int_{-\infty}^{\infty}e^{-i\varepsilon g(x-\varepsilon)/\hbar}\psi^*(x-\varepsilon)\,xe^{i\varepsilon g(x-\varepsilon)/\hbar}\psi(x-\varepsilon)\,dx \tag{23}$$
$$= \int_{-\infty}^{\infty}\psi^*(x-\varepsilon)\,x\psi(x-\varepsilon)\,dx \tag{24}$$
$$= \int_{-\infty}^{\infty}\psi^*\left(x'\right)\left(x'+\varepsilon\right)\psi\left(x'\right)dx' \tag{25}$$
$$= \langle\psi|X|\psi\rangle + \varepsilon \tag{26}$$

In the second line, we used the matrix element of X

$$\left\langle x\right|X\left|x'\right\rangle = x'\delta\left(x-x'\right) \tag{27}$$

and in the penultimate line, we again used the change of integration variable to $x' = x - \varepsilon$. Thus we regain 8.

The momentum transforms as follows.

$$\langle \psi_\varepsilon | P | \psi_\varepsilon \rangle = \int_{-\infty}^{\infty} \psi^* (x-\varepsilon) e^{-i\varepsilon g(x-\varepsilon)/\hbar} \left(-i\hbar \frac{d}{dx} \right) \left(e^{i\varepsilon g(x-\varepsilon)/\hbar} \psi (x-\varepsilon) \right) dx \tag{28}$$

$$= \int_{-\infty}^{\infty} \psi^* (x-\varepsilon) \left(\varepsilon \frac{d}{dx} (g(x-\varepsilon)) \psi (x-\varepsilon) - i\hbar \frac{d}{dx} (\psi (x-\varepsilon)) \right) dx \tag{29}$$

$$= \int_{-\infty}^{\infty} \psi^* (x') \left(\varepsilon \psi (x') \frac{d}{dx'} g(x') - i\hbar \frac{d}{dx'} \psi (x') \right) dx' \tag{30}$$

$$= \varepsilon \left\langle \frac{d}{dx} g(x) \right\rangle + \langle P \rangle \tag{31}$$

In the third line, we again transformed the integration variable to $x' = x - \varepsilon$, and used the fact that $dx = dx'$, so a derivative with respect to x is the same as a derivative with respect to x'. [This derivation is condensed a bit compared to the derivation of $\langle \psi_\varepsilon | X | \psi_\varepsilon \rangle$, but you can insert a couple of sets of complete states and do the extra integrals if you like.]

If we now impose the condition 9 so that the momentum is unchanged by the translation, this is equivalent to choosing the phase function $g(x) = 0$, and this is what is done in most applications.

Having explored the properties of the translation operator, we can now define what we mean by *translational invariance* in quantum mechanics. This is the requirement that the expectation value of the Hamiltonian is unchanged under the transformation. That is

$$\langle \psi | H | \psi \rangle = \langle \psi_\varepsilon | H | \psi_\varepsilon \rangle \tag{32}$$

For this, we need the explicit form of $T(\varepsilon)$. Since $\varepsilon = 0$ corresponds to no translation, we require $T(0) = I$. To first order in ε, we can then write

$$T(\varepsilon) = I - \frac{i\varepsilon}{\hbar} G \tag{33}$$

where G is some operator, called the generator of translations, that is to be determined. From 13 (with $g = 0$ from now on), we have

$$\langle x' + \varepsilon | x + \varepsilon \rangle = \left\langle x' \middle| T^\dagger (\varepsilon) T (\varepsilon) \middle| x \right\rangle = \delta (x' - x) = \langle x' | x \rangle \tag{34}$$

so we must have

$$T^{\dagger}(\varepsilon)T(\varepsilon) = I \tag{35}$$

so that T is unitary. Applying this condition to 33 up to order ε, we have

$$\begin{aligned} T^{\dagger}(\varepsilon)T(\varepsilon) &= \left(I + \frac{i\varepsilon}{\hbar}G^{\dagger}\right)\left(I - \frac{i\varepsilon}{\hbar}G\right) && (36)\\ &= I + \frac{i\varepsilon}{\hbar}\left(G^{\dagger} - G\right) + \mathcal{O}\left(\varepsilon^2\right) && (37)\end{aligned}$$

Requiring 35 shows that $G = G^{\dagger}$ so G is Hermitian. Now, from 19 ($g = 0$ again) we have

$$\langle x|T(\varepsilon)|\psi\rangle = \psi(x - \varepsilon) \tag{38}$$

We expand both sides to order ε:

$$\langle x|I|\psi\rangle - \frac{i\varepsilon}{\hbar}\langle x|G|\psi\rangle = \psi(x) - \varepsilon\frac{d\psi}{dx} \tag{39}$$

Since $\langle x|I|\psi\rangle = \langle x|\psi\rangle = \psi(x)$, we have

$$\langle x|G|\psi\rangle = -i\hbar\frac{d\psi}{dx} = \langle x|P|\psi\rangle \tag{40}$$

so $G = P$ and the momentum operator is the generator of translations, and the translation operator is, to order ε

$$T(\varepsilon) = I - \frac{i\varepsilon}{\hbar}P \tag{41}$$

By plugging this into 32 and expanding the RHS, we find that in order for the Hamiltonian to be invariant, the expectation value of the commutator $[P, H]$ must be zero (the derivation is done in Shankar's eqn 11.2.15). Using Ehrenfest's theorem we then find that the expectation value $\langle \dot{P} \rangle = \langle [P, H] \rangle = 0$, so that the expectation value of P is conserved over time.

Note that we *cannot* say that the momentum itself (rather than just its expectation value) is conserved since, due to the uncertainty principle, we never know what the exact momentum is at any given time.

PINGBACKS

Pingback: Correspondence between classical and quantum transformations

Pingback: Translation operator from passive transformations

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FINITE TRANSFORMATIONS: CORRESPONDENCE BETWEEN CLASSICAL AND QUANTUM

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 11, Exercise 11.2.3.

Post date: 2 Apr 2017

The translation operator for an infinitesimal translation ε is, to first order in ε:

$$T(\varepsilon) = I - \frac{i\varepsilon}{\hbar} P \tag{1}$$

where P, the momentum operator, serves as the generator of translations. To derive a formula for a finite (non-infinitesimal) translation over a distance a, we divide the interval a into N segments, each of width a/N, so that for very large N, the width becomes infinitesimal. Then we have

$$T(a) = \left(I - \frac{ia}{\hbar N} P \right)^N \tag{2}$$

This formula is reminiscent of one definition of the exponential function (which can be found in most introductory calculus texts):

$$e^{-ax} = \lim_{N \to \infty} \left(1 - \frac{ax}{N} \right)^N \tag{3}$$

When we try to apply a formula that is valid for ordinary numbers to a case containing operators, we need to take care that any commutation relations involving the operators are taken into account. In this case, 2 contains only the momentum operator and the identity operator, which commute with each other, so we can in fact apply the limit formula directly to the operator case. We therefore have

$$T(a) = \lim_{N \to \infty} \left(I - \frac{ia}{\hbar N} P \right)^N = e^{-iaP/\hbar} \tag{4}$$

In the position basis, $P = -i\hbar \frac{d}{dx}$, so if we apply $T(a)$ to a state vector $\psi(x) = \langle x | \psi \rangle$ we can expand the exponential in a Taylor series to get

$$\langle x | T(a) | \psi \rangle = \psi(x) - a \frac{d\psi}{dx} + \frac{a}{2!} \frac{d^2\psi}{dx^2} + \dots \tag{5}$$

We can extend our analysis of the correspondence between classical and quantum versions of translations. In the passive transformation model, the transformation is applied to operators rather than state vectors, so for a finite translation of an operator Ω we have

$$\Omega \to T^{\dagger}(a)\,\Omega T(a) = e^{iaP/\hbar}\Omega e^{-iaP/\hbar} \tag{6}$$

The operator expression on the RHS can be expanded using Hadamard's lemma, which for two operators A and B is

$$e^{-A}Be^{A} = B + [B,A] + \frac{1}{2!}[[B,A],A] + \ldots \tag{7}$$

where each term contains the commutator of the previous term's commutator with A.

In this case gives us

$$e^{iaP/\hbar}\Omega e^{-iaP/\hbar} = \Omega + a\left(-\frac{i}{\hbar}\right)[\Omega,P] + \frac{a^2}{2!}\left(-\frac{i}{\hbar}\right)^2[[\Omega,P],P] + \ldots \tag{8}$$

For example, in the case $\Omega = X$, $[X,P] = i\hbar I$ and all higher commutators are zero (since they involve the commutator of a constant with P), so we get

$$e^{iaP/\hbar}Xe^{-iaP/\hbar} = X + aI \tag{9}$$

so the system is translated by a distance a, as we'd expect.

For higher powers of X, we can use the result

$$[X^n,P] = i\hbar n X^{n-1} \tag{10}$$

We therefore get

$$\begin{aligned} e^{iaP/\hbar}X^n e^{-iaP/\hbar} &= X^n + anX^{n-1} + \frac{a^2}{2!}n(n-1)X^{n-2} + \ldots + \frac{a^n}{n!} && (11)\\ &= \sum_{m=0}^{n}\binom{n}{m}X^{n-m}(aI)^m && (12)\\ &= (X+aI)^n && (13)\end{aligned}$$

We're allowed to treat X as an ordinary number in these equations since it is (apart from I), the only operator present so all terms commute.

In the classical case, the infinitesimal change $\delta\omega$ of a variable ω under an infinitesimal displacement δa generated by the momentum p is given by the Poisson bracket

$$\delta\omega = \delta a \{\omega, p\} \tag{14}$$

We can write this as a derivative:

$$\frac{d\omega}{da} = \{\omega, p\} \tag{15}$$

For a finite translation by an amount a, we can write the value of ω as a Taylor series relative to some starting point a_0 as

$$\omega(a_0 + a) = \omega(a_0) + a\frac{d\omega}{da} + \frac{a^2}{2!}\frac{d^2\omega}{da^2} + \dots \tag{16}$$

where all derivatives are evaluated at $a = a_0$.

We can write all the derivatives in terms of Poisson brackets by using 15. For example

$$\frac{d^2\omega}{da^2} = \frac{d}{da}\left(\frac{d\omega}{da}\right) = \left\{\frac{d\omega}{da}, p\right\} = \{\{\omega, p\}, p\} \tag{17}$$

Thus the variable ω transforms according to

$$\omega(a_0 + a) = \omega + a\{\omega, p\} + \frac{a^2}{2!}\{\{\omega, p\}, p\} + \dots \tag{18}$$

Comparing this with 8, we see that the two expressions match if we use the usual recipe for converting classical Poisson brackets to quantum commutators, namely $\{a, b\} = -\frac{i}{\hbar}[A, B]$.

Although we've worked this out for the special case of translations, the same principle can be used for other transformations. For example, the angular momentum about the z axis is

$$\ell_z = xp_y - yp_x \tag{19}$$

and serves as the generator of rotations about the z axis. Suppose we have a rotation through an angle θ and we want to see how the two coordinates x and y transform. The expansion 18 becomes

$$\bar{x} = x + \theta\{x, \ell_z\} + \frac{\theta^2}{2!}\{\{x, \ell_z\}, \ell_z\} + \dots \tag{20}$$

The relevant Poisson brackets are (using the generic term q_i to represent the two coordinates x and y):

$$\{x,\ell_z\} = \sum_i \left[\frac{\partial x}{\partial q_i}\frac{\partial \ell_z}{\partial p_i} - \frac{\partial x}{\partial p_i}\frac{\partial \ell_z}{\partial q_i}\right] \tag{21}$$

$$= -y \tag{22}$$

$$\{y,\ell_z\} = \sum_i \left[\frac{\partial y}{\partial q_i}\frac{\partial \ell_z}{\partial p_i} - \frac{\partial y}{\partial p_i}\frac{\partial \ell_z}{\partial q_i}\right] \tag{23}$$

$$= x \tag{24}$$

Looking at how x transforms, we see that the Poisson brackets in 20 will cycle through the four values

$$\{x,\ell_z\} = -y \tag{25}$$

$$\{\{x,\ell_z\},\ell_z\} = -\{y,\ell_z\} = -x \tag{26}$$

$$\{\{\{x,\ell_z\},\ell_z\},\ell_z\} = -\{x,\ell_z\} = y \tag{27}$$

$$\{\{\{\{x,\ell_z\},\ell_z\},\ell_z\},\ell_z\} = \{y,\ell_z\} = x \tag{28}$$

The series 20 thus expands to

$$\bar{x} = x\left[1 - \frac{\theta^2}{2!} + \frac{\theta^4}{4!} - \ldots\right] - y\left[\theta - \frac{\theta^3}{3!} + \frac{\theta^5}{5!} - \ldots\right] \tag{29}$$

$$= x\cos\theta - y\sin\theta \tag{30}$$

We can do the same calculation for $\bar{y}$ to get

$$\bar{y} = x\sin\theta + y\cos\theta \tag{31}$$

PINGBACKS

Pingback: Translation invariance in two dimensions
Pingback: Rotations through a finite angle; use of polar coordinates
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Pingback: Goldstone's theorem

TIME TRANSLATION AND CONSERVATION OF ENERGY

Link to: physicspages home page.

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Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 11, Section 11.3.

Post date: 7 Apr 2017

We can investigate the effect of a quantum system being invariant under time translation by considering the evolution of a state vector using a propagator. A state at time t is given in terms of the state at time $t = 0$ according to

$$|\psi(t)\rangle = U(t)\,|\psi(0)\rangle = e^{-itH/\hbar}\,|\psi(0)\rangle \tag{1}$$

Strictly speaking, this equation is true only if H is time-independent, since in the time-dependent case, we need to express the propagator as a time-ordered integral. However, if we let the system evolve for only an infinitesimal time ε, we can ignore the complexities of the time-ordered integral and write, to first order in ε

$$U(\varepsilon) = e^{-i\varepsilon H(0)/\hbar} = I - \frac{i\varepsilon H(0)}{\hbar} \tag{2}$$

Note that it doesn't matter if we use the value of H at time $t = 0$ or $t = \varepsilon$ or at some time in between, since the differences between these values are of order ε, and thus make no difference to $U(\varepsilon)$ to first order in ε.

Now suppose we prepare the same system (which we'll call $|\psi_0\rangle$) at some time $t = t_1$ and consider how the system evolves over an infinitesimal time ε starting from $t = t_1$. We then have

$$|\psi(t_1+\varepsilon)\rangle = U(t_1+\varepsilon)\,|\psi_0\rangle \tag{3}$$

$$= \left(I - \frac{i\varepsilon H(t_1)}{\hbar}\right)|\psi_0\rangle \tag{4}$$

The idea behind time translation invariance is that it shouldn't make any difference at what time we prepare a system, provided that the system is prepared identically at whatever time we actually do prepare it. In other words, if we had prepared our system above at $t = t_2$ instead of $t = t_1$ and then let it evolve for an infinitesimal time ε, we should end up with exactly the same state. That is, we require that

$$|\psi(t_2+\varepsilon)\rangle = \left(I - \frac{i\varepsilon H(t_2)}{\hbar}\right)|\psi_0\rangle \tag{5}$$

$$= \left(I - \frac{i\varepsilon H(t_1)}{\hbar}\right)|\psi_0\rangle \tag{6}$$

Rearranging things, we get

$$-\frac{i\varepsilon}{\hbar}\left(H(t_2) - H(t_1)\right)|\psi_0\rangle = 0 \tag{7}$$

The initial state can be anything we like, so in order for this condition to be always true, we must have

$$H(t_2) = H(t_1) \tag{8}$$

Again, the two times t_1 and t_2 at which we prepared the system are arbitrary (and not necessarily separated by an infinitesimal time, so they could be years apart), so this condition implies that H itself must be constant in time. For a time-independent operator A, Ehrenfest's theorem says that

$$\left\langle \dot{A} \right\rangle = -\frac{i}{\hbar}\langle [A, H] \rangle \tag{9}$$

If $A = H$, then the commutator is $[H, H] = 0$, so time translation invariance implies that

$$\left\langle \dot{H} \right\rangle = 0 \tag{10}$$

That is, time translation invariance implies that the average energy of the system is conserved.

Clearly, energy is conserved if the system is in an energy eigenstate, since then the energy has a single, unchanging value. However, if we prepare the state as a combination of energy eigenstates, then the system has the form

$$\psi(x,t) = \sum_k c_k e^{-iE_k t/\hbar}\psi_k(x) \tag{11}$$

where the c_k are constant coefficients. A measurement of the energy on such a system can yield any of the energies E_k for which $c_k \neq 0$, so it might seem that we're violating the conservation of energy. The point is that, *on average*, the energy is

$$\langle E \rangle = \sum_k |c_k|^2 E_k \tag{12}$$

and it is this average that doesn't change with time. In dealing with averages, we're also retaining consistency with the infamous energy-time uncertainty relation.

PARITY TRANSFORMATIONS

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 11, Exercises 11.4.1 - 11.4.4.

Post date: 8 Apr 2017

A parity transformation reflects all the coordinate axes through the origin, so that, in one dimension $x \to -x$ and in three dimensions the position vector $\mathbf{r} \to -\mathbf{r}$. In one dimension, a parity transformation is the same as reflection in a point-sized mirror placed at the origin. It might seem that in three dimensions, parity is more than just a reflection in a plane mirror, but in fact it can be shown that it is equivalent to such a reflection followed by a rotation. To see this, suppose we place a mirror in the xy plane, so that the z axis gets reflected into $-z$. This converts a right-handed rectangular coordinate system (where the direction of the z axis is determined by the direction of your thumb on your right hand when you curl your fingers through the right angle between the positive x and y axes) into a left-handed coordinate system (the direction of the new $+z$ axis is found by doing the finger-curling maneuver with your left hand). However, merely reflecting the z axis in the xy plane leaves the x and y axes unchanged. Now if we rotate the xy plane by an angle π (or 180°) about the z axis, then the $+x$ axis gets rotated into the $-x$ axis, and the $+y$ axis gets rotated into the $-y$ axis. In this sense, the 3-d parity transformation is equivalent to a reflection (since pretty well every physical phenomenon is invariant under a rotation).

To apply parity to quantum state vectors, we define a parity operator Π to have the following action on the X basis:

$$\Pi|x\rangle = |-x\rangle \tag{1}$$

From this definition we can see the effect on an arbitrary state $|\psi\rangle$ by inserting a complete set of X states:

$$\Pi|\psi\rangle = \Pi\int_{-\infty}^{\infty}|x\rangle\langle x|\psi\rangle\,dx \tag{2}$$

$$= \int_{-\infty}^{\infty}|-x\rangle\langle x|\psi\rangle\,dx \tag{3}$$

$$= \int_{\infty}^{-\infty}\left|x'\right\rangle\left\langle -x'\right|\left.\psi\right\rangle\left(-dx'\right) \tag{4}$$

$$= \int_{-\infty}^{\infty}\left|x'\right\rangle\left\langle -x'\right|\left.\psi\right\rangle dx' \tag{5}$$

In the third line we made the substitution $x' = -x$, so that $dx = -dx'$ and the limits of integration get swapped. As a result of this, the effect of parity in the X basis representation $\langle x|\psi\rangle = \psi(x)$ of a state vector $|\psi\rangle$ is

$$\langle x|\Pi|\psi\rangle = \int_{-\infty}^{\infty}\left\langle x\right|\left.x'\right\rangle\left\langle -x'\right|\left.\psi\right\rangle dx' \tag{6}$$

$$= \int_{-\infty}^{\infty}\delta\left(x-x'\right)\left\langle -x'\right|\left.\psi\right\rangle dx' \tag{7}$$

$$= \psi(-x) \tag{8}$$

Parity therefore simply converts $x \to -x$ wherever it occurs in the function $\psi(x)$.

One special case of this is the momentum eigenstate $|p\rangle$ which has the form in the X basis of

$$\langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}}e^{ipx/\hbar} \tag{9}$$

The parity transformation gives

$$\langle x|\Pi|p\rangle = \frac{1}{\sqrt{2\pi\hbar}}e^{-ipx/\hbar} \tag{10}$$

Another way of looking at this is that parity changes p to $-p$ and leaves the x alone, so that

$$\Pi|p\rangle = |-p\rangle \tag{11}$$

[You might think that if parity transforms $x \to -x$ and $p \to -p$ then the effect on $e^{ipx/\hbar}$ should be to switch the signs of both x and p and thus leave the state unchanged. However, this isn't correct, as we can express a state vector in either the X basis (in which $x \to -x$) *or* in the P basis (in which $p \to -p$) but *not both at the same time*.]

A few properties of Π can be derived fairly easily. First, since applying Π twice in succession to the same state swaps $x \to -x$ and back again, it leaves that state unchanged. Since this is true for all states, we must have

$$\Pi^2 = I \tag{12}$$

from which we see that Π is its own inverse, so

$$\Pi^{-1} = \Pi \tag{13}$$

We can also see that Π is Hermitian by considering

$$\left\langle \psi \left| \Pi^\dagger \Pi \right| \psi \right\rangle = \langle \Pi\psi \,|\Pi\psi\rangle = \int_{-\infty}^{\infty} \psi^*(-x)\,\psi(-x)\,dx \tag{14}$$

$$= \int_{-\infty}^{\infty} \psi^*\left(x'\right)\psi\left(x'\right)dx' \tag{15}$$

$$= \langle \psi \,|\psi\rangle \tag{16}$$

In the second line we used the same trick as in the derivation of 5 to substitute $x' = -x$. Thus we see that

$$\Pi^\dagger \Pi = I \tag{17}$$

$$\Pi^\dagger = \Pi^{-1} = \Pi \tag{18}$$

The condition $\Pi^\dagger = \Pi$ shows that Π is Hermitian, and the condition $\Pi^\dagger = \Pi^{-1}$ shows that Π is unitary.

Finally, any operator whose square is the identity operator has eigenvalues ± 1, as we can see as follows. Suppose $|\psi\rangle$ is an eigenvector of Π with eigenvalue α. Then

$$\Pi|\psi\rangle = \alpha|\psi\rangle \tag{19}$$

$$\Pi^2|\psi\rangle = \alpha\Pi|\psi\rangle \tag{20}$$

$$= \alpha^2|\psi\rangle \tag{21}$$

$$= I|\psi\rangle \tag{22}$$

$$= |\psi\rangle \tag{23}$$

Therefore $\alpha^2 = 1$, so $\alpha = \pm 1$.

We can also define Π by examining its effect on operators, rather than states. Consider

$$\left\langle \Pi x' \,|X|\, \Pi x \right\rangle = \left\langle -x' \,|X|\, -x \right\rangle \tag{24}$$

$$= -x\delta\left(x' - x\right) \tag{25}$$

However, this is equivalent to

$$\left\langle \Pi x' \left| X \right| \Pi x \right\rangle = \left\langle x' \left| \Pi^\dagger X \Pi \right| x \right\rangle = -x\delta\left(x' - x\right) \tag{26}$$

Thus we can write

$$\Pi^\dagger X \Pi = -X \tag{27}$$

and similarly for the momentum

$$\Pi^\dagger P \Pi = -P \tag{28}$$

Eigenstates of parity are said to be even if the eigenvalue is $+1$ and odd if the eigenvalue is -1. Mathematically, the X basis representation of such eigenstates are even or odd functions of x, respectively.

The Hamiltonian is parity invariant if a parity transformation leaves it unchanged, so that

$$\Pi^\dagger H\left(X, P\right)\Pi = H\left(-X, -P\right) = H\left(X, P\right) \tag{29}$$

Since $\Pi^\dagger = \Pi$, this condition is equivalent to

$$\left[\Pi, H\right] = 0 \tag{30}$$

Using the same argument as with conservation of momentum, if this commutator is valid at all times (if H is time-independent this is automatic; if H is time-dependent, then we must impose the commutator at all times), then Π must also commute with the propagator $U\left(t\right)$, since U depends only on H. In this case, if we start with a system in a definite parity state (even or odd), then the parity of the state doesn't change with time. This follows because if $\left[\Pi, U\left(t\right)\right] = 0$ then if $\Pi\left|\psi\left(0\right)\right\rangle = \alpha\left|\psi\left(0\right)\right\rangle$ (where $\alpha = \pm 1$), then we can let the state evolve in time by applying the propagator to it, so that we have

$$\left|\psi\left(t\right)\right\rangle = U\left(t\right)\left|\psi\left(0\right)\right\rangle \tag{31}$$

Applying the parity operator to this and using the commutator, we have

$$\Pi\left|\psi\left(t\right)\right\rangle = \Pi U\left(t\right)\left|\psi\left(0\right)\right\rangle = U\left(t\right)\Pi\left|\psi\left(0\right)\right\rangle = \alpha U\left(t\right)\left|\psi\left(0\right)\right\rangle = \alpha\left|\psi\left(t\right)\right\rangle \tag{32}$$

Thus the parity of the evolved state is the same as the parity of the initial state.

Parity is not always conserved in physics. A notable parity-violating reaction is a decay involving the weak nuclear force. Shankar describes one such case with the decay of an isotope of cobalt: ${}^{60}\text{Co} \rightarrow {}^{60}\text{ Ni} + e^- + \bar{\nu}$. Another example is in Shankar's exercise 11.4.3.

Suppose that in one particular reaction which emits an electron, the electron's spin is observed to be always parallel to its momentum. For the purposes of this argument, we can regard an electron's spin as being caused by some physical rotation of the electron. Suppose in one such reaction, the electron's spin is in the $+z$ direction (using the right-hand rule for calculating the direction of angular momentum, so that viewed from above, the electron is rotating counterclockwise) and therefore its momentum is also in the $+z$ direction. Now reflect this reaction in a mirror lying in the yz plane. This reflection will invert the direction of rotation (think of viewing a spinning top in a mirror) so that the spin direction will now point in the $-z$ direction, but since the momentum vector is parallel to the plane of the mirror, it will *not* be inverted. Thus the spin and momentum are now antiparallel after a parity transformation, showing that parity in this case is not conserved.

Finally, Shankar includes a curious problem (11.4.2) which, as far as I can tell, doesn't have anything to do with parity, but I'll include it here for completeness. Suppose we have a particle that moves in a potential

$$V(x) = V_0 \sin\left(\frac{2\pi x}{a}\right) \tag{33}$$

This potential is periodic with a period of a, so if we translate the system according to $x \to x + ma$ for some integer m, the potential is unchanged. The problem is to show that momentum is not conserved in this case. The conservation of momentum argument, valid for infinitesimal translations, relied on Ehrenfest's theorem, which states that

$$\left\langle \dot{P} \right\rangle = -\frac{i}{\hbar} \langle [P, H] \rangle \tag{34}$$

If the momentum commutes with the Hamiltonian, then, on average, the momentum is conserved. Now in this case we can calculate the commutator $[P, V]$ using the result

$$[X^n, P] = i\hbar n X^{n-1} \tag{35}$$

We can write the potential as a series:

$$V(X) = V_0 \left[\frac{2\pi X}{a} - \frac{1}{3!}\left(\frac{2\pi X}{a}\right)^3 + \ldots\right] \tag{36}$$

The commutator is therefore

$$[V, P] = \frac{2\pi i\hbar V_0}{a}\left[1 - \frac{1}{2!}\left(\frac{2\pi X}{a}\right)^2 + \ldots\right] = \frac{2\pi i\hbar V_0}{a}\cos\left(\frac{2\pi X}{a}\right) \tag{37}$$

Therefore, Ehrenfest's theorem gives us (since H presumably is of the form $H = T + V$ with the kinetic energy depending only on P, so it commutes with P):

$$\left\langle \dot{P} \right\rangle = -\frac{2\pi V_0}{a} \left\langle \cos\left(\frac{2\pi X}{a}\right) \right\rangle \tag{38}$$

Since the cosine is periodic, we can't actually calculate a unique value for its average, although if we do the average over an exact number of periods, the average is still zero. I have a feeling that I'm missing something obvious here, so any suggestions are welcome.

COMMENTS

Remark 1. Aaron Stevens

Nov 21, 2017 10:40 PM

I am specifically referring to problem 11.4.2 in Shankar's Quantum Mechanics book (around equation 33 in the above link).

The final equation 38 you arrive at is valid, but then you say,

"Since the cosine is periodic, we can't actually calculate a unique value for its average, although if we do the average over an exact number of periods, the average is still zero. I have a feeling that I'm missing something obvious here, so any suggestions are welcome."

Let me see what you think: The final expression that results in the expectation value of the cosine function is not the same thing as the average of the cosine function. The only time the expectation value is equal to the average is when the probability distribution in question is the uniform distribution. In general, this expectation value is state dependent. It is a measure of what we would "expect" this cosine function to be given the probability distribution of finding the particle between x and x+dx in space (psi* times psi). We could contrive a state that gives 0 for this expectation value, but I doubt that the state will then evolve according to the Schrodinger's equation in such a way as to keep the expectation value set at 0.

To have momentum conservation, we need the expectation value of the commutator [P,H] to be 0 always, since momentum conservation is a property of the physical system in question, not on the states within that system. So since we get a "final answer" that is not identically 0, we must say that momentum is not conserved.

Another way I thought to solve the problem that is simpler but I am unsure is valid is that since the potential (and therefore Hamiltonian) is not invariant under infinitesimal translations that we cannot say momentum is conserved. Or thinking a little bit differently, just because we have found

points in space where the potential energy is the same does not mean momentum is conserved. It is like if you were to push a block down and back up a hill with friction so that it begins and ends at rest. If you are considering just the block as your system and then saying since it starts and stops with the same energy that its energy must have been conserved the entire time, you would not be correct.

I grade for a quantum class that uses this book, and I think a lot of the students refer to these solutions, so this is how I came across this. Thanks!

=========

I suspect you're right. The main point appears to be that in order to calculate $\left\langle \cos\left(\frac{2\pi X}{a}\right)\right\rangle$ we must do so in a particular state of the particle, and this will not in general be zero. However, I think your second solution is also valid - the derivation of constant momentum resulted from the invariance of the system under infinitesimal translations, and that's not true in this case.

==========

Aaron Stevens says:

December 19, 2017 at 4:05 pm

Awesome! Thanks! I agree, it requires some thought, and even though it all sounds good I still feel like I am doing some hand waving, especially with the infinitesimal translation argument. Thanks for looking it over!

PINGBACKS

Pingback: Time reversal, antiunitary operators and Wigner's theorem

Pingback: angular momentum and parity

Pingback: Parity transformation of creation and annihilation operators

TIME REVERSAL, ANTIUNITARY OPERATORS AND WIGNER'S THEOREM

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 11, Section 11.5.

Zee, A. (2016), *Group Theory in a Nutshell for Physicists*. Section IV.6.

Post date: 12 Apr 2017

Parity is one of the two main discrete symmetries treated in non-relativistic quantum mechanics. The other is time reversal, which we'll look at here.

First, we'll have a look at what time reversal symmetry means in classical physics. The idea is that if we can take a snapshot of the system at some time, each particle will have a given position x and a given momentum p. If we reverse the direction of time at that instant, the particle's position remains the same, but its momentum reverses. In other words $x \to x$ and $p \to -p$. Note the difference between time reversal and parity: in a parity operation, *both* position and momentum get 'reflected' into their negative values, while in time reversal, only momentum gets 'reflected'.

We can see how this works by looking at Newton's law in the form

$$F = m\frac{d^2x}{dt^2} \tag{1}$$

Time reversal invariance is valid if the same equation holds when we reverse the direction of time, that is, we let $t \to -t$. Since $x \to x$, the numerator on the RHS is unchanged. For the denominator $t \to -t$ means that $dt \to -dt$ and $(dt)^2 \to (-dt)^2 = dt^2$, so the acceleration is invariant. Newton's law is invariant under time reversal provided that the force on the LHS is invariant, which will be the case provided that F depends only on x and not on $\dot{x}$. This is true for forces such as Newtonian gravity and electrostatics, but is not true for the magnetic force felt by a charge q moving through a magnetic field $\mathbf{B}$ with velocity $\mathbf{v}$, where the Lorentz force law holds:

$$\mathbf{F} = q\mathbf{v} \times \mathbf{B} \tag{2}$$

This follows because $\mathbf{v} \to -\mathbf{v}$ so if the field $\mathbf{B}$ is the same after time reversal, $\mathbf{F} \to -\mathbf{F}$. However, because all magnetic fields are produced by the motion of charges, if we expand the time reversal to include the charges giving rise to the magnetic field $\mathbf{B}$, then the motion of all these charges would

reverse, which in turn would cause $\mathbf{B} \to -\mathbf{B}$. Thus if we time-reverse the *entire* electromagnetic system, the electromagnetic force is invariant under time reversal.

How does time reversal work in quantum mechanics? Shankar considers a particle in one dimension governed by a time-independent Hamiltonian, which obeys the Schrödinger equation, as usual:

$$i\hbar\frac{\partial\psi(x,t)}{\partial t} = H(x)\,\psi(x,t) \tag{3}$$

At this point, Shankar states that if we replace ψ by its complex conjugate ψ^*, we are implementing time reversal, claiming that it is 'clear' because ψ^* gives the same probability distribution as ψ. I cannot find any reason why this should be 'clear' from this statement, so let's try looking at the problem in a bit more detail. The clearest explanation I've found is in Zee's book, referenced above.

In order that the system be invariant under time reversal, we consider the transformation $t \to t' = -t$ and we wish to find some operator T which operates on the wave function $\psi(t)$ so that

$$T\psi(t) = \psi'\left(t'\right) = \psi'(-t) \tag{4}$$

[I'm suppressing the dependence on x for brevity; since time reversal doesn't affect x, it stays the same throughout this argument] satisfies the Schrödinger equation in the form

$$i\hbar\frac{\partial\psi'(t')}{\partial t'} = H\psi'\left(t'\right) \tag{5}$$

From this, we get

$$i\hbar\frac{\partial\left(T\psi(t)\right)}{\partial(-t)} = HT\psi(t) \tag{6}$$

Whatever this unknown operator T is, it has an inverse, so we can multiply on the left by T^{-1} to get

$$T^{-1}(-i)\,T\hbar\frac{\partial\psi(t)}{\partial t} = T^{-1}HT\psi(t) \tag{7}$$

Notice that we're not assuming that T has no effect on i (that is, we're not assuming that we can pull i out of the expression on the LHS). Now we know that T has an effect only if what it operates on depends on time (since it's the time reversal operator) so, since we're assuming that H is time-independent, we must have $[H,T] = 0$. Given this, we have

$$T^{-1}HT = T^{-1}TH = H \tag{8}$$

Thus, the RHS of 7 reduces to the RHS of the original Schrödinger equation 3. If the Schrödinger equation is to remain valid after time reversal, the LHS of 7 must also reduce to the LHS of 3. That is, we must have

$$T^{-1}(-i)T = i \tag{9}$$

Multiplying on the left by T we get

$$-iT = Ti \tag{10}$$

In other words, one of the effects of T is that it takes the complex conjugate of any expression that it operates on.

To find out exactly what T is, we can write it as the product of a unitary operator U and the operator K, whose only job is that it takes the complex conjugate. Since doing the complex conjugate operation twice in succession returns us to the original expression, $K^2 = I$, so $K = K^{-1}$. We get

$$\begin{aligned} T &= UK & (11)\\ T^{-1} &= K^{-1}U^{-1} = KU^{-1} & (12) \end{aligned}$$

Ordinary unitary operators are linear in the sense that $U(\alpha\psi) = \alpha U\psi$, where α is a complex number and ψ is some function, with a similar relation holding for U^{-1}. Combining the above few equations, we have

$$\begin{aligned} T^{-1}(-i)T &= KU^{-1}(-i)UK & (13)\\ &= K(-i)U^{-1}UK & (14)\\ &= iK^2 & (15)\\ &= i & (16) \end{aligned}$$

Thus the most general form for T is some unitary operator U multiplied by the complex conjugate operator K. We can see that, for such an operator, and complex constants $\alpha$and β and functions ψ and ϕ:

$$\begin{aligned} T(\alpha\psi + \beta\phi) &= UK(\alpha\psi + \beta\phi) & (17)\\ &= U(\alpha^* K\psi + \beta^* K\phi) & (18)\\ &= \alpha^* UK\psi + \beta^* UK\phi & (19)\\ &= \alpha^* T\psi + \beta^* T\phi & (20) \end{aligned}$$

An operator that obeys this relation is called *antilinear*. The operator T has the additional property

$$\langle T\psi\,|T\phi\rangle = \langle UK\psi\,|UK\phi\rangle \tag{21}$$
$$= \langle U\psi\,|U\phi\rangle^* \tag{22}$$
$$= \langle \psi\,|\phi\rangle^* \tag{23}$$
$$= \langle \phi\,|\psi\rangle \tag{24}$$

The third line follows from the fact that a unitary operator preserves inner products. An antilinear operator that satisfies the condition $\langle T\psi\,|T\phi\rangle = \langle \phi\,|\psi\rangle$ is called *antiunitary*. [The fact that time reversal is antiunitary was first derived by Eugene Wigner in 1932. A more general result, known as Wigner's theorem, states that any symmetry in a quantum system must be represented by either a unitary or an antiunitary operator.]

To find U in this case, consider a plane wave state

$$\psi\,(t) = e^{i(px-Et)/\hbar} \tag{25}$$

Applying T to this state, we have

$$T\psi\,(t) = UKe^{i(px-Et)/\hbar} \tag{26}$$
$$= Ue^{-i(px-Et)/\hbar} \tag{27}$$

In one dimension, the only unitary operator U is a phase factor like $e^{i\alpha}$ for some real α (since U has to preserve the inner product). We can take $U = 1$ since the phase factor cancels out when calculating $|T\psi\,(t)|^2$. Going back to 4, we see that the time-reversed wave function is

$$\psi'\,(-t) = T\psi\,(t) = e^{-i(px-Et)/\hbar} \tag{28}$$
$$\psi'\,(t) = e^{-i(px+Et)/\hbar} = e^{(-ipx-Et)/\hbar} \tag{29}$$

Since this is the same as the original wave function except that $p \to -p$, we see that it is indeed a valid time-reversed wave function. The energy is the same (the $-Et$ part of the exponent still has a minus sign) but the momentum has reversed, giving a wave that moves in the opposite direction.

Another way of looking at time reversal is as follows. Suppose we start with a system in the state $\psi\,(0)$ at $t = 0$. We can let it evolve for a time τ using the propagator to get the state at time $t = \tau$:

$$\psi\,(\tau) = e^{-iH\tau/\hbar}\psi\,(0) \tag{30}$$

Applying time reversal via the operator T to this state, we have (we're assuming that H is time-independent, but we're allowing it to be complex)

$$T\psi(\tau) = e^{iH^*\tau/\hbar}\psi^*(0) \tag{31}$$

If we now evolve this time-reversed state through the same time τ, we should end up back in the (time-reversed) original state if the system is invariant under time reversal. That is,

$$\psi(2\tau) = e^{-iH\tau/\hbar}e^{iH^*\tau/\hbar}\psi^*(0) = \psi^*(0) \tag{32}$$

[Note that we don't require $\psi(2\tau) = \psi(0)$ since $\psi(2\tau)$ is the system in its time-reversed state, where it's moving in the opposite direction to the original state. Think about time-reversing a bouncing ball. The ball becomes effectively time-reversed when it bounces. If the ball is travelling down at some speed v at a height h, then after bouncing (assuming an elastic bounce) it will be travelling at the same speed v when it bounces back to the height h, but it will be moving in the opposite direction.]

In this equation, we're working in the X basis, so the exponents are numerical functions, not operators, and we're free to combine the exponents without worrying about commutators. This means that in order for the system to be time-reversal invariant, we must have

$$H(x) = H^*(x) \tag{33}$$

In other words, the Hamiltonian must be real. The usual kinetic plus potential type of Hamiltonian satisfies this since it has the form

$$H = \frac{P^2}{2m} + V(x) \tag{34}$$

and although the quantum momentum operator is $P = -i\hbar\frac{d}{dx}$, its square is real. In the magnetic force case, the presence of the charge's velocity as a linear term (in $q\mathbf{v} \times \mathbf{B}$) means the momentum operator occurs as a linear term, making H complex, so time reversal invariance doesn't hold. Again, however, if we included the charges that give rise to the magnetic field, the discrepancy disappears.

PINGBACKS

Pingback: Generators of the Lorentz group

Pingback: Time reversal in the Dirac equation

TRANSLATION INVARIANCE IN TWO DIMENSIONS

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 12, Exercise 12.1.1.

Post date: 13 Apr 2017

In preparation for an examination of rotation invariance, we'll have a look at translational invariance in two dimensions. We can apply much of what we did with translation in one dimension, where we showed that the momentum P is the generator of translations. In particular, the translation operator $T(\varepsilon)$ for an infinitesimal translation ε is

$$T(\varepsilon) = I - \frac{i\varepsilon}{\hbar} P \tag{1}$$

In two dimensions, we can write an infinitesimal translation as $\boldsymbol{\delta} a$ where

$$\boldsymbol{\delta} a = \delta a_x \hat{\mathbf{x}} + \delta a_y \hat{\mathbf{y}} \tag{2}$$

In one dimension, we showed earlier that

$$\langle x | T(\varepsilon) | \psi \rangle = \psi(x - \varepsilon) \tag{3}$$

The analogous relation in two dimensions is

$$\langle x, y | T(\boldsymbol{\delta} a) | \psi \rangle = \psi(x - \delta a_x, y - \delta a_y) \tag{4}$$

We can verify that the correct form for $T(\boldsymbol{\delta} a)$ is

$$T(\boldsymbol{\delta} a) = I - \frac{i}{\hbar} \boldsymbol{\delta} a \cdot \mathbf{P} \tag{5}$$

$$= I - \frac{i}{\hbar} (\delta a_x P_x + \delta a_y P_y) \tag{6}$$

Using the representation of momentum in the position basis, which is

$$P_x = -i\hbar \frac{\partial}{\partial x} \tag{7}$$

$$P_y = -i\hbar \frac{\partial}{\partial y} \tag{8}$$

the LHS of 4 is, using $\langle x, y | \psi \rangle = \psi(x, y)$:

$$\langle x,y\left|T\left(\boldsymbol{\delta}a\right)\right|\psi\rangle=\left\langle x,y\left|I-\frac{i}{\hbar}\left(\delta a_{x}P_{x}+\delta a_{y}P_{y}\right)\right|\psi\right\rangle \tag{9}$$

$$=\psi\left(x,y\right)-\delta a_{x}\frac{\partial\psi}{\partial x}-\delta a_{y}\frac{\partial\psi}{\partial y} \tag{10}$$

The last line is also what we get if we expand the RHS of 4 to first order in $\boldsymbol{\delta}a$, which verifies that 5 is correct, so that the two-dimensional momentum $\mathbf{P}$ is the generator of two-dimensional translations.

We can apply the exponentiation technique we used in the one-dimensional case to obtain the translation operator for a finite translation in two dimensions. We need to be careful that we don't run into problems with non-commuting operators, but in view of 7 and 8 and the fact that derivatives with respect to different independent variables commute, we see that

$$\left[P_{x},P_{y}\right]=0 \tag{11}$$

We can divide a finite translation $\mathbf{a}$ into N small steps, each of size $\frac{\mathbf{a}}{N}$, so that the translation is

$$T\left(\mathbf{a}\right)=\left(I-\frac{i}{\hbar N}\mathbf{a}\cdot\mathbf{P}\right)^{N} \tag{12}$$

Because the two components of momentum commute, we can take the limit of this expression to get the exponential form:

$$T\left(\mathbf{a}\right)=\lim_{N\rightarrow\infty}\left(I-\frac{i}{\hbar N}\mathbf{a}\cdot\mathbf{P}\right)^{N}=e^{-i\mathbf{a}\cdot\mathbf{P}/\hbar} \tag{13}$$

Again, because the two components of momentum commute, we can combine two translations, by $\mathbf{a}$ and then by $\mathbf{b}$, to get

$$T\left(\mathbf{b}\right)T\left(\mathbf{a}\right)=e^{-i\mathbf{b}\cdot\mathbf{P}/\hbar}e^{-i\mathbf{a}\cdot\mathbf{P}/\hbar}=e^{-i(\mathbf{a}+\mathbf{b})\cdot\mathbf{P}/\hbar}=T\left(\mathbf{b}+\mathbf{a}\right) \tag{14}$$

PINGBACKS

Pingback: Combining translations and rotations

ROTATIONAL INVARIANCE IN TWO DIMENSIONS

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 12, Exercise 12.2.1.

Post date: 17 Apr 2017

As a first look at rotational invariance in quantum mechanics, we'll look at two-dimensional rotations about the z axis. Classically, a rotation by an angle ϕ_0 about the z axis is given by the matrix equation for the coordinates

$$\begin{bmatrix} \bar{x} \\ \bar{y} \end{bmatrix} = \begin{bmatrix} \cos\phi_0 & -\sin\phi_0 \\ \sin\phi_0 & \cos\phi_0 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} \tag{1}$$

The momenta transform the same way, since we are merely changing the direction of the x and y axes. Thus we have also

$$\begin{bmatrix} \bar{p}_x \\ \bar{p}_y \end{bmatrix} = \begin{bmatrix} \cos\phi_0 & -\sin\phi_0 \\ \sin\phi_0 & \cos\phi_0 \end{bmatrix} \begin{bmatrix} p_x \\ p_y \end{bmatrix} \tag{2}$$

The rotation matrix can be written as an operator, defined as

$$R(\phi_0\hat{\mathbf{z}}) = \begin{bmatrix} \cos\phi_0 & -\sin\phi_0 \\ \sin\phi_0 & \cos\phi_0 \end{bmatrix} \tag{3}$$

In quantum mechanics, due to the uncertainty principle we cannot specify position and momentum precisely at the same time, so as with the case of translational invariance, we deal with expectation values. As usual, a rotation is represented by a unitary operator $U[R(\phi_0\hat{\mathbf{z}})]$ so that a quantum state transforms according to

$$|\psi\rangle \rightarrow |\psi_R\rangle = U[R]\,|\psi\rangle \tag{4}$$

Dealing with expectation values means that the rotation operator must satisfy

$$\langle X\rangle_R = \langle X\rangle\cos\phi_0 - \langle Y\rangle\sin\phi_0 \tag{5}$$

$$\langle Y\rangle_R = \langle X\rangle\sin\phi_0 + \langle Y\rangle\cos\phi_0 \tag{6}$$

$$\langle P_x\rangle_R = \langle P_x\rangle\cos\phi_0 - \langle P_y\rangle\sin\phi_0 \tag{7}$$

$$\langle P_y\rangle_R = \langle P_x\rangle\sin\phi_0 + \langle P_y\rangle\cos\phi_0 \tag{8}$$

The expectation values on the LHS of these equations are calculated using the rotated state, so that

$$\langle X \rangle_R = \langle \psi_R | X | \psi_R \rangle \tag{9}$$

and so on.

In two dimensions, the position eigenkets depend on the two independent coordinates x and y, and each of these eigenkets transforms under rotation in the same way the position variables above. Operating on such an eigenket with the unitary rotation operator thus must give

$$U[R]|x,y\rangle = |x\cos\phi_0 - y\sin\phi_0, x\sin\phi_0 + y\cos\phi_0\rangle \tag{10}$$

As with the translation operator, we try to construct an explicity form for $U[R]$ by considering an infinitesimal rotation $\varepsilon_z\hat{\mathbf{z}}$ about the z axis. We propose that the unitary operator for this rotation is given by

$$U[R(\varepsilon_z\hat{\mathbf{z}})] = I - \frac{i\varepsilon_z L_z}{\hbar} \tag{11}$$

where L_z is, at this stage, an unknown operator called the generator of infinitesimal rotations (although, as the notation suggests, it will turn out to be the z component of angular momentum). Under this rotation, we have, to first order in ε_z:

$$U[R(\varepsilon_z\hat{\mathbf{z}})]|x,y\rangle = |x - y\varepsilon_z, x\varepsilon_z + y\rangle \tag{12}$$

Note that we've omitted a possible phase factor in this rotation. That is, we could have written

$$U[R(\varepsilon_z\hat{\mathbf{z}})]|x,y\rangle = e^{i\varepsilon_z g(x,y)/\hbar}|x - y\varepsilon_z, x\varepsilon_z + y\rangle \tag{13}$$

for some real function $g(x,y)$. Dropping the phase factor has the effect of making the momentum expectation values transform in the same way as the position expectaton values, as shown by Shankar in his equation 12.2.13, so we'll just take the phase factor to be 1 from now on.

We can now find the position space form of a general state vector $|\psi\rangle$ under an infinitesimal rotation by following a similar procedure to that for a translation.

We have

$$|\psi_{\varepsilon_z}\rangle = U\left[R\left(\varepsilon_z\hat{\mathbf{z}}\right)\right]|\psi\rangle \tag{14}$$

$$= U\left[R\left(\varepsilon_z\hat{\mathbf{z}}\right)\right]\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}|x,y\rangle\langle x,y|\psi\rangle\,dx\,dy \tag{15}$$

$$= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}U\left[R\left(\varepsilon_z\hat{\mathbf{z}}\right)\right]|x,y\rangle\langle x,y|\psi\rangle\,dx\,dy \tag{16}$$

$$= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}|x-y\varepsilon_z, x\varepsilon_z+y\rangle\langle x,y|\psi\rangle\,dx\,dy \tag{17}$$

We can now change integration variables if we define

$$x' \equiv x-y\varepsilon_z \tag{18}$$

$$y' = x\varepsilon_z+y \tag{19}$$

The differentials transform by considering terms only up to first order in infinitesimal quantities, so we have

$$dx' = dx-\varepsilon_z dy = dx \tag{20}$$

$$dy' = \varepsilon_z dx+dy = dy \tag{21}$$

Also, to first order in infinitesimal quantities, we can invert the variables to get

$$x'+\varepsilon_z y' = x-y\varepsilon_z+x\varepsilon_z^2+y\varepsilon_z = x \tag{22}$$

$$y'-\varepsilon_z x' = x\varepsilon_z+y-x\varepsilon_z+y\varepsilon_z^2 = y \tag{23}$$

The ranges of integration are still $\pm\infty$, so we end up with

$$|\psi_{\varepsilon_z}\rangle = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\left|x',y'\right\rangle\left\langle x'+\varepsilon_z y', y'-\varepsilon_z x'\,|\psi\right\rangle dx'\,dy' \tag{24}$$

Multiplying on the left by the bra $\langle x,y|$ we have

$$\langle x,y\,|\psi_{\varepsilon_z}\rangle = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\left\langle x,y\left|x',y'\right.\right\rangle\left\langle x'+\varepsilon_z y', y'-\varepsilon_z x'\,|\psi\right\rangle dx'\,dy' \tag{25}$$

$$= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\delta\left(x-x'\right)\delta\left(y-y'\right)\left\langle x'+\varepsilon_z y', y'-\varepsilon_z x'\,|\psi\right\rangle dx'\,dy' \tag{26}$$

$$= \langle x+\varepsilon_z y, y-\varepsilon_z x\,|\psi\rangle \tag{27}$$

$$= \psi\left(x+\varepsilon_z y, y-\varepsilon_z x\right) \tag{28}$$

This can now be expanded in a 2-variable Taylor series to give, to first order in ε_z:

$$\psi\left(x+\varepsilon_z y, y-\varepsilon_z x\right)=\psi\left(x,y\right)+y\varepsilon_z\frac{\partial\psi}{\partial x}-x\varepsilon_z\frac{\partial\psi}{\partial y} \tag{29}$$

We can compare this with 11 inserted into 14:

$$\begin{aligned}\left\langle x,y\left|\psi_{\varepsilon_z}\right.\right\rangle &= \left\langle x,y\left|U\left[R\left(\varepsilon_z\hat{\mathbf{z}}\right)\right]\right|\psi\right\rangle &(30)\\ &= \left\langle x,y\left|I-\frac{i\varepsilon_z L_z}{\hbar}\right|\psi\right\rangle &(31)\\ &= \psi\left(x,y\right)-\frac{i\varepsilon_z}{\hbar}\left\langle x,y\left|L_z\right|\psi\right\rangle &(32)\end{aligned}$$

Setting 32 equal to 29 we have

$$\begin{aligned}-\frac{i\varepsilon_z}{\hbar}\left\langle x,y\left|L_z\right|\psi\right\rangle &= y\varepsilon_z\frac{\partial\psi}{\partial x}-x\varepsilon_z\frac{\partial\psi}{\partial y} &(33)\\ \left\langle x,y\left|L_z\right|\psi\right\rangle &= x\left(-i\hbar\frac{\partial\psi}{\partial y}\right)-y\left(-i\hbar\frac{\partial\psi}{\partial x}\right) &(34)\end{aligned}$$

Using the position-space forms of the momenta

$$\begin{aligned}P_x &= -i\hbar\frac{\partial}{\partial x} &(35)\\ P_y &= -i\hbar\frac{\partial}{\partial y} &(36)\end{aligned}$$

we see that L_z is given by

$$L_z = XP_y - YP_x \tag{37}$$

which is the quantum equivalent of the z component of angular momentum, as promised.

PINGBACKS

Pingback: Rotational transformations using passive transformations
Pingback: Rotations through a finite angle; use of polar coordinates
Pingback: Combining translations and rotations
Pingback: Angular momentum in three dimensions
Pingback: Rotation of a vector wave function
Pingback: Spherical tensor operators; commutators

ROTATIONAL TRANSFORMATIONS USING PASSIVE TRANSFORMATIONS

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Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 12, Exercise 12.2.2.

Post date: 18 Apr 2017

We can also derive the generator of rotations L_z by considering passive transformations of the position and momentum operators, in a way similar to that used for deriving the generator of translations. In a passive transformation, the operators are modified while the state vectors remain the same. For an infinitesimal rotation $\varepsilon_z \hat{\mathbf{z}}$ about the z axis in two dimensions, the unitary operator has the form

$$U\left[R\left(\varepsilon_z \hat{\mathbf{z}}\right)\right] = I - \frac{i\varepsilon_z L_z}{\hbar} \tag{1}$$

For a finite rotation by $\phi_0 \hat{\mathbf{z}}$ the transformations are given by

$$\langle X\rangle_R = \langle X\rangle \cos\phi_0 - \langle Y\rangle \sin\phi_0 \tag{2}$$
$$\langle Y\rangle_R = \langle X\rangle \sin\phi_0 + \langle Y\rangle \cos\phi_0 \tag{3}$$
$$\langle P_x\rangle_R = \langle P_x\rangle \cos\phi_0 - \langle P_y\rangle \sin\phi_0 \tag{4}$$
$$\langle P_y\rangle_R = \langle P_x\rangle \sin\phi_0 + \langle P_y\rangle \cos\phi_0 \tag{5}$$

For the infinitesimal transformation, $\phi_0 = \varepsilon_z$ and these equations reduce to

$$\langle X\rangle_R = \langle X\rangle - \langle Y\rangle \varepsilon_z \tag{6}$$
$$\langle Y\rangle_R = \langle X\rangle \varepsilon_z + \langle Y\rangle \tag{7}$$
$$\langle P_x\rangle_R = \langle P_x\rangle - \langle P_y\rangle \varepsilon_z \tag{8}$$
$$\langle P_y\rangle_R = \langle P_x\rangle \varepsilon_z + \langle P_y\rangle \tag{9}$$

In the passive transformation scheme, we move the transformation to the operators to get

$$U^{\dagger}[R]XU[R] = X - Y\varepsilon_z \tag{10}$$
$$U^{\dagger}[R]YU[R] = X\varepsilon_z + Y \tag{11}$$
$$U^{\dagger}[R]P_xU[R] = P_x - P_y\varepsilon_z \tag{12}$$
$$U^{\dagger}[R]P_yU[R] = P_x\varepsilon_z + P_y \tag{13}$$

Substituting 1 into these equations gives us the commutation relations satisfied by L_z. For example, in the first equation we have

$$U^{\dagger}[R]XU[R] = \left(I + \frac{i\varepsilon_z L_z}{\hbar}\right) X \left(I - \frac{i\varepsilon_z L_z}{\hbar}\right) \tag{14}$$
$$= X + \frac{i\varepsilon_z}{\hbar}(L_z X - X L_z) \tag{15}$$
$$= X - Y\varepsilon_z \tag{16}$$

Equating the last two lines, we get

$$[X, L_z] = -i\hbar Y \tag{17}$$

Similarly, for the other three equations we get

$$[Y, L_z] = i\hbar X \tag{18}$$
$$[P_x, L_z] = -i\hbar P_y \tag{19}$$
$$[P_y, L_z] = i\hbar P_x \tag{20}$$

We can use these commutation relations to derive the form of L_z by using the commutation relations for coordinates and momenta:

$$[X, P_x] = [Y, P_y] = i\hbar \tag{21}$$

with all other commutators involving X, Y, P_x and P_y being zero. Starting with 17, we see that

$$[X, L_z] = -[X, P_x]Y \tag{22}$$

We can therefore deduce that

$$L_z = -P_x Y + f(X, Y, P_y) \tag{23}$$

where f is some unknown function. We must include f since the commutators of X with X, Y and P_y are all zero, so adding on f still satisfies 17. (You can think of it as similar to adding on the constant in an indefinite integral.)

Now from 18, we have

$$[Y, L_z] = [Y, P_y] X \tag{24}$$

so combining this with 23 we have

$$L_z = -P_x Y + P_y X + g(X, Y) \tag{25}$$

The undetermined function is now a function only of X and Y, since the dependence of L_z on P_x and P_y has been determined uniquely by the commutators 17 and 18.

From 19 we have

$$[P_x, L_z] = [P_x, X] P_y \tag{26}$$

We can see that this is satisfied already by 25, except that we now know that the function g cannot depend on X, since then $[P_x, g] \neq 0$. Thus we have narrowed down L_z to

$$L_z = -P_x Y + P_y X + h(Y) \tag{27}$$

Finally, from 20 we have

$$[P_y, L_z] = -[P_y, Y] P_x \tag{28}$$

This is satisfied by 27 if we take $h = 0$ (well, technically, we could take h to be some constant, but we might as well take the constant to be zero), giving us the final form for L_z:

$$L_z = -P_x Y + P_y X \tag{29}$$

PINGBACKS

Pingback: Combining translations and rotations

Pingback: Two-dimensional harmonic oscillator - Part 1

ROTATIONS THROUGH A FINITE ANGLE; USE OF POLAR COORDINATES

Link to: physicspages home page.

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Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 12, Exercise 12.2.3.

Post date: 20 Apr 2017

The angluar momentum operator L_z is the generator of rotations in the xy plane. We did the derivation for infinitesimal rotations, but we can generalize this to finite rotations in a similar manner to that used for translations. The unitary transformation for an infinitesimal rotation is

$$U\left[R\left(\varepsilon_z\hat{\mathbf{z}}\right)\right] = I - \frac{i\varepsilon_z L_z}{\hbar} \tag{1}$$

For rotation through a finite angle ϕ_0, we divide up the angle into N small angles, so $\varepsilon_z = \phi_0/N$. Rotation through the full angle ϕ_0 is then given by

$$U\left[R\left(\phi_0\hat{\mathbf{z}}\right)\right] = \lim_{N\to\infty}\left(I - \frac{i\phi_0 L_z}{N\hbar}\right)^N = e^{-i\phi_0 L_z/\hbar} \tag{2}$$

The limit follows because the only non-trivial operator involved is L_z, so no commutation problems arise.

In rectangular coordinates, L_z has the relatively non-obvious form

$$\begin{aligned} L_z &= XP_y - YP_x & (3)\\ &= -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) & (4)\end{aligned}$$

so it's not immediately clear that 2 does in fact lead to the desired rotation. Trying to calculate the exponential with L_z expressed this way is not easy, given that the two terms $x\frac{\partial}{\partial y}$ and $y\frac{\partial}{\partial x}$ don't commute.

It turns out that L_z has a much simpler form in polar coordinates, and there are two ways of converting it to polar form. First, we recall the transformation equations.

$$x = \rho\cos\phi \tag{5}$$
$$y = \rho\sin\phi \tag{6}$$
$$\rho = \sqrt{x^2+y^2} \tag{7}$$
$$\phi = \tan^{-1}\frac{y}{x} \tag{8}$$

From the chain rule, we can convert the derivatives:

$$\frac{\partial}{\partial x} = \frac{\partial\rho}{\partial x}\frac{\partial}{\partial\rho} + \frac{\partial\cos\phi}{\partial x}\frac{\partial}{\partial(\cos\phi)} \tag{9}$$
$$= \frac{\partial\rho}{\partial x}\frac{\partial}{\partial\rho} - \sin\phi\frac{\partial\phi}{\partial x}\frac{\partial}{(-\sin\phi)\,\partial\phi} \tag{10}$$
$$= \frac{x}{\rho}\frac{\partial}{\partial\rho} - \sin\phi\frac{-y/x^2}{1+y^2/x^2}\left(\frac{-1}{\sin\phi}\right)\frac{\partial}{\partial\phi} \tag{11}$$
$$= \frac{x}{\rho}\frac{\partial}{\partial\rho} - \frac{y}{\rho^2}\frac{\partial}{\partial\phi} \tag{12}$$

Using similar methods, we get for the other derivative

$$\frac{\partial}{\partial y} = \frac{\partial\rho}{\partial y}\frac{\partial}{\partial\rho} + \frac{\partial\sin\phi}{\partial x}\frac{\partial}{\partial(\sin\phi)} \tag{13}$$
$$= \frac{y}{\rho}\frac{\partial}{\partial\rho} + \frac{x}{\rho^2}\frac{\partial}{\partial\phi} \tag{14}$$

Plugging these into 4 we have

$$L_z = -i\hbar\left[x\left(\frac{y}{\rho}\frac{\partial}{\partial\rho} + \frac{x}{\rho^2}\frac{\partial}{\partial\phi}\right) - y\left(\frac{x}{\rho}\frac{\partial}{\partial\rho} - \frac{y}{\rho^2}\frac{\partial}{\partial\phi}\right)\right] \tag{15}$$
$$= -i\hbar\frac{x^2+y^2}{\rho^2}\frac{\partial}{\partial\phi} \tag{16}$$
$$= -i\hbar\frac{\partial}{\partial\phi} \tag{17}$$

Another method of converting L_z to polar coordinates is to consider the effect of $U[R]$ for an infinitesimal rotation ε_z on a state vector expressed in polar coordinates $\psi(\rho,\phi)$. Shankar states that

$$\langle\rho,\phi\,|U[R]|\,\psi(\rho,\phi)\rangle = \psi(\rho,\phi-\varepsilon_z) \tag{18}$$

If you don't believe this, it can be shown using a method similar to that for the one-dimensional translation. In this case, we're dealing with position eigenkets in polar coordinates, so we have

$$U\left[R\right]\left|\rho,\phi\right\rangle = \left|\rho,\phi+\varepsilon_z\right\rangle \tag{19}$$

Applying this, we get

$$\begin{aligned}
\left|\psi_{\varepsilon_z}\right\rangle &= U\left[R\right]\left|\psi\right\rangle && (20)\\
&= U\left[R\right]\int_0^{2\pi}\int_0^{\infty}\left|\rho,\phi\right\rangle\left\langle\rho,\phi\left|\psi\right.\right\rangle\rho d\rho\, d\phi && (21)\\
&= \int_0^{2\pi}\int_0^{\infty}\left|\rho,\phi+\varepsilon_z\right\rangle\left\langle\rho,\phi\left|\psi\right.\right\rangle\rho d\rho\, d\phi && (22)\\
&= \int_0^{2\pi}\int_0^{\infty}\left|\rho',\phi'\right\rangle\left\langle\rho',\phi'-\varepsilon_z\left|\psi\right.\right\rangle\rho' d\rho'\, d\phi' && (23)
\end{aligned}$$

where in the last line, we used the substitution $\phi' = \phi + \varepsilon_z$. (The substitution $\rho' = \rho$ is used just to give the radial variable a different name in the integrand.) We can use the same limits of integration for ϕ and ϕ', since we just need to ensure that the integral covers the total range of angles. It then follows that

$$\begin{aligned}
\left\langle\rho,\phi\left|\psi_{\varepsilon_z}\right.\right\rangle &= \int_0^{2\pi}\int_0^{\infty}\left\langle\rho,\phi\left|\rho',\phi'\right.\right\rangle\left\langle\rho',\phi'-\varepsilon_z\left|\psi\right.\right\rangle\rho' d\rho'\, d\phi' && (24)\\
&= \int_0^{2\pi}\int_0^{\infty}\delta\left(\rho-\rho'\right)\delta\left(\phi-\phi'\right)\left\langle\rho',\phi'-\varepsilon_z\left|\psi\right.\right\rangle\rho' d\rho'\, d\phi' && (25)\\
&= \psi\left(\rho,\phi-\varepsilon_z\right) && (26)
\end{aligned}$$

Combining this with 1 we have

$$\left\langle\rho,\phi\left|I-\frac{i\varepsilon_z L_z}{\hbar}\right|\psi\right\rangle = \psi\left(\rho,\phi-\varepsilon_z\right) \tag{27}$$

Expanding the RHS to order ε_z we have

$$\left\langle\rho,\phi\left|I-\frac{i\varepsilon_z L_z}{\hbar}\right|\psi\right\rangle = \psi\left(\rho,\phi\right)-\varepsilon_z\frac{\partial\psi}{\partial\phi} \tag{28}$$

from which 17 follows again.

Once we have L_z in this form, the exponential form of a finite rotation is easier to interpret, for we have, from 2

$$e^{-i\phi_0 L_z/\hbar} = \exp\left[-\phi_0 \frac{\partial}{\partial\phi}\right] \tag{29}$$

$$= 1 - \phi_0 \frac{\partial}{\partial\phi} + \frac{\phi_0^2}{2!}\frac{\partial^2}{\partial\phi^2} + \dots \tag{30}$$

Applying this to a state function $\psi(\rho,\phi)$, we see that we get the Taylor series for $\psi(\rho,\phi-\phi_0)$, so the exponential does indeed represent a rotation through a finite angle.

PINGBACKS

Pingback: Eigenvalues of two-dimensional angular momentum

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COMBINING TRANSLATIONS AND ROTATIONS

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Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 12, Exercise 12.2.4.

Post date: 24 Apr 2017

[If some equations are too small to read easily, use your browser's magnifying option (Ctrl + on Chrome, probably something similar on other browsers).]

When it comes to symmetries in quantum mechanics, we've looked at translations and rotations in two dimensions, and found that the generators are the momenta P_x and P_y for translations, and the angular momentum L_z for rotations.

From the fact that L_z does not commute with either momentum or position operators, you might guess that if we performed some sequence of translations and rotations on a system that the order in which these operations are done matters. In fact, you can see this by considering simple two-dimensional geometry, without reference to quantum mechanics. Consider the x and y axes on a sheet of graph paper. First, translate these axes by adding the vector $\mathbf{r}$ to all points, so that the new origin of coordinates lies at position $\mathbf{r}$ as referenced in the original coordinates. Next, do a rotation *about the original origin* by some angle ϕ. This will move the new origin around the original z axis. Now, do the inverse of the original translation by adding $-\mathbf{r}$ to all points. Finally, do the inverse of the rotation by rotating the system by $-\phi$ around the *original* z axis. You'll find that the xy axes that have undergone this sequence of transformations does not coincide with the original xy axes. However, if you did the same set of four transformations in the order: translate by $\mathbf{r}$, translate by $-\mathbf{r}$, rotate by ϕ, rotate by $-\phi$, the transformed axes *would* coincide with the original axes.

To see how this works in quantum mechanics, we can again consider infinitesimal translations and rotations. If we start with a point at location $[x, y]$ and apply the four transformations described above, but now for an infinitesimal translation $\boldsymbol{\varepsilon} = \varepsilon_x\hat{\mathbf{x}} + \varepsilon_y\hat{\mathbf{y}}$ and rotation $\varepsilon_z\hat{\mathbf{z}}$, then the successive transformations work as follows. In each case, we'll retain terms up to order $\varepsilon_x\varepsilon_z$ and $\varepsilon_y\varepsilon_z$ but discard terms of order ε_x^2, ε_y^2, ε_z^2 and higher. [I'm not quite sure of the rationale that allows us to do this, apart from the fact that it gives the right answer.]

$$\begin{bmatrix} x \\ y \end{bmatrix} \xrightarrow[T(\boldsymbol{\varepsilon})]{} \begin{bmatrix} x+\varepsilon_x \\ y+\varepsilon_y \end{bmatrix} \tag{1}$$

$$\begin{bmatrix} x+\varepsilon_x \\ y+\varepsilon_y \end{bmatrix} \xrightarrow[R(\varepsilon_z\hat{\mathbf{z}})]{} \begin{bmatrix} x+\varepsilon_x-(y+\varepsilon_y)\varepsilon_z \\ y+\varepsilon_y+(x+\varepsilon_x)\varepsilon_z \end{bmatrix} \tag{2}$$

$$\begin{bmatrix} x+\varepsilon_x-(y+\varepsilon_y)\varepsilon_z \\ y+\varepsilon_y+(x+\varepsilon_x)\varepsilon_z \end{bmatrix} \xrightarrow[T(-\boldsymbol{\varepsilon})]{} \begin{bmatrix} x+\varepsilon_x-(y+\varepsilon_y)\varepsilon_z-\varepsilon_x \\ y+\varepsilon_y+(x+\varepsilon_x)\varepsilon_z-\varepsilon_y \end{bmatrix} \tag{3}$$

$$= \begin{bmatrix} x-(y+\varepsilon_y)\varepsilon_z \\ y+(x+\varepsilon_x)\varepsilon_z \end{bmatrix} \tag{4}$$

$$\begin{bmatrix} x-(y+\varepsilon_y)\varepsilon_z \\ y+(x+\varepsilon_x)\varepsilon_z \end{bmatrix} \xrightarrow[R(-\varepsilon_z\hat{\mathbf{z}})]{} \begin{bmatrix} x-(y+\varepsilon_y)\varepsilon_z+[y+(x+\varepsilon_x)\varepsilon_z]\varepsilon_z \\ y+(x+\varepsilon_x)\varepsilon_z-[x-(y+\varepsilon_y)\varepsilon_z]\varepsilon_z \end{bmatrix} \tag{5}$$

$$= \begin{bmatrix} x-\varepsilon_y\varepsilon_z \\ y+\varepsilon_x\varepsilon_z \end{bmatrix} \tag{6}$$

Thus, to this order in the infinitesimals, the combination of translation-rotation-translation-rotation is equivalent to a single translation by a distance $[-\varepsilon_y\varepsilon_z, \varepsilon_x\varepsilon_z]$. We can write this in terms of the unitary quantum operators for translations and rotations as

$$U\left[R\left(-\varepsilon_z\hat{\mathbf{z}}\right)\right]T\left(-\boldsymbol{\varepsilon}\right)U\left[R\left(\varepsilon_z\hat{\mathbf{z}}\right)\right]T\left(\boldsymbol{\varepsilon}\right) = T\left(-\varepsilon_y\varepsilon_z\hat{\mathbf{x}}+\varepsilon_x\varepsilon_z\hat{\mathbf{y}}\right) \tag{7}$$

Using the forms of these operators for infinitesimal transformations, we can expand both sides to give

$$\left(I+\frac{i\varepsilon_z}{\hbar}L_z\right)\left[I+\frac{i}{\hbar}\left(\varepsilon_x P_x+\varepsilon_y P_y\right)\right]\times \tag{8}$$

$$\left(I-\frac{i\varepsilon_z}{\hbar}L_z\right)\left[I-\frac{i}{\hbar}\left(\varepsilon_x P_x+\varepsilon_y P_y\right)\right] = I-\frac{i}{\hbar}\left(-\varepsilon_y\varepsilon_z P_x+\varepsilon_x\varepsilon_z P_y\right) \tag{9}$$

Since the infinitesimal displacements are arbitrary, this equation can be valid only if the coefficients of each combination of $\varepsilon_x, \varepsilon_y$ and ε_z are equal on both sides. As above, we'll discard any terms of order ε_x^2, ε_y^2, ε_z^2 and higher. The algebra is straightforward although a bit tedious, so I'll just give a couple of examples here.

The coefficient of ε_z on its own is, on the LHS

$$\frac{i\varepsilon_z}{\hbar}L_z-\frac{i\varepsilon_z}{\hbar}L_z = 0 \tag{10}$$

On the RHS, there is no term in ε_z, so we get 0 on the RHS. In this case, we see the equation is consistent.

For the $\varepsilon_x\varepsilon_z$ term, we get on the LHS:

$$\varepsilon_x\varepsilon_z\frac{i^2}{\hbar^2}\left(L_zP_x - L_zP_x - P_xL_z + L_zP_x\right) = -\varepsilon_x\varepsilon_z\frac{i^2}{\hbar^2}\left[P_x, L_z\right] \tag{11}$$

On the RHS, the term is

$$-\frac{i}{\hbar}\varepsilon_x\varepsilon_zP_y \tag{12}$$

Thus the condition here becomes

$$\left[P_x, L_z\right] = -i\hbar P_y \tag{13}$$

which agrees with the commutation relation we found earlier. By considering the coefficient of $\varepsilon_y\varepsilon_z$, we arrive at the other condition, which is

$$\left[P_y, L_z\right] = i\hbar P_x \tag{14}$$

The result of this calculation doesn't tell us anything new about the translation or rotation operators, but it does show that the condition 7 is consistent with what we already know about the commutators of position, momentum and angular momentum.

As Shankar points out, we might think that we need to verify the conditions for an infinite number of combinations of rotations and translations, since each such combination gives rise to a different overall transformation. He says that it has actually been shown that the example above is sufficient to guarantee that all such combinations do in fact give valid results, although he doesn't give the details. We are, however, given the exercise of verifying this claim for one special case, which we'll consider now.

In this example, we'll consider the same four transformations, in the same order, as above except that we'll take the translation to be entirely in the x direction so that $\varepsilon_y = 0$. This time, we'll retain terms up to $\varepsilon_x\varepsilon_z^2$ and see what we get. We start by repeating the calculations in 1 through 6. However, because we're saving higher order terms, we need to represent the infinitesimal rotations by

$$R\left(\varepsilon_z\hat{\mathbf{z}}\right) = \begin{bmatrix} 1 - \frac{\varepsilon_z^2}{2} & -\varepsilon_z \\ \varepsilon_z & 1 - \frac{\varepsilon_z^2}{2} \end{bmatrix} \tag{15}$$

That is, we're approximating $\cos\varepsilon_z$ by the first two terms in its expansion. Using this, we have

$$\begin{bmatrix} x \\ y \end{bmatrix} \longrightarrow \begin{bmatrix} x+\varepsilon_x \\ y \end{bmatrix} \tag{16}$$

$$\begin{bmatrix} x+\varepsilon_x \\ y \end{bmatrix} \longrightarrow \begin{bmatrix} (x+\varepsilon_x)\left(1-\frac{\varepsilon_z^2}{2}\right)-y\varepsilon_z \\ y\left(1-\frac{\varepsilon_z^2}{2}\right)+(x+\varepsilon_x)\varepsilon_z \end{bmatrix} \tag{17}$$

$$\begin{bmatrix} x+\varepsilon_x-y\varepsilon_z \\ y+(x+\varepsilon_x)\varepsilon_z \end{bmatrix} \longrightarrow \begin{bmatrix} (x+\varepsilon_x)\left(1-\frac{\varepsilon_z^2}{2}\right)-y\varepsilon_z-\varepsilon_x \\ y\left(1-\frac{\varepsilon_z^2}{2}\right)+(x+\varepsilon_x)\varepsilon_z \end{bmatrix} \tag{18}$$

$$= \begin{bmatrix} x\left(1-\frac{\varepsilon_z^2}{2}\right)-y\varepsilon_z-\frac{1}{2}\varepsilon_x\varepsilon_z^2 \\ y\left(1-\frac{\varepsilon_z^2}{2}\right)+\varepsilon_z x+\varepsilon_x\varepsilon_z \end{bmatrix} \tag{19}$$

$$\begin{bmatrix} x-y\varepsilon_z \\ y+(x+\varepsilon_x)\varepsilon_z \end{bmatrix} \longrightarrow \begin{bmatrix} \left[x\left(1-\frac{\varepsilon_z^2}{2}\right)-y\varepsilon_z-\frac{1}{2}\varepsilon_x\varepsilon_z^2\right]\left(1-\frac{\varepsilon_z^2}{2}\right)+\left[y\left(1-\frac{\varepsilon_z^2}{2}\right)+\varepsilon_z x+\varepsilon_x\varepsilon_z\right]\varepsilon_z \\ \left[y\left(1-\frac{\varepsilon_z^2}{2}\right)+\varepsilon_z x+\varepsilon_x\varepsilon_z\right]\left(1-\frac{\varepsilon_z^2}{2}\right)-\left[x\left(1-\frac{\varepsilon_z^2}{2}\right)-y\varepsilon_z-\frac{1}{2}\varepsilon_x\varepsilon_z^2\right]\varepsilon_z \end{bmatrix} \tag{20}$$

$$= \begin{bmatrix} x\left(1+\frac{\varepsilon_z^4}{4}\right)+\frac{1}{2}\varepsilon_x\varepsilon_z^2+\frac{1}{4}\varepsilon_x\varepsilon_z^4 \\ y\left(1+\frac{\varepsilon_z^4}{4}\right)+\varepsilon_x\varepsilon_z \end{bmatrix} \tag{21}$$

To get the last line, I used Maple to do the algebra in multiplying out the terms. At this point, we can neglect the terms in ε_z^4, leaving us with the overall transformation:

$$\begin{bmatrix} x \\ y \end{bmatrix} \longrightarrow \begin{bmatrix} x+\frac{1}{2}\varepsilon_x\varepsilon_z^2 \\ y+\varepsilon_x\varepsilon_z \end{bmatrix} \tag{22}$$

This is equivalent to a translation by $\boldsymbol{\varepsilon} = \frac{1}{2}\varepsilon_x\varepsilon_z^2\hat{\mathbf{x}} + \varepsilon_x\varepsilon_z\hat{\mathbf{y}}$, so by analogy with 7, we have the condition

$$U\left[R(-\varepsilon_z\hat{\mathbf{z}})\right]T(-\boldsymbol{\varepsilon})\,U\left[R(\varepsilon_z\hat{\mathbf{z}})\right]T(\boldsymbol{\varepsilon}) = T\left(\frac{1}{2}\varepsilon_x\varepsilon_z^2\hat{\mathbf{x}}+\varepsilon_x\varepsilon_z\hat{\mathbf{y}}\right) \tag{23}$$

To expand the operators on the LHS and retain terms up to $\varepsilon_x\varepsilon_z^2$, we need to expand the rotation operators up to order ε_z^2. Treating the rotation operator as an exponential, this expansion is

$$R(\varepsilon_z\hat{\mathbf{z}}) = I - \frac{i\varepsilon_z}{\hbar}L_z + \frac{i^2\varepsilon_z^2}{2\hbar^2}L_z^2 + \ldots \tag{24}$$

Using this approximation gives us

$$\left(I+\frac{i\varepsilon_z}{\hbar}L_z+\frac{i^2\varepsilon_z^2}{2\hbar^2}L_z^2\right)\left[I+\frac{i}{\hbar}\varepsilon_x P_x\right]\left(I-\frac{i\varepsilon_z}{\hbar}L_z+\frac{i^2\varepsilon_z^2}{2\hbar^2}L_z^2\right)\left[I-\frac{i}{\hbar}\varepsilon_x P_x\right] \;=\; I-\frac{i}{\hbar}\left(\frac{1}{2}\varepsilon_x\varepsilon_z^2 P_x+\right.$$

By equating the coefficients of $\varepsilon_x\varepsilon_z$ we regain 13, so that condition checks out.

Extracting the coefficient of $\varepsilon_x\varepsilon_z^2$ on the LHS gives

$$\frac{i^3}{\hbar^3}\varepsilon_x\varepsilon_z^2\left(-L_zP_xL_z+\frac{L_z^2P_x}{2}-\frac{L_z^2P_x}{2}+\frac{P_xL_z^2}{2}-\frac{L_z^2P_x}{2}+L_z^2P_x\right) \;=\; \frac{i^3}{\hbar^3}\varepsilon_x\varepsilon_z^2\left(-L_zP_xL_z+\frac{L_z^2P_x}{2}+\right.$$

Matching this to the $\varepsilon_x\varepsilon_z^2$ term on the RHS of 25, we get the condition specified in Shankar's problem:

$$-2L_zP_xL_z+L_z^2P_x+P_xL_z^2=\hbar^2P_x \tag{27}$$

We can show that this condition reduces to the already-known commutators by using the identity

$$\begin{aligned}[\Lambda,[\Lambda,\Omega]] &= \Lambda(\Lambda\Omega-\Omega\Lambda)-(\Lambda\Omega-\Omega\Lambda)\Lambda &(28)\\ &= -2\Lambda\Omega\Lambda+\Lambda^2\Omega+\Omega\Lambda^2 &(29)\end{aligned}$$

Applying this to 27 we have

$$\begin{aligned}-2L_zP_xL_z+L_z^2P_x+P_xL_z^2 &= [L_z,[L_z,P_x]] &(30)\\ &= i\hbar[L_z,P_y] &(31)\\ &= i\hbar(-i\hbar P_x) &(32)\\ &= \hbar^2P_x &(33)\end{aligned}$$

Thus the more complicated condition 27 actually reduces to existing commutators.

EIGENVALUES OF TWO-DIMENSIONAL ANGULAR MOMENTUM

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Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 12, Exercise 12.3.1.

Post date: 28 Apr 2017

[If some equations are too small to read easily, use your browser's magnifying option (Ctrl + on Chrome, probably something similar on other browsers).]

The angular momentum operator L_z for rotations in two dimensions has the form, in polar coordinates, of

$$L_z = -i\hbar\frac{\partial}{\partial\phi} \tag{1}$$

To find the eigenvalues and eigenfunctions, we need to solve

$$L_z\left|\ell_z\right\rangle = \ell_z\left|\ell_z\right\rangle \tag{2}$$

where $|\ell_z\rangle$ is the eigenfunction and ℓ_z is the corresponding eigenvalue. Using polar coordinates, we must solve

$$-i\hbar\frac{\partial}{\partial\phi}\psi_{\ell_z}(\rho,\phi) = \ell_z\psi_{\ell_z}(\rho,\phi) \tag{3}$$

where ρ is the radial coordinate. As the only derivative here is with respect to ϕ, we can solve this using separation of variables by proposing a solution of form

$$\psi_{\ell_z}(\rho,\phi) = R(\rho)\,\Phi(\phi) \tag{4}$$

Substituting this and cancelling off $R(\rho)$ we get

$$-i\hbar\frac{\partial}{\partial\phi}\Phi(\phi) = \ell_z\Phi(\phi) \tag{5}$$

which has the solution

$$\Phi(\phi) = Ae^{i\ell_z\phi/\hbar} \tag{6}$$

for some constant A, which we can absorb into $R(\rho)$ to give the general solution

$$\psi_{\ell_z}(\rho,\phi) = R(\rho)\, e^{i\ell_z\phi/\hbar} \tag{7}$$

[This is actually the two-dimensional version of the more general 3-d case, in which the solution involved a radial function multiplied by a spherical harmonic.]

At this stage, the eigenvalue ℓ_z could be any number, real or complex, since they all satisfy 3. However, since L_z is an observable, it must be hermitian, which implies that $L_z^\dagger = L_z$, so that

$$\langle\psi_1|L_z|\psi_2\rangle = \langle\psi_2|L_z|\psi_1\rangle^* \tag{8}$$

In the coordinate basis, we have

$$\int_0^\infty\int_0^{2\pi}\psi_1^*\left(-i\hbar\frac{\partial}{\partial\phi}\right)\psi_2 d\phi\, d\rho = \left[\int_0^\infty\int_0^{2\pi}\psi_2^*\left(-i\hbar\frac{\partial}{\partial\phi}\right)\psi_1 d\phi\, d\rho\right]^* \tag{9}$$

Integrating the LHS by parts, we have

$$\int_0^\infty\int_0^{2\pi}\psi_1^*\left(-i\hbar\frac{\partial}{\partial\phi}\right)\psi_2 d\phi\, d\rho = -i\hbar\int_0^\infty\psi_1^*\psi_2|_0^{2\pi}\, d\rho + i\hbar\int_0^\infty\int_0^{2\pi}\frac{\partial\psi_1^*}{\partial\phi}\psi_2 d\phi\, d\rho \tag{10}$$

The second term on the RHS is seen to be equal to the RHS of 9, so in order for 9 to be true, we must have

$$\int_0^\infty\psi_1^*\psi_2|_0^{2\pi}\, d\rho = 0 \tag{11}$$

Although two different eigenfunctions ψ_1 and ψ_2 are orthogonal and thus would satisfy this condition automatically, the condition must also be true when $\psi_1 = \psi_2$. This gives us the condition that

$$\psi_{\ell_z}(2\pi) = \psi_{\ell_z}(0) \tag{12}$$

That is, the eigenfunctions must be periodic with period 2π. Looking back at 7, we see that this forces the eigenvalues ℓ_z to be integral multiples of $\hbar$:

$$\ell_z = m\hbar \tag{13}$$

$$m = 0, \pm1, \pm2, \ldots \tag{14}$$

Here m is the *magnetic quantum number*, not the mass.

PINGBACKS

Pingback: Eigenvalues of angular momentum

Pingback: Angular momentum: probabilities of eigenvalues in two dimensions

Pingback: Radially symmetric potentials, angular momentum and centrifugal force

Pingback: Angular momentum of circular motion

Pingback: Harmonic oscillator in 2 dimensions: comparison with rectangular coordinates

EIGENVALUES OF ANGULAR MOMENTUM

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 12, Exercise 12.3.2.

Post date: 29 Apr 2017

[If some equations are too small to read easily, use your browser's magnifying option (Ctrl + on Chrome, probably something similar on other browsers).]

One consequence of requiring the angular momentum operator L_z to be hermitian is that the eigenvalues must be integral multiples of $\hbar$, so that $\ell_z = m\hbar$ for $m = 0, \pm 1, \pm 2, \ldots$. Shankar proposes another method by which we might try to obtain this restriction on ℓ_z. We start with a superposition of two eigenstates of L_z, so that

$$\psi(\rho,\phi) = A(\rho)\, e^{i\phi\ell_z/\hbar} + B(\rho)\, e^{i\phi\ell'_z/\hbar} \tag{1}$$

$$= e^{i\phi\ell'_z/\hbar}\left[A(\rho)\, e^{i\phi(\ell_z-\ell'_z)/\hbar} + B(\rho)\right] \tag{2}$$

where A and B are two unknown functions of the radial coordinate ρ, and ℓ_z and ℓ'_z are two eigenvalues of L_z. If we rotate the system by a complete circle, so that $\phi \to \phi + 2\pi$, the physical state should remain unchanged. This means that

$$|\psi(\rho,\phi+2\pi)| = |\psi(\rho,\phi)| \tag{3}$$

so that $\psi(\rho,\phi+2\pi)$ may differ from $\psi(\rho,\phi)$ by a phase factor. From 2

$$\psi(\rho,\phi+2\pi) = e^{i(\phi+2\pi)\ell'_z/\hbar}\left[A(\rho)\, e^{i(\phi+2\pi)(\ell_z-\ell'_z)/\hbar} + B(\rho)\right] \tag{4}$$

The phase factor of $e^{i(\phi+2\pi)\ell'_z/\hbar}$ on the RHS can be anything (provided the exponent is purely imaginary), but the quantity in the square brackets must be numerically the same as the corresponding quantity in 2. This means that

$$\frac{(\phi+2\pi)(\ell_z-\ell'_z)}{\hbar} = \frac{\phi(\ell_z-\ell'_z)}{\hbar} + 2m\pi \tag{5}$$

where m is an integer. This gives the condition

$$\ell_z - \ell'_z = m\hbar \tag{6}$$

To proceed further, we need to argue that ℓ_z is symmetric about zero, that is, if ℓ_z is an eigenvalue, then so is $-\ell_z$. I'm not sure if Shankar expects us to prove this rigorously, but it seems plausible, since the only difference between $+\ell_z$ and $-\ell_z$ is (classically, anyway) that the direction of rotation is reversed. Given this condition, ℓ_z must be a multiple of $\frac{1}{2}\hbar$, since any other value doesn't satisfy both the conditions of symmetry about zero, and 6. (For example, if we try $\ell_z = \frac{1}{4}\hbar$, then the symmetry requirement means we must also allow $\ell_z = -\frac{1}{4}\hbar$, but this violates 6.) If ℓ_z is an odd multiple of $\frac{1}{2}\hbar$, then we get the sequence $\ldots, -\frac{3}{2}\hbar$,-$\frac{1}{2}\hbar, +\frac{1}{2}\hbar, +\frac{3}{2}\hbar, \ldots$ while if ℓ_z is an even multiple of $\frac{1}{2}\hbar$ we get the sequence $\ldots, -2\hbar, -\hbar, 0, +\hbar, +2\hbar, \ldots$. In reality, only the latter sequence is correct, but we can't show that from this argument.

ANGULAR MOMENTUM: PROBABILITIES OF EIGENVALUES IN TWO DIMENSIONS

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 12, Exercises 12.3.3 - 12.3.4.

Post date: 2 May 2017

[If some equations are too small to read easily, use your browser's magnifying option (Ctrl + on Chrome, probably something similar on other browsers).]

We've seen that the eigenfunctions of two-dimensional angular momentum have the form

$$\psi(\rho,\phi) = R(\rho)\, e^{i\ell_z \phi/\hbar} \tag{1}$$

where ℓ_z (the eigenvalue) is an integral multiple of $\hbar$ and $R(\rho)$ is some function of the radial coordinate ρ which depends on the particular potential function in the hamiltonian. It's more convenient to write the angular function as

$$\Phi_m(\phi) = \frac{1}{\sqrt{2\pi}} e^{im\phi} \tag{2}$$

This set of functions is orthonormal over the interval $\phi \in [0, 2\pi]$, that is

$$\int_0^{2\pi} \Phi_m^*(\phi)\, \Phi_{m'}(\phi)\, d\phi = \delta_{mm'} \tag{3}$$

This set of functions forms the angular part of the eigenfunctions of L_z, which in some cases allows us to determine the probabilities of a system being in a particular eigenstate of L_z. Here are a couple of examples.

Example 1. A particle is described by the wave function

$$\psi(\rho,\phi) = Ae^{-\rho^2/2\Delta^2} \cos^2\phi \tag{4}$$

where A is a normalization constant, and Δ is another constant.

We can use the trig identity

$$\cos^2\phi = \frac{1}{2}(1+\cos 2\phi) \tag{5}$$

to write this wave function as

$$\psi(\rho,\phi) = \frac{A}{2} e^{-\rho^2/2\Delta^2} [1+\cos 2\phi] \tag{6}$$

$$= \frac{A}{2} e^{-\rho^2/2\Delta^2} \left(1 + \frac{e^{2i\phi}+e^{-2i\phi}}{2}\right) \tag{7}$$

$$= \frac{A\sqrt{2\pi}}{2} e^{-\rho^2/2\Delta^2} \left(\Phi_0 + \frac{1}{2}(\Phi_2+\Phi_{-2})\right) \tag{8}$$

Thus the wave function has the form

$$\psi(\rho,\phi) = c_0\Phi_0 + c_2\Phi_2 + c_{-2}\Phi_{-2} \tag{9}$$

where the coefficients c_m can be found by comparison with 8. Since the Φ_m are orthonormal functions, the probability of the particle being in state i is

$$P(\ell_z = m\hbar) = \frac{|c_m|^2}{\sum_j |c_j|^2} \tag{10}$$

We can see from this formula that the factor of $\frac{A\sqrt{2\pi}}{2} e^{-\rho^2/2\Delta^2}$ cancels out of the probability formula, so we have

$$P(\ell_z = 0) = \frac{|c_0|^2}{\sum_j |c_j|^2} \tag{11}$$
$$= \frac{1}{1+\frac{1}{4}+\frac{1}{4}} \tag{12}$$
$$= \frac{2}{3} \tag{13}$$
$$P(\ell_z = 2\hbar) = \frac{|c_2|^2}{\sum_j |c_j|^2} \tag{14}$$
$$= \frac{\frac{1}{4}}{1+\frac{1}{4}+\frac{1}{4}} \tag{15}$$
$$= \frac{1}{6} \tag{16}$$
$$P(\ell_z = -2\hbar) = \frac{|c_{-2}|^2}{\sum_j |c_j|^2} \tag{17}$$
$$= \frac{\frac{1}{4}}{1+\frac{1}{4}+\frac{1}{4}} \tag{18}$$
$$= \frac{1}{6} \tag{19}$$

Example 2. Now we have the wave function

$$\psi(\rho,\phi) = Ae^{-\rho^2/2\Delta^2}\left(\frac{\rho}{\Delta}\cos\phi + \sin\phi\right) \tag{20}$$

Again, we write the trig functions in terms of Φ_m to get

$$\psi(\rho,\phi) = Ae^{-\rho^2/2\Delta^2}\left(\frac{\rho}{\Delta}\frac{e^{i\phi}+e^{-i\phi}}{2} + \frac{e^{i\phi}-e^{-i\phi}}{2i}\right) \tag{21}$$
$$= A\sqrt{2\pi}e^{-\rho^2/2\Delta^2}\left[\left(\frac{\rho}{2\Delta}+\frac{1}{2i}\right)\Phi_1 + \left(\frac{\rho}{2\Delta}-\frac{1}{2i}\right)\Phi_{-1}\right] \tag{22}$$

As above, the factor of $A\sqrt{2\pi}e^{-\rho^2/2\Delta^2}$ cancels out when calculating probabilities, so we have

$$P(\ell_z = \hbar) = \frac{|c_1|^2}{|c_1|^2 + |c_{-1}|^2} \tag{23}$$

$$= \frac{\left|\frac{\rho}{2\Delta} + \frac{1}{2i}\right|^2}{\left|\frac{\rho}{2\Delta} + \frac{1}{2i}\right|^2 + \left|\frac{\rho}{2\Delta} - \frac{1}{2i}\right|^2} \tag{24}$$

$$= \frac{\left(\frac{\rho}{2\Delta}\right)^2 + \frac{1}{4}}{2\left[\left(\frac{\rho}{2\Delta}\right)^2 + \frac{1}{4}\right]} \tag{25}$$

$$= \frac{1}{2} \tag{26}$$

$$P(\ell_z = -\hbar) = \frac{|c_{-1}|^2}{|c_1|^2 + |c_{-1}|^2} \tag{27}$$

$$= \frac{\left|\frac{\rho}{2\Delta} - \frac{1}{2i}\right|^2}{\left|\frac{\rho}{2\Delta} + \frac{1}{2i}\right|^2 + \left|\frac{\rho}{2\Delta} - \frac{1}{2i}\right|^2} \tag{28}$$

$$= \frac{\left(\frac{\rho}{2\Delta}\right)^2 + \frac{1}{4}}{2\left[\left(\frac{\rho}{2\Delta}\right)^2 + \frac{1}{4}\right]} \tag{29}$$

$$= \frac{1}{2} \tag{30}$$

Thus in this case, the ρ dependence cancels out when calculating the probabilities, although we can't expect this to be true in general.

RADIALLY SYMMETRIC POTENTIALS, ANGULAR MOMENTUM AND CENTRIFUGAL FORCE

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 12, Exercise 12.3.5.

Post date: 4 May 2017

[If some equations are too small to read easily, use your browser's magnifying option (Ctrl + on Chrome, probably something similar on other browsers).]

We've seen that the eigenfunctions of two-dimensional angular momentum have the form

$$\psi(\rho,\phi) = R(\rho)\,\Phi_m(\phi) \tag{1}$$

where

$$\Phi_m(\phi) = \frac{1}{\sqrt{2\pi}} e^{im\phi} \tag{2}$$

In 2 dimensions and polar coordinates, the hamiltonian can be written as

$$H = -\frac{\hbar^2}{2\mu}\left(\frac{\partial^2}{\partial\rho^2} + \frac{1}{\rho}\frac{\partial}{\partial\rho} + \frac{1}{\rho^2}\frac{\partial^2}{\partial\phi^2}\right) + V(\rho,\phi) \tag{3}$$

If the potential is radially symmetric, that is, it doesn't depend on ϕ, then

$$H = -\frac{\hbar^2}{2\mu}\left(\frac{\partial^2}{\partial\rho^2} + \frac{1}{\rho}\frac{\partial}{\partial\rho} + \frac{1}{\rho^2}\frac{\partial^2}{\partial\phi^2}\right) + V(\rho) \tag{4}$$

In polar coordinates, the angular momentum operator has the form

$$L_z = -i\hbar\frac{\partial}{\partial\phi} \tag{5}$$

Thus L_z commutes with every term in the hamiltonian 4, so for $V = V(\rho)$, we find

$$[H, L_z] = 0 \tag{6}$$

meaning that we can find a set of functions that are simultaneously eigenfunctions of both H and L_z. Since we already know what the most general

eigenfunctions of L_z are (eqn 1), the problem is then to find the radial function $R(\rho)$ so that

$$H\left[R(\rho)\,\Phi_m(\phi)\right] = ER(\rho)\,\Phi_m(\phi) \tag{7}$$

If we use 4 for H and 2 for Φ we find that we must solve the differential equation

$$-\frac{\hbar^2}{2\mu}\left(\frac{d^2R}{d\rho^2}+\frac{1}{\rho}\frac{dR}{d\rho}-\frac{m^2}{\rho^2}R\right)+V(\rho)\,R = ER \tag{8}$$

We've replaced the partial derivatives in 4 by ordinary derivatives, since we now have an ODE in one independent variable, namely ρ.

The term arising from the $\frac{1}{\rho^2}\frac{\partial^2}{\partial\phi^2}$ term in 4 is similar to a potential term, since it doesn't involve any derivatives of R. The potential term is

$$V_c = \frac{\hbar^2}{2\mu}\frac{m^2}{\rho^2} \tag{9}$$

We can find the force corresponding to V_c by taking the negative gradient, which in this case amounts to

$$F_c = -\frac{\partial V_c}{\partial\rho} = \frac{\hbar^2 m^2}{\mu\rho^3} \tag{10}$$

Since the quantum angular momentum is $\ell_z = m\hbar$, this can be written as

$$F_c = \frac{\ell_z^2}{\mu\rho^3} \tag{11}$$

If the particle is in a circular orbit, then $\ell_z = \rho p$ where p is its momentum, so this becomes

$$F_c = \frac{p^2}{\mu\rho} \tag{12}$$

Classically, $p = \mu v$ so this is equivalent to

$$F_c = \frac{\mu v^2}{\rho} \tag{13}$$

which is the formula for centrifugal force in Newtonian physics.

PINGBACKS

Pingback: Two-dimensional harmonic oscillator - Part 1

ANGULAR MOMENTUM OF CIRCULAR MOTION

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 12, Exercise 12.3.6.

Post date: 14 May 2017

[If some equations are too small to read easily, use your browser's magnifying option (Ctrl + on Chrome, probably something similar on other browsers).]

A particle of mass μ constrained to move (at constant speed v, we assume) on a circle of radius a centred at the origin in the xy plane has a constant kinetic energy of $\frac{1}{2}\mu v^2$. As its momentum **p** is always perpendicular to the radius vector **r**, the angular momentum is given by

$$\mathbf{L} = \mathbf{r} \times \mathbf{p} = \mu a v \hat{\mathbf{z}} = L_z \hat{\mathbf{z}} \tag{1}$$

The energy can thus be written as

$$H = \frac{1}{2}\mu v^2 = \frac{L_z^2}{2\mu a^2} \tag{2}$$

In polar coordinates, the angular momentum operator is

$$L_z = -i\hbar \frac{\partial}{\partial \phi} \tag{3}$$

The eigenvalue problem for this system is therefore

$$H\psi = E\psi \tag{4}$$

$$-\frac{\hbar^2}{2\mu a^2}\frac{\partial^2 \psi}{\partial \phi^2} = E\psi \tag{5}$$

The eigenvalues of L_z are the solutions of

$$-\hbar^2 \frac{\partial^2 \psi}{\partial \phi^2} = \ell_z \psi \tag{6}$$

which are

$$\psi = Ae^{i\ell_z \phi/\hbar} = Ae^{im\phi} \tag{7}$$

for some constant A, with the quantization condition (arising from the requirement that $\psi(\phi + 2\pi) = \psi(\phi)$)

$$\ell_z = m\hbar \tag{8}$$

where m is an integer (positive, negative or zero). Plugging this into 5 we find

$$E = \frac{\hbar^2 m^2}{2\mu a^2} \tag{9}$$

Each energy is two-fold degenerate since $\pm m$ both give the same energy. This corresponds to the particle moving round the circle in the clockwise or counterclockwise direction.

TWO-DIMENSIONAL HARMONIC OSCILLATOR - PART 1

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 12, Exercise 12.3.7 (1) - (5).

Post date: 4 May 2017

[If some equations are too small to read easily, use your browser's magnifying option (Ctrl + on Chrome, probably something similar on other browsers).]

In this problem, we'll look at solving the 2-dimensional isotropic harmonic oscillator. The solution is fairly lengthy, so we'll split it into two posts, with this being the first. The method of solution is similar to that used in the one-dimensional harmonic oscillator, so you may wish to refer back to that before proceeding.

The Hamiltonian is, in rectangular coordinates:

$$H = \frac{P_x^2 + P_y^2}{2\mu} + \frac{1}{2}\mu\omega^2\left(X^2 + Y^2\right) \tag{1}$$

The potential term is radially symmetric (it doesn't depend on the polar angle ϕ) so we have a problem of the form considered earlier. We saw there that for such potentials $[H, L_z] = 0$. [If you don't believe this, you can grind through the calculations using the commutation relations for L_z with the rectangular momenta and coordinates, but I won't go through that here.]

As a result, L_z and H have simultaneous eigenfunctions of form

$$\psi(\rho, \phi) = R(\rho)\,\Phi_m(\phi) \tag{2}$$

where

$$\Phi_m(\phi) = \frac{1}{\sqrt{2\pi}} e^{im\phi} \tag{3}$$

The radial function satisfies the ODE

$$-\frac{\hbar^2}{2\mu}\left(\frac{d^2R}{d\rho^2} + \frac{1}{\rho}\frac{dR}{d\rho} - \frac{m^2}{\rho^2}R\right) + V(\rho)\,R = ER \tag{4}$$

where in this case

$$V(\rho) = \frac{1}{2}\mu\omega^2\rho^2 \tag{5}$$

Thus the equation we must solve is

$$-\frac{\hbar^2}{2\mu}\left(\frac{d^2}{d\rho^2}+\frac{1}{\rho}\frac{d}{d\rho}-\frac{m^2}{\rho^2}\right)R+\frac{1}{2}\mu\omega^2\rho^2R=ER \tag{6}$$

To get a feel for the solution, we examine the behaviour in two limiting cases: $\rho\to 0$ and $\rho\to\infty$. It's actually easier if we introduce dimensionless variables now, rather than in Shankar's step 4, so we define

$$y \equiv \sqrt{\frac{\mu\omega}{\hbar}}\rho \tag{7}$$

$$\varepsilon \equiv \frac{E}{\hbar\omega} \tag{8}$$

This transforms 6 to

$$-\frac{\hbar^2}{2\mu}\left(\frac{\mu\omega}{\hbar}\right)\left(\frac{d^2}{dy^2}+\frac{1}{y}\frac{d}{dy}-\frac{m^2}{y^2}\right)R+\frac{1}{2}\hbar\omega y^2R=ER \tag{9}$$

$$-\left(\frac{d^2}{dy^2}+\frac{1}{y}\frac{d}{dy}-\frac{m^2}{y^2}+2\varepsilon\right)R+y^2R=0 \tag{10}$$

We can now look at $y\to 0$, and we neglect the terms $2\varepsilon R$ and y^2R to get

$$\left(\frac{d^2}{dy^2}+\frac{1}{y}\frac{d}{dy}-\frac{m^2}{y^2}\right)R=0 \tag{11}$$

If we try a solution of form

$$R=y^{|m|} \tag{12}$$

we have

$$|m|\left(|m|-1\right)y^{|m|-2}+|m|\,y^{|m|-2}-m^2y^{|m|-2}=0 \tag{13}$$

Thus 12 is indeed a solution in this limiting case.
For $y\to\infty$, we can ignore the terms $\frac{1}{y}\frac{d}{dy}$, $\frac{m^2}{y^2}R$ and $2\varepsilon R$ to get

$$-\frac{d^2}{dy^2}R+y^2R=0 \tag{14}$$

or

$$R''=y^2R \tag{15}$$

We try a solution of form

$$R=y^ae^{-y^2/2} \tag{16}$$

where a is some constant. We find

$$R' = \left(ay^{a-1} - y^{a+1}\right) e^{-y^2/2} \tag{17}$$

$$R'' = \left(a\left(a-1\right) y^{a-2} - \left(a+1\right) y^a - ay^a + y^{a+2}\right) e^{-y^2/2} \tag{18}$$

$$= y^{a+2}\left(\frac{a\left(a-1\right)}{y^4} - \frac{2a+1}{y^2} + 1\right) e^{-y^2/2} \tag{19}$$

As $y \to \infty$, the last line tends to

$$R'' \to y^{a+2} e^{-y^2/2} = y^2 R \tag{20}$$

so in this limit 16 is a solution. We can therefore propose that R has the general form

$$R\left(y\right) = y^{|m|} e^{-y^2/2} U\left(y\right) \tag{21}$$

where U is a function to be determined by solving the exact ODE 10. We can get an ODE for U by substituting 21 into 10, although the calculation gets somewhat messy. As Shankar suggests, we can do this in two stages. First, we substitute

$$R = y^{|m|} f\left(y\right) \tag{22}$$

where

$$f\left(y\right) = e^{-y^2/2} U\left(y\right) \tag{23}$$

The required derivatives are (To make the notation simpler, I'll drop the absolute value signs around m; you should assume that wherever m occurs, it should really be $|m|$. We can replace the absolute value sign at the end.)

$$R' = my^{m-1} f + y^m f' \tag{24}$$

$$R'' = m\left(m-1\right) y^{m-2} f + 2my^{m-1} f' + y^m f'' \tag{25}$$

Plugging these into 10 we have

$$-\left(m\left(m-1\right) y^{m-2} f + 2my^{m-1} f' + y^m f''\right) - \left(my^{m-2} f + y^{m-1} f'\right) + \ldots \tag{26}$$

$$m^2 y^{m-2} f - 2\varepsilon y^m f + y^{m+2} f = 0 \tag{27}$$

Collecting terms and dividing through by $-y^m$, we get

$$f'' + f'\left(\frac{2m+1}{y}\right) + f\left(2\varepsilon - y^2\right) = 0 \tag{28}$$

We now get the derivatives of f:

$$f' = -ye^{-y^2/2}U + e^{-y^2/2}U' \tag{29}$$

$$= e^{-y^2/2}\left(U' - yU\right) \tag{30}$$

$$f'' = \left[-y\left(U' - yU\right) + U'' - U - yU'\right]e^{-y^2/2} \tag{31}$$

$$= \left(U'' - 2yU' + \left(y^2 - 1\right)U\right)e^{-y^2/2} \tag{32}$$

When we plug these into 28, the exponential factor cancels out, so we get

$$U'' - 2yU' + \left(y^2 - 1\right)U + \frac{2m+1}{y}\left(U' - yU\right) + U\left(2\varepsilon - y^2\right) = 0 \tag{33}$$

Collecting terms, we get, upon restoring the absolute values:

$$U'' + \left(\frac{2\,|m|+1}{y} - 2y\right)U' + (2\varepsilon - 2\,|m| - 2)\,U = 0 \tag{34}$$

We can solve this ODE using a power series in y, but we'll leave that till the next post.

PINGBACKS

Pingback: Two-dimensional harmonic oscillator – Part 2: Series solution
Pingback: Harmonic oscillator in a magnetic field

TWO-DIMENSIONAL HARMONIC OSCILLATOR – PART 2: SERIES SOLUTION

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 12, Exercise 12.3.7 (6) - (7).

Post date: 6 May 2017

[If some equations are too small to read easily, use your browser's magnifying option (Ctrl + on Chrome, probably something similar on other browsers).]

In this post, we'll continue with the solution of the 2-d isotropic harmonic oscillator. In the last post, we started with the ODE for the radial function in the form

$$-\frac{\hbar^2}{2\mu}\left(\frac{d^2}{d\rho^2}+\frac{1}{\rho}\frac{d}{d\rho}-\frac{m^2}{\rho^2}\right)R+\frac{1}{2}\mu\omega^2\rho^2R=ER \tag{1}$$

We introduced dimensionless variables

$$y \equiv \sqrt{\frac{\mu\omega}{\hbar}}\rho \tag{2}$$

$$\varepsilon \equiv \frac{E}{\hbar\omega} \tag{3}$$

and found that R could be written as

$$R(y)=y^{|m|}e^{-y^2/2}U(y) \tag{4}$$

with U given by the solution of the ODE

$$U''+\left(\frac{2|m|+1}{y}-2y\right)U'+(2\varepsilon-2|m|-2)U=0 \tag{5}$$

We can solve this by using a power series of the form

$$U(y)=\sum_{r=0}^{\infty}C_r y^r \tag{6}$$

where the coefficients C_r are constants.

The derivatives are

$$U' = \sum_{r=0}^{\infty} C_r r y^{r-1} \tag{7}$$

$$= 0 + C_1 + 2C_2 y + 3C_3 + y^2 + \dots \tag{8}$$

$$= \sum_{r=0}^{\infty} C_{r+1} (r+1) y^r \tag{9}$$

$$U'' = \sum_{r=0}^{\infty} C_{r+1} r (r+1) y^{r-1} \tag{10}$$

$$= 0 + (1)(2) C_2 + (2)(3) C_3 y + \dots \tag{11}$$

$$= \sum_{r=0}^{\infty} C_{r+2} (r+1)(r+2) y^r \tag{12}$$

Plugging these into 5 we have (we'll drop the absolute value signs on $|m|$ to make the notation simpler; we can restore them at the end):

$$\sum_{r=0}^{\infty} C_{r+2} (r+1)(r+2) y^r + (2m+1) \sum_{r=0}^{\infty} C_r r y^{r-2} - \dots \tag{13}$$

$$2 \sum_{r=0}^{\infty} C_r r y^r + 2(\varepsilon - m - 1) \sum_{r=0}^{\infty} C_r y^r = 0 \tag{14}$$

The second sum in the first line is

$$\sum_{r=0}^{\infty} C_r r y^{r-2} = 0 + C_1 y^{-1} + 2C_2 + 3C_3 y + \dots \tag{15}$$

$$= \sum_{r=-1}^{\infty} C_{r+2} (r+2) y^r \tag{16}$$

The sum thus becomes

$$(2m+1) C_1 y^{-1} + \sum_{r=0}^{\infty} y^r C_{r+2} (r+2)^2 + 2 \sum_{r=0}^{\infty} y^r C_r [-r + \varepsilon - m - 1] = 0 \tag{17}$$

A basic theorem about power series is that if the sum of the series equals zero for all y, then the coefficient of each power must be zero. This shows that $C_1 = 0$ since otherwise the series would blow up as $y \to 0$. This results in a recursion relation for the C_r:

$$C_{r+2} = \frac{2(r + m + 1 - \varepsilon)}{(r+2)^2} C_r \tag{18}$$

Since $C_1 = 0$, all $C_r = 0$ for odd r. For large r we have

$$\frac{C_{r+2}}{C_r} \to \frac{2}{r} \tag{19}$$

If the series is allowed to be infinite, this leads to a divergent series as we can see from the following (based on Shankar's section 7.3). Suppose we look at $y^m e^{y^2}$, which clearly goes to infinity at large y (remember, m is positive). In series form this is

$$y^m e^{y^2} = \sum_{k=0}^{\infty} \frac{y^{2k+m}}{k!} \tag{20}$$

The coefficient C_n of y^n , with $n = 2k + m$ in this series is

$$C_n = \frac{1}{[(n-m)/2]!} \tag{21}$$

Similarly,

$$C_{n+2} = \frac{1}{[(n+2-m)/2]!} \tag{22}$$

The ratio is

$$\begin{aligned} \frac{C_{n+2}}{C_n} &= \frac{[(n-m)/2]!}{[(n+2-m)/2]!} && (23) \\ &= \frac{1}{(n-m)/2+1} && (24) \\ &\to \frac{2}{n} && (25) \end{aligned}$$

In other words, the coefficients of our series solution have the same behaviour 19 for large r as those in the series for $y^m e^{y^2}$. Referring back to 4, we see that this gives an overall behaviour for the radial function R of

$$R \to y^m e^{-y^2/2} y^m e^{y^2} = y^{2m} e^{y^2/2} \tag{26}$$

Thus if we allow the series for U to be infinite, the overall solution diverges, which is not acceptable. We therefore require that the series terminates at some finite value of r, and from 18 we see that this happens if

$$\varepsilon = r + m + 1 \tag{27}$$

for some r. From the definition 3 this gives us the allowed values for the energy:

$$E = \hbar\omega\left(r+|m|+1\right) \tag{28}$$
$$= \hbar\omega\left(2k+|m|+1\right) \tag{29}$$

where the last line follows because r must be even. If

$$n \equiv 2k+|m| \tag{30}$$

then the allowed energies are

$$E = \hbar\omega\left(n+1\right) \tag{31}$$

PINGBACKS

Pingback: Two-dimensional harmonic oscillator - Part 1

Pingback: Harmonic oscillator in 2 dimensions: comparison with rectangular coordinates

Pingback: Harmonic oscillator in a magnetic field

HARMONIC OSCILLATOR IN 2 DIMENSIONS: COMPARISON WITH RECTANGULAR COORDINATES

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 12, Exercise 12.3.7 (8) - (10).

Post date: 9 May 2017

[If some equations are too small to read easily, use your browser's magnifying option (Ctrl + on Chrome, probably something similar on other browsers).]

In this post, we'll continue with the solution of the 2-d isotropic harmonic oscillator. In the previous post, we found that the radial equation R can be written as

$$R(y) = y^{|m|}e^{-y^2/2}U(y) \tag{1}$$

where the dimensionless variables are given by

$$y \equiv \sqrt{\frac{\mu\omega}{\hbar}}\rho \tag{2}$$

$$\varepsilon \equiv \frac{E}{\hbar\omega} \tag{3}$$

and U has a solution as a power series

$$U(y) = \sum_{r=0}^{\infty} C_r y^r \tag{4}$$

The coefficients C_r satisfy the recursion relation

$$C_{r+2} = \frac{2(r+|m|+1-\varepsilon)}{(r+2)^2}C_r \tag{5}$$

Only C_r for even r are non-zero.

In order for U to remain finite for large y, the series must terminate, which gives the allowable values for the energy as

$$E = \hbar\omega(n+1) \tag{6}$$

with

$$n \equiv 2k + |m| \tag{7}$$

and $k = 0, 1, 2, \ldots$.

We can now compare the solution obtained in polar coordinates with our earlier solution in terms of rectangular coordinates. First, what are the possible values for m for a given energy $E = \hbar\omega\,(n+1)$? From the relation 7, we can look at even and odd n separately. For even n, k can take values $0, 1, \ldots, \frac{n}{2} - 1, \frac{n}{2}$. The first $\frac{n}{2}$ of these values for k (that is, for $k = 0, 1, \ldots, \frac{n}{2} - 1$) each allow two values of m such that $|m| = n - 2k$, namely $m = \pm\,(n - 2k)$. If $k = \frac{n}{2}$, then we must have $m = 0$. Thus for even n the total number of combinations is $2 \times \frac{n}{2} + 1 = n + 1$.

For odd n, k can take on values $0, 1, \ldots, \frac{n-1}{2}$, giving a total of $\frac{n+1}{2}$ possible values. (If this isn't obvious, write it out for the first few values of odd n to see the pattern.) For each of these values of k, m can take on the two values $m = \pm\,(n - 2k)$, thus there are again $2 \times \frac{n+1}{2} = n + 1$ different combinations. Thus a state with energy $E = \hbar\omega\,(n+1)$ has a degeneracy $n + 1$.

We can construct the actual eigenfunctions for a couple of values of n by plugging in the appropriate formulas. For $n = 0$ there is only one function, which we find by setting $k = m = 0$. From 4, we have

$$U_0\,(y) = C_0 \tag{8}$$

and from 1 we have

$$R_0\,(y) = C_0 e^{-y^2/2} \tag{9}$$

or, in terms of the original variables

$$R_0\,(\rho) = C_0 e^{-\mu\omega\rho^2/2\hbar} \tag{10}$$

The complete solution is given by

$$\begin{aligned} \psi_m\,(\rho, \phi) &= R(\rho)\,\Phi_m\,(\phi) && (11) \\ &= \frac{1}{\sqrt{2\pi}} R(\rho)\, e^{im\phi} && (12) \end{aligned}$$

so for $m = 0$ we have

$$\psi_0\,(\rho, \phi) = \frac{C_0}{\sqrt{2\pi}} e^{-\mu\omega\rho^2/2\hbar} \tag{13}$$

The constant C_0 can be found by normalizing:

$$1 = \int_0^\infty \int_0^{2\pi} |\psi_0|^2 \rho d\phi d\rho \tag{14}$$

$$= |C_0|^2 \int_0^\infty e^{-\mu\omega\rho^2/\hbar} \rho d\rho \tag{15}$$

$$= |C_0|^2 \frac{\hbar}{2\mu\omega} \tag{16}$$

$$C_0 = \sqrt{\frac{2\mu\omega}{\hbar}} \tag{17}$$

$$\psi_0(\rho, \phi) = \sqrt{\frac{\mu\omega}{\pi\hbar}} e^{-\mu\omega\rho^2/2\hbar} \tag{18}$$

This agrees with the earlier result in rectangular coordinates (eqn 26 in this post). This must be the case, since the $n = 0$ state is non-degenerate.

For $n = 1$, we have $k = 0$ and $m = \pm 1$ so we have two solutions:

$$\psi_1 = \frac{C_0}{\sqrt{2\pi}} \sqrt{\frac{\mu\omega}{\hbar}} \rho e^{-\mu\omega\rho^2/2\hbar} e^{i\phi} \tag{19}$$

$$\psi_{-1} = \frac{C_0}{\sqrt{2\pi}} \sqrt{\frac{\mu\omega}{\hbar}} \rho e^{-\mu\omega\rho^2/2\hbar} e^{-i\phi} \tag{20}$$

Again, we normalize

$$1 = \int_0^\infty \int_0^{2\pi} |\psi_{\pm 1}|^2 \rho d\phi d\rho \tag{21}$$

$$= \frac{\mu\omega}{\hbar} |C_0|^2 \int_0^\infty e^{-\mu\omega\rho^2/\hbar} \rho^3 d\rho \tag{22}$$

$$C_0 = \sqrt{\frac{2\mu\omega}{\hbar}} \tag{23}$$

$$\psi_{\pm 1} = \frac{\mu\omega}{\hbar\sqrt{\pi}} \rho e^{-\mu\omega\rho^2/2\hbar} e^{\pm i\phi} \tag{24}$$

These solutions are linear combinations of the corresponding solutions in rectangular coordinates:

$$\psi_{10} = \frac{\sqrt{2}\mu\omega}{\hbar\sqrt{\pi}} e^{-\mu\omega\rho^2/2\hbar} \rho \cos\phi \tag{25}$$

$$\psi_{01} = \frac{\sqrt{2}\mu\omega}{\hbar\sqrt{\pi}} e^{-\mu\omega\rho^2/2\hbar} \rho \sin\phi \tag{26}$$

The combinations are

$$\psi_{+1} = \frac{1}{\sqrt{2}}(\psi_{10} + i\psi_{01}) \tag{27}$$

$$\psi_{-1} = \frac{1}{\sqrt{2}}(\psi_{10} - i\psi_{01}) \tag{28}$$

The parity of the states is found from their behaviour under the transformation (in rectangular coordinates) $x \to -x$ and $y \to -y$. In polar coordinates this is equivalent to the transformation $\phi \to \phi + \pi$ and from 18 and 24 we see that

$$\psi_0(\rho, \phi + \pi) = \psi_0(\rho, \phi) \tag{29}$$

$$\psi_{\pm 1}(\rho, \phi + \pi) = \psi_{\pm 1}(\rho, \phi)\, e^{\pm \pi} \tag{30}$$

$$= -\psi_{\pm 1}(\rho, \phi) \tag{31}$$

Thus the parity of $n = 0$ is even, and that of $n = 1$ is odd. In general, since the ϕ dependence enters only through the term $e^{im\phi} = e^{in\phi}e^{-2ik\phi}$, we see that adding π to ϕ leaves the $e^{-2ik\phi}$ term unchanged and multiplies the $e^{in\phi}$ term by $e^{in\pi\phi} = (-1)^n$, so the parity of state n is $(-1)^n$.

PINGBACKS

Pingback: Harmonic oscillator in a magnetic field

Pingback: Rotation of a vector wave function

HARMONIC OSCILLATOR IN A MAGNETIC FIELD

Link to: physicspages home page.

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Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 12, Exercise 12.3.8.

Post date: 12 May 2017

[If some equations are too small to read easily, use your browser's magnifying option (Ctrl + on Chrome, probably something similar on other browsers).]

As another example of the harmonic oscillator, we'll look at a charged particle moving in a magnetic field. The field **B** is given in terms of the magnetic vector potential

$$\mathbf{A} = \frac{B}{2}\left(-y\hat{\mathbf{x}} + x\hat{\mathbf{y}}\right) \tag{1}$$

The field is

$$\begin{aligned} \mathbf{B} &= \nabla \times \mathbf{A} && (2)\\ &= \left(\frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y}\right)\hat{\mathbf{z}} && (3)\\ &= B\hat{\mathbf{z}} && (4) \end{aligned}$$

If the particle is confined to the xy plane and the magnetic field provides the only force, the force is given by the Lorentz force law

$$\mathbf{F} = q\mathbf{v} \times \mathbf{B} \tag{5}$$

Since **F** is always perpendicular to the direction of motion **v**, the magnetic force does no work, so the kinetic energy and hence the speed v of the particle is constant. Classically, the particle is thus confined to move in a circle with **F** providing the centripetal force, so we have

$$\begin{aligned} qvB &= \frac{\mu v^2}{\rho} && (6)\\ v &= \frac{qB\rho}{\mu} && (7) \end{aligned}$$

where q is the charge, μ is the mass and ρ is the radius of the circle. The period of the orbit is

$$T = \frac{2\pi\rho}{v} = \frac{2\pi\mu}{qB} \tag{8}$$

which gives an angular frequency of

$$\omega_0 = \frac{2\pi}{T} = \frac{qB}{\mu} \tag{9}$$

This is the result in SI units; Shankar uses Gaussian units, in which the magnetic field picks up a factor of $\frac{1}{c}$, so in Shankar's notation, this is

$$\omega_0 = \frac{qB}{\mu c} \tag{10}$$

As the rest of the problem relies on Gaussian units, we'll stick to them from now on.

Classically, the Hamiltonian for the electromagnetic force is

$$H = \frac{|\mathbf{p} - q\mathbf{A}/c|^2}{2\mu} + q\phi \tag{11}$$

where ϕ is the electric potential, which is zero here. Thus using 1, we have for the quantum version in which **p** and the position vector are replaced by operators

$$H = \frac{(P_x + qYB/2c)^2}{2\mu} + \frac{(P_y - qXB/2c)^2}{2\mu} \tag{12}$$

We can perform a canonical transformation by defining

$$Q \equiv \frac{1}{qB}\left(cP_x + \frac{qYB}{2}\right) \tag{13}$$

$$P \equiv P_y - \frac{qXB}{2c} \tag{14}$$

We can verify that these coordinates are canonical by checking their commutator:

$$[Q, P] = \frac{1}{qB}\left[cP_x + \frac{qYB}{2}, P_y - \frac{qXB}{2c}\right] \tag{15}$$

$$= \frac{1}{qB}\left(-\frac{qB}{2}[P_x, X] + \frac{qB}{2}[Y, P_y]\right) \tag{16}$$

$$= \frac{i\hbar}{2} + \frac{i\hbar}{2} \tag{17}$$

$$= i\hbar \tag{18}$$

Thus Q and P have the correct commutator for a pair of position and momentum variables.

Rewriting 12 in terms of Q and P, we have

$$H = \frac{q^2B^2}{2\mu c^2}Q^2 + \frac{P^2}{2\mu} \tag{19}$$

$$= \frac{P^2}{2\mu} + \frac{\mu}{2}\omega_0^2 Q^2 \tag{20}$$

Thus H has the same form as that for a one-dimensional harmonic oscillator with frequency ω_0, so the energy levels of this system must be

$$E = \left(n + \frac{1}{2}\right)\hbar\omega_0 \tag{21}$$

We can expand 12 in terms of the original position and momentum variables to get

$$H = \frac{P_x^2 + P_y^2}{2\mu} + \frac{1}{2}\mu\left(\frac{qB}{2\mu c}\right)^2\left(X^2 + Y^2\right) + \frac{qB}{2\mu c}\left(P_xY - P_yX\right) \tag{22}$$

$$= \frac{P_x^2 + P_y^2}{2\mu} + \frac{1}{2}\mu\left(\frac{\omega_0}{2}\right)^2\left(X^2 + Y^2\right) - \frac{\omega_0}{2}\left(XP_y - YP_x\right) \tag{23}$$

$$= H\left(\frac{\omega_0}{2}, \mu\right) - \frac{\omega_0}{2}L_z \tag{24}$$

where $H\left(\frac{\omega_0}{2}, \mu\right)$ is the hamiltonian for a 2-dim harmonic oscillator with frequency $\omega_0/2$. As we saw when solving that system, the Hamiltonian for the isotropic oscillator commutes with L_z since the potential is radially symmetric, thus the eigenfunctions of H are also eigenfunctions of L_z. In terms of the present problem, this means that the eigenfunctions of $H\left(\frac{\omega_0}{2}, \mu\right)$ are also eigenfunctions of L_z and thus also eigenfunctions of H. In our solution of the 2-dim isotropic oscillator, we found that the energy levels are given by

$$E = \hbar\omega\left(2k + |m| + 1\right) \tag{25}$$

where $k = 0, 1, 2, \ldots$ and m is the angular momentum (in units of $\hbar$). Thus for the oscillator with Hamiltonian $H\left(\frac{\omega_0}{2}, \mu\right)$, the energy levels are

$$E = \frac{1}{2}\hbar\omega_0\left(2k + |m| + 1\right) \tag{26}$$

$$= \hbar\omega_0\left(k + \frac{1}{2}|m| + \frac{1}{2}\right) \tag{27}$$

The energy levels of the original H are therefore, from 24

$$E = \hbar\omega_0 \left(k + \frac{1}{2}|m| + \frac{1}{2} \right) - \frac{\omega_0}{2} m\hbar \tag{28}$$

$$= \hbar\omega_0 \left(k + \frac{1}{2}|m| - \frac{1}{2}m + \frac{1}{2} \right) \tag{29}$$

[Shankar says the k can be 'any integer', but from our original derivation of 25, we found that k is a non-negative integer.] Equation 29 gives the same energies as 21, since if $m > 0$, we get $E = \hbar\omega_0 \left(k + \frac{1}{2}\right)$, while if $m < 0$ we have $E = \hbar\omega_0 \left(k + |m| + \frac{1}{2}\right)$. Both $k + \frac{1}{2}$ and $k + |m| + \frac{1}{2}$ give the same sequence of values as $n + \frac{1}{2}$. [I'm not quite sure the two methods are equivalent, though, since 21, being the solution of a one-dimensional system is non-degenerate, while 29, being a two-dimensional system does have degenerate energy levels.]

LEVI-CIVITA ANTISYMMETRIC TENSOR, VECTOR PRODUCTS AND SYSTEMS OF 3 FERMIONS

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Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 12, Exercise 12.4.1.

Post date: 16 May 2017

[If some equations are too small to read easily, use your browser's magnifying option (Ctrl + on Chrome, probably something similar on other browsers).]

The Levi-Civita symbol ε_{ijk} is defined as $+1$ if i, j, k have the values 1,2,3 (in that order), 2,3,1 or 3,1,2. Swapping any pair of indices multiplies the value by -1, so that, for example, $\varepsilon_{123} = +1$ and $\varepsilon_{213} = -1$. If two indices are the same, such as $i = j = 1$, then swapping them leaves ε_{11k} unchanged so the requirement that $\varepsilon_{ijk} = -\varepsilon_{jik}$ means that $\varepsilon_{ijk} = 0$ if any two of its indices are equal.

The symbol is actually an antisymmetric tensor of rank 3, and is found frequently in physical and mathematical equations. One example is in the cross product of two 3-d vectors. If

$$\mathbf{c} = \mathbf{a} \times \mathbf{b} \tag{1}$$

we can work out the components of **c** in the usual way by calculating the determinant:

$$\mathbf{c} = \begin{vmatrix} \hat{\mathbf{x}}_1 & \hat{\mathbf{x}}_2 & \hat{\mathbf{x}}_3 \\ a_1 & a_2 & a_3 \\ b_1 & b_2 & b_3 \end{vmatrix} \tag{2}$$

$$= (a_2 b_3 - b_2 a_3)\,\hat{\mathbf{x}}_1 - (a_1 b_3 - b_1 a_3)\,\hat{\mathbf{x}}_2 + (a_1 b_2 - b_2 a_1)\,\hat{\mathbf{x}}_3 \tag{3}$$

where I've used $\hat{\mathbf{x}}_1 = \hat{\mathbf{x}}$, $\hat{\mathbf{x}}_2 = \hat{\mathbf{y}}$ and $\hat{\mathbf{x}}_3 = \hat{\mathbf{z}}$.

Using ε_{ijk} we can write this in the compact form

$$\mathbf{c} = \sum_{i,j,k} \varepsilon_{ijk} \hat{\mathbf{x}}_i a_j b_k \tag{4}$$

as can be verified by expanding the sum and comparing with 3.

The Levi-Civita symbol can be used to write a completely antisymmetric wave function for a set of three fermions. Suppose the wave function for a single fermion in state n with coordinate x_a is $U_n(x_a)$ (where both n and a

can take values 1, 2 or 3). Then a completely antisymmetric wave function is

$$\psi_A(x_1, x_2, x_3) = \frac{1}{\sqrt{6}} \sum_{i,j,k} \varepsilon_{ijk} U_i(x_1) U_j(x_2) U_k(x_3) \tag{5}$$

The factor of $\frac{1}{\sqrt{6}}$ is for normalization and assumes that the U_n are all normalized wave functions.

Swapping the locations x_1 and x_2, for example, is equivalent to swapping i and j in the sum, which produces the negative of the original sum. That is

$$\psi_A(x_2, x_1, x_3) = \frac{1}{\sqrt{6}} \sum_{i,j,k} \varepsilon_{ijk} U_i(x_2) U_j(x_1) U_k(x_3) \tag{6}$$

$$= \frac{1}{\sqrt{6}} \sum_{i,j,k} \varepsilon_{jik} U_i(x_1) U_j(x_2) U_k(x_3) \tag{7}$$

$$= -\frac{1}{\sqrt{6}} \sum_{i,j,k} \varepsilon_{ijk} U_i(x_1) U_j(x_2) U_k(x_3) \tag{8}$$

$$= -\psi_A(x_1, x_2, x_3) \tag{9}$$

The same argument applies to swapping the other pairs of locations.

PINGBACKS

Pingback: Vector operators; transformation under rotation
Pingback: Pauli matrices: properties
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Pingback: Electromagnetic Lorentz invariant

ANGULAR MOMENTUM IN THREE DIMENSIONS

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Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 12, Exercise 12.4.2.

Post date: 17 May 2017

[If some equations are too small to read easily, use your browser's magnifying option (Ctrl + on Chrome, probably something similar on other browsers).]

We can now generalize our treatment of rotation, originally studied in two dimensions, to three dimensions. We'll view a 3-d rotation as a combination of rotations about the x, y and z axes, each of which can be represented by a 3×3 matrix. These matrices are as follows:

$$R(\theta\hat{\mathbf{x}}) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos\theta & -\sin\theta \\ 0 & \sin\theta & \cos\theta \end{bmatrix} \tag{1}$$

$$R(\theta\hat{\mathbf{y}}) = \begin{bmatrix} \cos\theta & 0 & \sin\theta \\ 0 & 1 & 0 \\ -\sin\theta & 0 & \cos\theta \end{bmatrix} \tag{2}$$

$$R(\theta\hat{\mathbf{z}}) = \begin{bmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{bmatrix} \tag{3}$$

We're interested in infinitesimal rotations, for which we retain terms up to first order in the rotation angle ε_i, so that $\cos\varepsilon_i = 1$ and $\sin\varepsilon_i = \varepsilon_i$. This gives the infinitesimal rotation matrices as

$$R(\varepsilon_x\hat{\mathbf{x}}) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & -\varepsilon_x \\ 0 & \varepsilon_x & 1 \end{bmatrix} \tag{4}$$

$$R(\varepsilon_y\hat{\mathbf{y}}) = \begin{bmatrix} 1 & 0 & \varepsilon_y \\ 0 & 1 & 0 \\ -\varepsilon_y & 0 & 1 \end{bmatrix} \tag{5}$$

$$R(\varepsilon_z\hat{\mathbf{z}}) = \begin{bmatrix} 1 & -\varepsilon_z & 0 \\ \varepsilon_z & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \tag{6}$$

We now consider the series of rotations as follows: first, a rotation by $\varepsilon_x\hat{\mathbf{x}}$, then by $\varepsilon_y\hat{\mathbf{y}}$, then by $-\varepsilon_x\hat{\mathbf{x}}$ and finally by $-\varepsilon_y\hat{\mathbf{y}}$. Because the various rotations don't commute, we don't end up back where we started. We can calculate the matrix products to find the final rotation.

$$R = R(-\varepsilon_y\hat{\mathbf{y}})\,R(-\varepsilon_x\hat{\mathbf{x}})\,R(\varepsilon_y\hat{\mathbf{y}})\,R(\varepsilon_x\hat{\mathbf{x}}) \tag{7}$$

$$= \begin{bmatrix} 1 & 0 & -\varepsilon_y \\ 0 & 1 & 0 \\ \varepsilon_y & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & \varepsilon_x \\ 0 & -\varepsilon_x & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & \varepsilon_y \\ 0 & 1 & 0 \\ -\varepsilon_y & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & -\varepsilon_x \\ 0 & \varepsilon_x & 1 \end{bmatrix} \tag{8}$$

$$= \begin{bmatrix} 1 & \varepsilon_x\varepsilon_y & -\varepsilon_y \\ 0 & 1 & \varepsilon_x \\ \varepsilon_y & -\varepsilon_x & 1 \end{bmatrix} \begin{bmatrix} 1 & \varepsilon_x\varepsilon_y & \varepsilon_y \\ 0 & 1 & -\varepsilon_x \\ -\varepsilon_y & \varepsilon_x & 1 \end{bmatrix} \tag{9}$$

$$= \begin{bmatrix} 1+\varepsilon_y^2 & \varepsilon_x\varepsilon_y & -\varepsilon_x^2\varepsilon_y \\ -\varepsilon_x\varepsilon_y & 1+\varepsilon_x^2 & 0 \\ 0 & \varepsilon_x\varepsilon_y^2 & 1+\varepsilon_x^2+\varepsilon_y^2 \end{bmatrix} \tag{10}$$

To get the third line, we multiplied the first two matrices in the second line, and the last two matrices in the second line. In the final result, we can discard terms containing ε_x^2 or ε_y^2 to get

$$R = \begin{bmatrix} 1 & \varepsilon_x\varepsilon_y & 0 \\ -\varepsilon_x\varepsilon_y & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} = R(-\varepsilon_x\varepsilon_y\hat{\mathbf{z}}) \tag{11}$$

Thus the result of the four rotations about the x and y axes is a single rotation about the z axis.

To convert this to quantum operators, we define the operator $U[R]$ by comparison with the procedure we used for 2-d rotations. That is, the operator U is given by the corresponding angular momentum operator L_x, L_y or L_z as

$$U[R(\varepsilon_x \hat{\mathbf{x}})] = I - \frac{i\varepsilon_x L_x}{\hbar} \quad (12)$$

$$U[R(\varepsilon_y \hat{\mathbf{y}})] = I - \frac{i\varepsilon_y L_y}{\hbar} \quad (13)$$

$$U[R(\varepsilon_z \hat{\mathbf{z}})] = I - \frac{i\varepsilon_z L_z}{\hbar} \quad (14)$$

By comparing 7 and 11 we thus require these U operators to satisfy

$$U[R(-\varepsilon_y \hat{\mathbf{y}})]\,U[R(-\varepsilon_x \hat{\mathbf{x}})]\,U[R(\varepsilon_y \hat{\mathbf{y}})]\,U[R(\varepsilon_x \hat{\mathbf{x}})] = U[R(-\varepsilon_x \varepsilon_y \hat{\mathbf{z}})] \quad (15)$$

We can get the commutation relation $[L_x, L_y]$ by matching coefficients of $\varepsilon_x \varepsilon_y$ on each side of this equation. On the RHS, the coefficient is $\frac{iL_z}{\hbar}$. On the LHS, we can pick out the terms involving $\varepsilon_x \varepsilon_y$ to get

$$-\frac{1}{\hbar^2}\left(L_y L_x - L_y L_x - L_x L_y + L_y L_x\right) = \frac{1}{\hbar^2}\left[L_x, L_y\right] \quad (16)$$

The first term on the LHS comes from the ε_x term in the first U in 15 multiplied by the ε_y term in the second U (with the I term in the other two Us); the second term on the LHS comes from the ε_x term in the first U in 15 multiplied by the ε_y term in the fourth U, and so on.

Matching the two sides, we get

$$[L_x, L_y] = i\hbar L_z \quad (17)$$

By comparison with the classical definitions of the three components of $\mathbf{L}$, we can write the quantum operators in terms of position and momentum operators as

$$L_x = YP_z - ZP_y \quad (18)$$

$$L_y = ZP_x - XP_z \quad (19)$$

$$L_z = XP_y - YP_x \quad (20)$$

From the commutators of position and momentum $[X, P_x] = i\hbar$ and so on, we can verify 17 from these relations as well.

$$
\begin{aligned}
[L_x, L_y] &= [YP_z - ZP_y, ZP_x - XP_z] && (21)\\
&= [YP_z, ZP_x - XP_z] - [ZP_y, ZP_x - XP_z] && (22)\\
&= -i\hbar YP_x + i\hbar P_y X && (23)\\
&= i\hbar\,(XP_y - YP_x) && (24)\\
&= i\hbar L_z && (25)
\end{aligned}
$$

The third line follows because $[YP_z, XP_z] = [ZP_y, ZP_x] = 0$. The other two commutation relations follow by cyclic permutation of x, y and z:

$$
\begin{aligned}
[L_y, L_z] &= i\hbar L_x && (26)\\
[L_z, L_x] &= i\hbar L_y && (27)
\end{aligned}
$$

PINGBACKS

Pingback: Finite rotations about an arbitrary axis in three dimensions
Pingback: Vector operators; transformation under rotation
Pingback: spherical harmonics: rotation about the x axis
Pingback: General infinitesimal Lorentz transformation

FINITE ROTATIONS ABOUT AN ARBITRARY AXIS IN THREE DIMENSIONS

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 12, Exercise 12.4.3.

Post date: 19 May 2017

[If some equations are too small to read easily, use your browser's magnifying option (Ctrl + on Chrome, probably something similar on other browsers).]

The operators for an infinitesimal rotation in 3-d are

$$U\left[R(\varepsilon_x\hat{\mathbf{x}})\right] = I - \frac{i\varepsilon_x L_x}{\hbar} \tag{1}$$

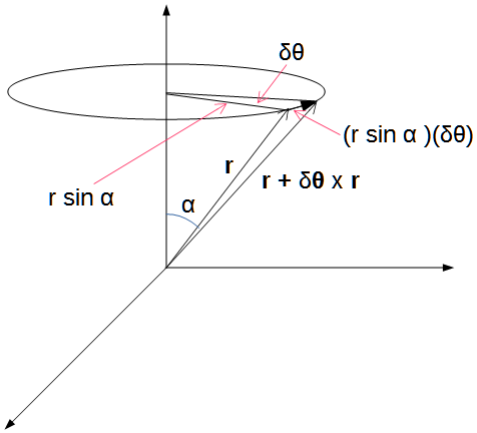
$$U\left[R(\varepsilon_y\hat{\mathbf{y}})\right] = I - \frac{i\varepsilon_y L_y}{\hbar} \tag{2}$$

$$U\left[R(\varepsilon_z\hat{\mathbf{z}})\right] = I - \frac{i\varepsilon_z L_z}{\hbar} \tag{3}$$

If we have a finite (larger than infinitesimal) rotation about one of the coordinate axes, we can create the operator by dividing up the finite rotation angle θ into N small increments and take the limit as $N \to \infty$, just as we did with finite translations. For example, for a finite rotation about the x axis, we have

$$U\left[R(\theta\hat{\mathbf{x}})\right] = \lim_{N\to\infty}\left(I - \frac{i\theta L_x}{N\hbar}\right)^N = e^{-i\theta L_x/\hbar} \tag{4}$$

What if we have a finite rotation about some arbitrarily directed axis? Suppose we have a vector $\mathbf{r}$ as shown in the figure:



The vector **r** makes an angle α with the z axis, and we wish to rotate **r** about the z axis by an angle $\delta\theta$. Note that this argument is completely general, since if the axis of rotation is not the z axis, we can rotate the entire coordinate system so that the axis of rotation *is* the z axis. The generality enters through the fact that we're keeping the angle α arbitrary.

The rotation by $\delta\theta\hat{\mathbf{z}} \equiv \delta\boldsymbol{\theta}$ shifts the tip of **r** along the circle shown by a distance $(r\sin\alpha)\,\delta\theta$ in a counterclockwise direction (looking down the z axis). This shift is in a direction that is perpendicular to both $\hat{\mathbf{z}}$ and **r**, so the little vector representing the shift in **r** is

$$\delta\mathbf{r} = (\delta\boldsymbol{\theta}) \times \mathbf{r} \tag{5}$$

Thus under the rotation $\delta\boldsymbol{\theta}$, a vector transforms as

$$\mathbf{r} \to \mathbf{r} + (\delta\boldsymbol{\theta}) \times \mathbf{r} \tag{6}$$

Just as with translations, if we rotate the coordinate system by an amount $\delta\boldsymbol{\theta}$, this is equivalent to rotating the wave function $\psi(\mathbf{r})$ by the same angle, but in the opposite direction, so we require

$$\psi(\mathbf{r}) \to \psi(\mathbf{r} - (\delta\boldsymbol{\theta}) \times \mathbf{r}) \tag{7}$$

A first order Taylor expansion of the quantity on the RHS gives

$$\psi(\mathbf{r} - (\delta\boldsymbol{\theta}) \times \mathbf{r}) = \psi(\mathbf{r}) - (\delta\boldsymbol{\theta} \times \mathbf{r}) \cdot \nabla\psi \tag{8}$$

The operator generating this rotation will have the form (in analogy with the forms for the coordinate axes above):

$$U[R(\delta\boldsymbol{\theta})] = I - \frac{i\delta\theta}{\hbar} L_{\hat{\theta}} \tag{9}$$

where $L_{\hat{\theta}}$ is an angular momentum operator to be determined.

Writing out the RHS of 8, we have

$$\psi(\mathbf{r}) - (\delta\boldsymbol{\theta} \times \mathbf{r}) \cdot \nabla\psi = \psi(\mathbf{r}) - (\delta\theta_y z - \delta\theta_z y)\frac{\partial\psi}{\partial x} + (\delta\theta_x z - \delta\theta_z x)\frac{\partial\psi}{\partial y} - (\delta\theta_x y - \delta\theta_y x)\frac{\partial\psi}{\partial z} \tag{10}$$

$$= \psi(\mathbf{r}) - \delta\theta_x\left(y\frac{\partial\psi}{\partial z} - z\frac{\partial\psi}{\partial y}\right) - \delta\theta_y\left(z\frac{\partial\psi}{\partial x} - x\frac{\partial\psi}{\partial z}\right) - \delta\theta_z\left(x\frac{\partial\psi}{\partial y} - y\frac{\partial\psi}{\partial x}\right) \tag{11}$$

$$= \psi(\mathbf{r}) - \delta\boldsymbol{\theta} \cdot \frac{i}{\hbar}\mathbf{r} \times \mathbf{p}\psi \tag{12}$$

$$= \psi(\mathbf{r}) - \frac{i}{\hbar}\delta\boldsymbol{\theta} \cdot \mathbf{L}\psi \tag{13}$$

$$= U[R(\delta\boldsymbol{\theta})]\psi \tag{14}$$

Comparing this with 9, we see that

$$L_{\hat{\theta}} = \hat{\boldsymbol{\theta}} \cdot \mathbf{L} \tag{15}$$

where $\hat{\boldsymbol{\theta}}$ is the unit vector along the axis of rotation. Since all rotations about the same axis commute, we can use the same procedure as above to generate a finite rotation $\boldsymbol{\theta}$ about an arbitrary axis and get

$$U[R(\boldsymbol{\theta})] = e^{-i\boldsymbol{\theta}\cdot\mathbf{L}/\hbar} \tag{16}$$

PINGBACKS

Pingback: Vector operators; transformation under rotation

Pingback: total angular momentum finite rotations

Pingback: Effective magnetic field in rotating frame - axis of rotation not parallel

VECTOR OPERATORS; TRANSFORMATION UNDER ROTATION

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 12, Exercise 12.4.4.

Post date: 20 May 2017

[If some equations are too small to read easily, use your browser's magnifying option (Ctrl + on Chrome, probably something similar on other browsers).]

A vector operator $\mathbf{V}$ is defined as an operator whose components transform under rotation according to

$$U^{\dagger}[R]\, V_i U[R] = \sum_j R_{ij} V_j \tag{1}$$

where R is the rotation matrix in either 2 or 3 dimensions. We've seen that, for an infinitesimal rotation about an arbitrary axis $\delta\boldsymbol{\theta}$, a vector transforms like

$$\mathbf{V} \rightarrow \mathbf{V} + \delta\boldsymbol{\theta} \times \mathbf{V} \tag{2}$$

This can be written more compactly using the Levi-Civita tensor, since component i of a cross product is

$$(\delta\boldsymbol{\theta} \times \mathbf{V})_i = \sum_{j,k} \varepsilon_{ijk} (\delta\theta)_j V_k \tag{3}$$

We get

$$\sum_j R_{ij} V_j = V_i + \sum_{j,k} \varepsilon_{ijk} (\delta\theta)_j V_k \tag{4}$$

The operator $U[R]$ is given by

$$U[R(\delta\boldsymbol{\theta})] = I - \frac{i}{\hbar} \delta\boldsymbol{\theta} \cdot \mathbf{L} \tag{5}$$

where $\mathbf{L}$ is the angular momentum. Plugging this into 1, we have, to first order in $\delta\boldsymbol{\theta}$ (remembering that the components of $\mathbf{L}$ do not commute with each other and, in general also do not commute with the components of $\mathbf{V}$):

$$\left(I+\frac{i}{\hbar}\delta\boldsymbol{\theta}\cdot\mathbf{L}\right)V_i\left(I-\frac{i}{\hbar}\delta\boldsymbol{\theta}\cdot\mathbf{L}\right)=V_i+\frac{i}{\hbar}\sum_j\left(\delta\theta_j L_j\right)V_i-\frac{i}{\hbar}V_i\sum_j\left(\delta\theta_j L_j\right) \tag{6}$$

$$=V_i+\frac{i}{\hbar}\sum_j\delta\theta_j\left[L_j,V_i\right] \tag{7}$$

Setting this equal to the RHS of 4 we have, equating coefficients of $\delta\theta_j$:

$$\frac{i}{\hbar}\left[L_j,V_i\right] = \sum_k\varepsilon_{ijk}V_k \tag{8}$$

$$\left[V_i,L_j\right] = i\hbar\sum_k\varepsilon_{ijk}V_k \tag{9}$$

With $\mathbf{V}=\mathbf{L}$, we regain the commutation relations for the components of angular momentum

$$\left[L_x,L_y\right] = i\hbar L_z \tag{10}$$

$$\left[L_y,L_z\right] = i\hbar L_x \tag{11}$$

$$\left[L_z,L_x\right] = i\hbar L_y \tag{12}$$

By the way, it is possible to write these commutation relations in the compact form

$$\mathbf{L}\times\mathbf{L}=i\hbar\mathbf{L} \tag{13}$$

This looks wrong if you're used to the standard definition of the cross product for vectors whose components are ordinary numbers, since for such a vector $\mathbf{a}$, we always have $\mathbf{a}\times\mathbf{a}=0$. However, if the components of the vector are *operators* that don't commute, then the result is not zero, as we can see:

$$\left(\mathbf{L}\times\mathbf{L}\right)_i = \sum_{j,k}\varepsilon_{ijk}L_jL_k \tag{14}$$

If $i=x$, for example, then the sum on the RHS gives

$$\left(\mathbf{L}\times\mathbf{L}\right)_x = \sum_{j,k}\varepsilon_{xjk}L_jL_k \tag{15}$$

$$= L_yL_z-L_zL_y \tag{16}$$

$$= \left[L_y,L_z\right] \tag{17}$$

From 13, this gives

$$[L_y, L_z] = i\hbar L_x \tag{18}$$

PINGBACKS

Pingback: Spherical tensor operators; commutators

ROTATION OF A VECTOR WAVE FUNCTION

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 12, Exercise 12.5.1.

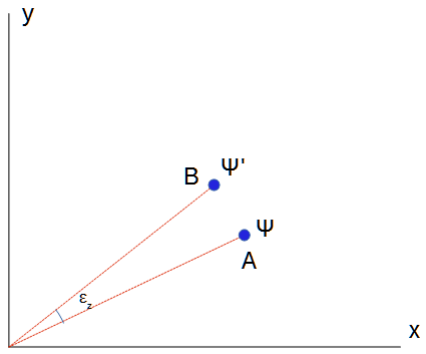
Post date: 22 May 2017

[If some equations are too small to read easily, use your browser's magnifying option (Ctrl + on Chrome, probably something similar on other browsers).]

We've seen that, for a rotation by an infinitesimal angle ε_z about the z axis, a scalar wave function transforms according to

$$\psi(x,y) \rightarrow \psi(x+\varepsilon_z y, y-\varepsilon_z x) \tag{1}$$

The meaning of this transformation can be seen in the figure:



The physical system represented by the wave function Ψ is rigidly rotated by the angle ε_z, so that the value of Ψ at point A is now sitting over the point B. However, in the primed (rotated) coordinate system, the numerical value of the coordinates of the point B in the figure are the same as the numerical values that the point A had in the original, unrotated coordinates. That is

$$\left(x'_B, y'_B\right) = (x_A, y_A) \tag{2}$$

Just as B is obtained from A by rotating A by $+\varepsilon_z$, we can obtain A from B by rotating by $-\varepsilon_z$. For any given point, the primed (rotated) and unprimed (unrotated) coordinates are related by (all relations are to first order in ε_z):

$$x' = x - y\varepsilon_z \quad (3)$$
$$y' = y + x\varepsilon_z \quad (4)$$

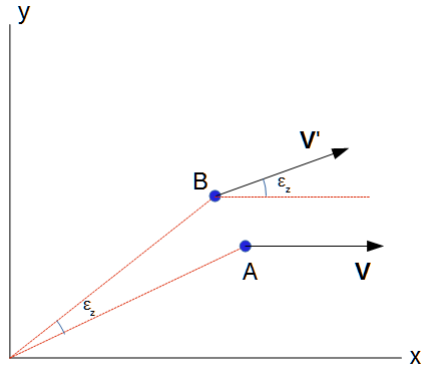
The inverse relations are obtained by a rotation by $-\varepsilon_z$:

$$x = x' + y'\varepsilon_z \quad (5)$$
$$y = y' - x'\varepsilon_z \quad (6)$$

After rotation, the values of Ψ' are related to the values Ψ before rotation by rotating through the angle $-\varepsilon_z$, so that

$$\Psi'(x,y) = \Psi(x + y\varepsilon_z, y - x\varepsilon_z) \quad (7)$$

Now suppose the wave function is a vector $\mathbf{V} = V_x\hat{\mathbf{x}} + V_y\hat{\mathbf{y}}$. The situation is as shown:



The initial unrotated vector $\mathbf{V}$ is the value of the wave function at point A (and is entirely in the x direction for convenience). After rotation, the vector gets moved to B and is also rotated so that it now makes an angle ε_z with the *original* x axis. However, its direction is now along the x' axis, which makes an angle of ε_z with the original x axis.

In this case, each component of $\mathbf{V}$ still gets transformed in the same way as the scalar function above, but the vector itself is also rotated. If the components V_x and V_y of the vector were constants, then the rotated vector is given by applying the 2-d rotation matrix

$$R = \begin{bmatrix} 1 & -\varepsilon_z \\ \varepsilon_z & 1 \end{bmatrix} \quad (8)$$

so we get $\mathbf{V}' = R\mathbf{V}$, or, in components:

$$V_x' = V_x - V_y\varepsilon_z \tag{9}$$
$$V_y' = V_y + V_x\varepsilon_z \tag{10}$$

If V_x and V_y vary from point to point, then we must apply the transformation 1 to each component, so that the overall transformation is

$$V_x' = V_x\left(x+\varepsilon_z y, y-\varepsilon_z x\right) - V_y\left(x+\varepsilon_z y, y-\varepsilon_z x\right)\varepsilon_z \tag{11}$$
$$V_y' = V_y\left(x+\varepsilon_z y, y-\varepsilon_z x\right) + V_x\left(x+\varepsilon_z y, y-\varepsilon_z x\right)\varepsilon_z \tag{12}$$

The operator that generates the transformation of a scalar function by an infinitesimal angle $\delta\boldsymbol{\theta}$ is

$$U\left[R\left(\delta\boldsymbol{\theta}\right)\right] = I - \frac{i}{\hbar}\delta\boldsymbol{\theta}\cdot\mathbf{L} \tag{13}$$

In this case, the rotation is about the z axis so

$$\delta\boldsymbol{\theta} = \varepsilon_z\hat{\mathbf{z}} \tag{14}$$
$$\delta\boldsymbol{\theta}\cdot\mathbf{L} = \varepsilon_z L_z \tag{15}$$

Thus we have

$$V_{x,y}\left(x+\varepsilon_z y, y-\varepsilon_z x\right) = \left(I - \frac{i}{\hbar}\varepsilon_z L_z\right) V_{x,y}\left(x,y\right) \tag{16}$$

Plugging this into 11 and keeping terms only up to order ε_z we have

$$V_x' = \left(I - \frac{i}{\hbar}\varepsilon_z L_z\right) V_x - V_y\varepsilon_z \tag{17}$$
$$V_y' = \left(I - \frac{i}{\hbar}\varepsilon_z L_z\right) V_y + V_x\varepsilon_z \tag{18}$$

In matrix form, this is

$$\begin{bmatrix} V_x' \\ V_y' \end{bmatrix} = \left(\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} - \frac{i\varepsilon_z}{\hbar}\begin{bmatrix} L_z & 0 \\ 0 & L_z \end{bmatrix} - \varepsilon_z\begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}\right)\begin{bmatrix} V_x \\ V_y \end{bmatrix} \tag{19}$$
$$= \left(\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} - \frac{i\varepsilon_z}{\hbar}\begin{bmatrix} L_z & 0 \\ 0 & L_z \end{bmatrix} - \frac{i\varepsilon_z}{\hbar}\begin{bmatrix} 0 & -i\hbar \\ i\hbar & 0 \end{bmatrix}\right)\begin{bmatrix} V_x \\ V_y \end{bmatrix} \tag{20}$$
$$= \left(I - \frac{i\varepsilon_z}{\hbar}J_z\right)\begin{bmatrix} V_x \\ V_y \end{bmatrix} \tag{21}$$

This has the same form as 13, except that the angular momentum generator is now the sum of L_z and the final matrix on the RHS above, which Shankar calls suggestively S_z, in anticipation of spin which at this stage he hasn't considered. That is,

$$J_z = L_z + S_z \tag{22}$$

$$= \begin{bmatrix} L_z & 0 \\ 0 & L_z \end{bmatrix} + \begin{bmatrix} 0 & -i\hbar \\ i\hbar & 0 \end{bmatrix} \tag{23}$$

The eigenvalues of the second matrix here are just $\pm\hbar$, so we haven't yet encountered half-integral values of angular momentum.

PINGBACKS

Pingback: Total angular momentum - matrix elements and commutation relations

Pingback: total angular momentum finite rotations

Pingback: kinematics of spin: hilbert space for an electron

TOTAL ANGULAR MOMENTUM - MATRIX ELEMENTS AND COMMUTATION RELATIONS

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 12, Exercise 12.5.2.

Post date: 24 May 2017

[If some equations are too small to read easily, use your browser's magnifying option (Ctrl + on Chrome, probably something similar on other browsers).]

In Shankar's Chapter 12 treatment of the eigenvalues of the angular momentum operators L^2 and L_z, he retraces much of what we've already covered as a result of working through Griffiths's book. He defines raising and lowering operators for angular momentum as

$$L_{\pm} \equiv L_x \pm iL_y \tag{1}$$

These operators can be used to discover the eigenvalues of L^2 to be $\ell(\ell+1)\hbar^2$, where $\ell = 0, \frac{1}{2}, 1, \frac{3}{2}, \ldots$ and the eigenvalues of L_z are $m\hbar$ where m ranges from $-\ell$ to $+\ell$ in integer steps. The eigenvalues of $L_{\pm}$ can also be found to satisfy

$$L_{\pm}|\ell m\rangle = \hbar\sqrt{(\ell \mp m)(\ell \pm m + 1)}\,|\ell, m \pm 1\rangle \tag{2}$$

When dealing with vector wave functions (as opposed to scalar ones) in two dimensions, we found that a quantity J_z is the generator of infinitesimal rotations about the z axis, where

$$J_z = L_z + S_z \tag{3}$$

and the operator producing the rotation by ε_z is

$$U\left[R(\varepsilon_z \hat{\mathbf{z}})\right] = I - \frac{i\varepsilon_z}{\hbar} J_z \tag{4}$$

For a scalar wave function in three dimensions, we found that the properties of two successive rotations by ε_x about the x axis and ε_y about the y axis led to the commutations

$$[L_x, L_y] = i\hbar L_z \quad (5)$$
$$[L_y, L_z] = i\hbar L_x \quad (6)$$
$$[L_z, L_x] = i\hbar L_y \quad (7)$$

For a vector wave function, the rotation is generated by J_i rather than L_i but because the effects of rotations are the same, the J_i must have the same commutation relations, so that

$$[J_x, J_y] = i\hbar J_z \quad (8)$$
$$[J_y, J_z] = i\hbar J_x \quad (9)$$
$$[J_z, J_x] = i\hbar J_y \quad (10)$$

We can do the same analysis on J as we did above with L to define the raising and lowering operators

$$J_\pm \equiv J_x \pm i J_y \quad (11)$$

and get the same eigenvalue relations

$$J_\pm |jm\rangle = \hbar\sqrt{(j \mp m)(j \pm m + 1)}\, |j, m \pm 1\rangle \quad (12)$$

The three components of $\mathbf{J}$ are then J_z and

$$J_x = \frac{1}{2}(J_+ + J_-) \quad (13)$$
$$J_y = \frac{1}{2i}(J_+ - J_-) \quad (14)$$

Using these three equations, we can generate the matrix elements of the components of $\mathbf{J}$ in the orthonormal basis $|jm\rangle$ (that is, the basis consisting of eigenfunctions with total angular momentum number j and J_z number m). These matrix elements are

$$\langle j'm' | J_x | jm \rangle = \frac{1}{2}\langle j'm' | J_+ + J_- | jm \rangle \quad (15)$$
$$= \frac{\hbar}{2}\sqrt{(j-m)(j+m+1)}\,\langle j'm' | j, m+1 \rangle + \quad (16)$$
$$\frac{\hbar}{2}\sqrt{(j+m)(j-m+1)}\,\langle j'm' | j, m-1 \rangle \quad (17)$$
$$= \frac{\hbar}{2}\left[\sqrt{(j-m)(j+m+1)}\delta_{j'j}\delta_{m',m+1} + \sqrt{(j+m)(j-m+1)}\delta_{j'j}\delta_{m',m-1}\right] \quad (18)$$

$$\left\langle j'm' \left| J_y \right| jm \right\rangle = \frac{1}{2i} \left\langle j'm' \left| J_+ - J_- \right| jm \right\rangle \tag{19}$$

$$= \frac{\hbar}{2i} \sqrt{(j-m)(j+m+1)} \left\langle j'm' \left| j, m+1 \right. \right\rangle - \tag{20}$$

$$\frac{\hbar}{2i} \sqrt{(j+m)(j-m+1)} \left\langle j'm' \left| j, m-1 \right. \right\rangle \tag{21}$$

$$= \frac{\hbar}{2i} \left[\sqrt{(j-m)(j+m+1)} \delta_{j'j} \delta_{m',m+1} - \sqrt{(j+m)(j-m+1)} \delta_{j'j} \delta_{m',m-1} \right] \tag{22}$$

$$\left\langle j'm' \left| J_z \right| jm \right\rangle = m\hbar \delta_{j'j} \delta_{m',m} \tag{23}$$

The full matrix for each component J_i is actually infinite-dimensional, since j can be any half-integer from 0 up to infinity. However, the sub-matrix for each value of j is completely orthogonal to all other sub-matrices with different j values, so the complete matrix for each J_i is block-diagonal. Shankar gives the matrices for J_x and J_y up to $j = 1$ in his equations 12.5.23 and 12.5.24. This means that the commutation relations 9 should be obeyed for each set of sub-matrices corresponding to a particular j value.

For $j = \frac{1}{2}$ we have for the 3 sub-matrices (we can copy these from Shankar or use the above formulas to work them out). The values of m are $+\frac{1}{2}$ and $-\frac{1}{2}$ in that order, from top to bottom and left to right.

$$J_x^{(1/2)} = \frac{\hbar}{2} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \tag{24}$$

$$J_y^{(1/2)} = \frac{\hbar}{2i} \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \tag{25}$$

$$= \frac{i\hbar}{2} \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} \tag{26}$$

$$\left[J_x^{(1/2)}, J_y^{(1/2)} \right] = \frac{i\hbar^2}{4} \left(\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} - \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix} \right) \tag{27}$$

$$\frac{i\hbar^2}{2} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \tag{28}$$

$$= i\hbar J_z^{(1/2)} \tag{29}$$

For $j = 1$ we have for the 3 sub-matrices

$$J_x^{(1)} = \frac{\hbar}{\sqrt{2}} \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \tag{30}$$

$$J_y^{(1)} = \frac{i\hbar}{\sqrt{2}} \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & -1 \\ 0 & 1 & 0 \end{bmatrix} \tag{31}$$

$$\left[J_x^{(1)}, J_y^{(1)}\right] = \frac{i\hbar^2}{2} \left(\begin{bmatrix} 1 & 0 & -1 \\ 0 & 0 & 0 \\ 1 & 0 & -1 \end{bmatrix} - \begin{bmatrix} -1 & 0 & -1 \\ 0 & 0 & 0 \\ 1 & 0 & 1 \end{bmatrix} \right) \tag{32}$$

$$= i\hbar^2 \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix} \tag{33}$$

$$= i\hbar J_z^{(1)} \tag{34}$$

For $j = \frac{3}{2}$ we need to work out the matrices from the formulas above for the matrix elements. Ordering the values of $m = \frac{3}{2}, \frac{1}{2}, -\frac{1}{2}, \frac{3}{2}$ from left to right (columns) and top to bottom (rows), we get

$$J_x^{(3/2)} = \frac{\hbar}{2}\begin{bmatrix} 0 & \sqrt{3} & 0 & 0 \\ \sqrt{3} & 0 & 2 & 0 \\ 0 & 2 & 0 & \sqrt{3} \\ 0 & 0 & \sqrt{3} & 0 \end{bmatrix} \tag{35}$$

$$J_y^{(3/2)} = \frac{\hbar}{2i}\begin{bmatrix} 0 & \sqrt{3} & 0 & 0 \\ -\sqrt{3} & 0 & 2 & 0 \\ 0 & -2 & 0 & \sqrt{3} \\ 0 & 0 & -\sqrt{3} & 0 \end{bmatrix} \tag{36}$$

$$= \frac{i\hbar}{2}\begin{bmatrix} 0 & -\sqrt{3} & 0 & 0 \\ \sqrt{3} & 0 & -2 & 0 \\ 0 & 2 & 0 & -\sqrt{3} \\ 0 & 0 & \sqrt{3} & 0 \end{bmatrix} \tag{37}$$

$$\left[J_x^{(3/2)}, J_y^{(3/2)}\right] = \frac{i\hbar^2}{4}\left(\begin{bmatrix} 3 & 0 & -2\sqrt{3} & 0 \\ 0 & 1 & 0 & -2\sqrt{3} \\ 2\sqrt{3} & 0 & -1 & 0 \\ 0 & 2\sqrt{3} & 0 & -3 \end{bmatrix} - \begin{bmatrix} -3 & 0 & -2\sqrt{3} & 0 \\ 0 & -1 & 0 & -2\sqrt{3} \\ 2\sqrt{3} & 0 & 1 & 0 \\ 0 & 2\sqrt{3} & 0 & 3 \end{bmatrix}\right) \tag{38}$$

$$= i\hbar^2\begin{bmatrix} \frac{3}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & -\frac{1}{2} & 0 \\ 0 & 0 & 0 & -\frac{3}{2} \end{bmatrix} \tag{39}$$

$$= i\hbar J_z^{(3/2)} \tag{40}$$

Thus the commutation relation $[J_x, J_y] = i\hbar J_z$ is satisfied for these three sets of sub-matrices.

PINGBACKS

Pingback: angular momentum in 3-d expectation values and uncertainty principle

Pingback: total angular momentum finite rotations

ANGULAR MOMENTUM IN 3-D EXPECTATION VALUES AND UNCERTAINTY PRINCIPLE

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Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 12, Exercise 12.5.3.

Post date: 25 May 2017

[If some equations are too small to read easily, use your browser's magnifying option (Ctrl + on Chrome, probably something similar on other browsers).]

For 3-d angular momentum, we've seen that the components J_x and J_y can be written in terms of raising and lowering operators

$$J_\pm \equiv J_x \pm iJ_y \tag{1}$$

In the basis of eigenvectors of J^2 and J_z (that is, the states $|jm\rangle$) the raising and lowering operators have the following effects:

$$J_\pm |jm\rangle = \hbar\sqrt{(j\mp m)(j\pm m+1)}\,|j,m\pm 1\rangle \tag{2}$$

We can use these relations to construct the matrix elements of J_x and J_y in this basis. We can also use these relations to work out expectation values and uncertainties for the angular momentum components in this basis.

First, since diagonals of both the J_x and J_y matrices have only zero elements,

$$\langle J_x\rangle = \langle jm|J_x|jm\rangle = 0 \tag{3}$$

$$\langle J_y\rangle = \langle jm|J_y|jm\rangle = 0 \tag{4}$$

To work out $\langle J_x^2\rangle$ and $\langle J_y^2\rangle$, we can write these operators in terms of the raising and lowering operators:

$$J_x = \frac{1}{2}(J_+ + J_-) \tag{5}$$

$$J_y = \frac{1}{2i}(J_+ - J_-) \tag{6}$$

We can then use the fact that the basis states are orthonormal, so that

$$\langle j'm'|jm\rangle = \delta_{j'j}\delta_{m'm} \tag{7}$$

The required squares are

$$J_x^2 = \frac{1}{4}\left(J_+^2 + J_+J_- + J_-J_+ + J_-^2\right) \tag{8}$$

$$J_y^2 = -\frac{1}{4}\left(J_+^2 - J_+J_- - J_-J_+ + J_-^2\right) \tag{9}$$

$$= \frac{1}{4}\left(-J_+^2 + J_+J_- + J_-J_+ - J_-^2\right) \tag{10}$$

The diagonal matrix elements $\left\langle jm\left|J_x^2\right|jm\right\rangle$ and $\left\langle jm\left|J_y^2\right|jm\right\rangle$ will get non-zero contributions only from those terms that leave j and m unchanged when operating on $|jm\rangle$. This means that only the terms that contain an equal number of J_+ and J_- terms will contribute. We therefore have

$$\left\langle jm\left|J_x^2\right|jm\right\rangle = \frac{1}{4}\left\langle jm\left|J_+J_- + J_-J_+\right|jm\right\rangle \tag{11}$$

$$= \frac{\hbar}{4}\sqrt{(j+m)(j-m+1)}\left\langle jm\left|J_+\right|j,m-1\right\rangle + \tag{12}$$

$$\frac{\hbar}{4}\sqrt{(j-m)(j+m+1)}\left\langle jm\left|J_-\right|j,m+1\right\rangle \tag{13}$$

$$= \frac{\hbar^2}{4}\sqrt{(j+m)(j-m+1)}\sqrt{(j-m+1)(j+m)} + \tag{14}$$

$$\frac{\hbar^2}{4}\sqrt{(j-m)(j+m+1)}\sqrt{(j+m+1)(j-m)} \tag{15}$$

$$= \frac{\hbar^2}{4}\left((j+m)(j-m+1) + (j-m)(j+m+1)\right) \tag{16}$$

$$= \frac{\hbar^2}{4}\left(j^2 - m^2 + j + m + j^2 - m^2 + j - m\right) \tag{17}$$

$$= \frac{\hbar^2}{2}\left(j(j+1) - m^2\right) \tag{18}$$

From 10 we see that the only terms that contribute to $\left\langle jm\left|J_y^2\right|jm\right\rangle$ are the same as the corresponding terms in $\left\langle jm\left|J_x^2\right|jm\right\rangle$, so the result is the same:

$$\left\langle jm\left|J_y^2\right|jm\right\rangle = \frac{\hbar^2}{2}\left(j(j+1) - m^2\right) \tag{19}$$

We can check that J_x and J_y satisfy the uncertainty principle, as derived by Shankar. That is, we want to verify that

$$\Delta J_x \cdot \Delta J_y \geq \left|\left\langle jm\left|\left(J_x - \langle J_x\rangle\right)\left(J_y - \langle J_y\rangle\right)\right|jm\right\rangle\right| \tag{20}$$

On the LHS

$$\Delta J_x = \sqrt{\langle J_x^2\rangle - \langle J_x\rangle^2} \tag{21}$$

$$= \sqrt{\langle J_x^2\rangle} \tag{22}$$

$$= \sqrt{\frac{\hbar^2}{2}\left(j\left(j+1\right)-m^2\right)} \tag{23}$$

$$\Delta J_y = \sqrt{\frac{\hbar^2}{2}\left(j\left(j+1\right)-m^2\right)} \tag{24}$$

$$\Delta J_x \cdot \Delta J_y = \frac{\hbar^2}{2}\left(j\left(j+1\right)-m^2\right) \tag{25}$$

On the RHS

$$\left|\langle jm\left|\left(J_x - \langle J_x\rangle\right)\left(J_y - \langle J_y\rangle\right)\right|jm\rangle\right| = \left|\langle jm\left|J_xJ_y\right|jm\rangle\right| \tag{26}$$

Using the same technique as that above for deriving $\left\langle jm\left|J_x^2\right|jm\right\rangle$ we have

$$\langle jm\left|J_xJ_y\right|jm\rangle = \frac{1}{4i}\langle jm\left|\left(J_+ + J_-\right)\left(J_+ - J_-\right)\right|jm\rangle \tag{27}$$

$$= \frac{1}{4i}\langle jm\left|J_-J_+ - J_+J_-\right|jm\rangle \tag{28}$$

$$= \frac{\hbar^2}{4i}\left(\left(j-m\right)\left(j+m+1\right) - \left(j+m\right)\left(j-m+1\right)\right) \tag{29}$$

$$= -\frac{\hbar^2 m}{2i} \tag{30}$$

We therefore need to verify that

$$j\left(j+1\right) - m^2 \geq |m| \tag{31}$$

for all allowed values of m. We know that $-j \leq m \leq +j$, so

$$j\left(j+1\right) - m^2 \geq j^2 + j - j^2 = j \geq |m| \tag{32}$$

Thus the inequality is indeed satisfied.
In the case $|m| = j$ we have

$$j\left(j+1\right) - j^2 = j = |m| \tag{33}$$

so the inequality saturates (becomes an equality) in that case.

TOTAL ANGULAR MOMENTUM FINITE ROTATIONS

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 12, Exercises 12.5.4 - 12.5.5.

Post date: 29 May 2017

[If some equations are too small to read easily, use your browser's magnifying option (Ctrl + on Chrome, probably something similar on other browsers).]

For infinitesimal 3-d rotations, we've seen that the generator is $\hat{\boldsymbol{\theta}} \cdot \mathbf{L}$ where $\hat{\boldsymbol{\theta}}$ is a unit vector along the axis of rotation. Generalizing this to the total angular momentum $\mathbf{J}$ we have the operator for a general 3-d rotation through an infinitesimal angle:

$$U\left[R\left(\delta\boldsymbol{\theta}\right)\right] = I - \frac{i\delta\boldsymbol{\theta} \cdot \mathbf{J}}{\hbar} \tag{1}$$

In principle 'all' we need to do to get the operator for a finite 3-d rotation is take the exponential, in the form

$$e^{-i\boldsymbol{\theta}\cdot\mathbf{J}/\hbar} \tag{2}$$

The problem is that in this case, $\mathbf{J}$ is infinite dimensional, so the exponential of such a matrix cannot be calculated. However, because the components of $\mathbf{J}$ are block diagonal (see Shankar's equations 12.5.23 and 12.5.24), all powers of these components are also block diagonal, and thus so is the exponential. For a given value of the total momentum quantum number j, the corresponding block is a $(2j+1) \times (2j+1)$ sub-matrix $J_i^{(j)}$ (where the suffix i refers to x, y or z), so the block in the exponential, defined as $D^{(j)}\left[R\left(\boldsymbol{\theta}\right)\right]$ is calculated as

$$D^{(j)}\left[R\left(\boldsymbol{\theta}\right)\right] = \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{-i\theta}{\hbar}\right)^n \left(\hat{\boldsymbol{\theta}} \cdot \mathbf{J}\right)^n \tag{3}$$

This may still look pretty hopeless in terms of actual calculation, but for small values of j, we can actually get closed-form solutions.

First, we look at the eigenvalues of $\hat{\boldsymbol{\theta}} \cdot \mathbf{J}$. If we review the calculations by which we found that the eigenvalues of L_z (and thus also J_z) were $-j, -j+1, \ldots, j-1, j$ (multiplied by $\hbar$), we see that there's nothing special about the fact that we chose the z direction over any other direction

as the component of **J** for which we calculated the eigenvalues. We could, for example, go through exactly the same calculations taking L_x to be the chosen component. We would then define raising and lowering operators as $J_\pm = J_y \pm iJ_z$ and come out with the conclusion that the eigenvalues of L_x are also $-j, -j+1, \ldots, j-1, j$ (multiplied by $\hbar$). We can generalize even further and choose the 'special' direction to be the axis of rotation, however that axis may be oriented in space. This would lead us to the conclusion that the eigenvalues of $\hat{\boldsymbol{\theta}} \cdot \mathbf{J}$ are the same as those of J_z.

Now consider the operator (where $J \equiv \hat{\boldsymbol{\theta}} \cdot \mathbf{J}$):

$$(J - j\hbar)(J - (j-1)\hbar)(J - (j-2)\hbar)\ldots(J + (j-1)\hbar)(J + j\hbar) \quad (4)$$

First, suppose that $J = J_z$ (so that $\hat{\boldsymbol{\theta}}$ is along the z axis). Then if we're in an eigenstate $|jm\rangle$ of J_z, the term $(J - m\hbar)$ in this operator will give zero when operating on this state. Thus the operator 4 will always give zero when operating on an eigenstate of J_z. However, since the set of eigenstates of J_z span the space in which the total angular momentum number is j, any state in this space can be expressed as a linear combination of eigenstates of J_z, so when 4 operates on this state, there is always one factor in the operator that gives zero for each term in the linear combination. Thus this operator *always* gives zero when operating on any state with angular momentum j. [Note that the order in which we write the factors in 4 doesn't matter; the only operator in the expression is J, so all the factors commute with each other.] That is, we have

$$(J - j\hbar)(J - (j-1)\hbar)(J - (j-2)\hbar)\ldots(J + (j-1)\hbar)(J + j\hbar) = 0 \quad (5)$$

If we multiply out this operator, we get a polynomial of degree $2j+1$ in J. The highest power can thus be written as a linear combination of lower powers:

$$J^{2j+1} = \sum_{n=0}^{2j} a_n J^n \quad (6)$$

where the coefficients a_n can be found by expanding the formula (which we won't need to do here). But this implies that all higher powers of J can also be written as linear combinations of powers up to J^{2j}. To see this, consider

$$
\begin{aligned}
J^{2j+2} &= J \times J^{2j+1} && (7)\\
&= \sum_{n=0}^{2j} a_n J^{n+1} && (8)\\
&= \sum_{n=1}^{2j} a_{n-1} J^n + a_{2j} J^{2j+1} && (9)\\
&= \sum_{n=1}^{2j} a_{n-1} J^n + a_{2j} \sum_{n=0}^{2j} a_n J^n && (10)
\end{aligned}
$$

Thus J^{2j+2} can be written as a linear combination of powers of J up to J^{2j}. By iterating this process, we can express all higher powers of J as a linear combination of powers of J up to J^{2j}. Here are a couple of examples. [Shankar marks these as 'hard', though I can't see that they are any more difficult than most of his other problems, so hopefully I'm not missing anything.]

Consider $D^{(1/2)}[R]$, starting from 3. We first use 5 with $j = \frac{1}{2}$:

$$
\begin{aligned}
\left(J - \frac{\hbar}{2}\right)\left(J + \frac{\hbar}{2}\right) &= 0 && (11)\\
J^2 &= \frac{\hbar^2}{4} && (12)
\end{aligned}
$$

We can now iterate this formula as described above to get (to be accurate, all the I and J terms should have a superscript $(1/2)$ to indicate that they refer to the subspace with $j = \frac{1}{2}$, but this would clutter the notation).

$$
\begin{aligned}
J^0 &= I && (13)\\
J^1 &= J && (14)\\
J^2 &= \left(\frac{\hbar}{2}\right)^2 I && (15)\\
J^3 &= \left(\frac{\hbar}{2}\right)^2 J && (16)\\
J^4 &= \left(\frac{\hbar}{2}\right)^4 I && (17)\\
&\vdots && (18)
\end{aligned}
$$

From 3 we have

$$D^{(1/2)}[R] = \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{-i\theta}{\hbar} \right)^n J^n \tag{19}$$

We can consider the even and odd terms in this sum separately. For the evens:

$$\left(D^{(1/2)}[R] \right)_{even} = \sum_{n\,even} \frac{1}{n!} \left(\frac{-i\theta}{\hbar} \right)^n \left(\frac{\hbar}{2} \right)^n I \tag{20}$$

$$= \sum_{n\,even} \frac{1}{n!} \left(\frac{-i\theta}{2} \right)^n I \tag{21}$$

$$= \left[1 - \left(\frac{\theta}{2} \right)^2 \frac{1}{2!} + \left(\frac{\theta}{2} \right)^4 \frac{1}{4!} - \ldots \right] I \tag{22}$$

$$= I \cos \frac{\theta}{2} \tag{23}$$

For the odds:

$$\left(D^{(1/2)}[R] \right)_{odd} = \sum_{n\,odd} \frac{1}{n!} \left(\frac{-i\theta}{\hbar} \right)^n \left(\frac{\hbar}{2} \right)^{n-1} J \tag{24}$$

$$= \frac{2J}{\hbar} \sum_{n\,odd} \frac{(-i)^n}{n!} \left(\frac{\theta}{2} \right)^n \tag{25}$$

$$= \frac{2J}{\hbar} \left[-\frac{\theta}{2} i + \left(\frac{\theta}{2} \right)^3 \frac{i}{3!} - \left(\frac{\theta}{2} \right)^5 \frac{i}{5!} + \ldots \right] \tag{26}$$

$$= -\frac{2iJ}{\hbar} \sin \frac{\theta}{2} \tag{27}$$

Thus we get

$$D^{(1/2)}[R] = I \cos \frac{\theta}{2} - \frac{2iJ}{\hbar} \sin \frac{\theta}{2} \tag{28}$$

$$= I^{(1/2)} \cos \frac{\theta}{2} - \frac{2i\hat{\boldsymbol{\theta}} \cdot \mathbf{J}^{(1/2)}}{\hbar} \sin \frac{\theta}{2} \tag{29}$$

(I've restored the superscript $(1/2)$.)
Going through the same process for $j = 1$, we first look at 5 to get

$$(J - \hbar) J (J + \hbar) = 0 \tag{30}$$

$$J^3 = \hbar^2 J \tag{31}$$

Again, by iterating we find the pattern:

$$\begin{aligned} J^0 &= I && (32)\\ J^1 &= J && (33)\\ J^2 &= J^2 && (34)\\ J^3 &= \hbar^2 J && (35)\\ J^4 &= \hbar^2 J^2 && (36)\\ &\vdots && (37) \end{aligned}$$

We then have

$$D^{(1)}[R] = \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{-i\theta}{\hbar} \right)^n J^n \tag{38}$$

Again, we can consider evens and odds separately:

$$\begin{aligned} \left(D^{(1)}[R] \right)_{even} &= \sum_{n\,even} \frac{1}{n!} \left(\frac{-i\theta}{\hbar} \right)^n J^n && (39)\\ &= I + \sum_{n=2,4,\ldots} \frac{1}{n!} \left(\frac{-i\theta}{\hbar} \right)^n \hbar^{n-2} J^2 && (40)\\ &= I + \frac{J^2}{\hbar^2} \sum_{n=2,4,\ldots} \frac{(-i\theta)^n}{n!} && (41)\\ &= I + \frac{J^2}{\hbar^2} (\cos\theta - 1) && (42) \end{aligned}$$

For the odds:

$$\begin{aligned} \left(D^{(1)}[R] \right)_{even} &= \sum_{n\,odd} \frac{1}{n!} \left(\frac{-i\theta}{\hbar} \right)^n \hbar^{n-1} J && (43)\\ &= \frac{J}{\hbar} \sum_{n\,odd} \frac{(-i\theta)^n}{n!} && (44)\\ &= -\frac{iJ}{\hbar} \sin\theta && (45) \end{aligned}$$

We have

$$D^{(1)}[R] = I + \frac{J^2}{\hbar^2}(\cos\theta - 1) - \frac{iJ}{\hbar}\sin\theta \tag{46}$$

$$= I^{(1)} + \frac{\left(\hat{\boldsymbol{\theta}}\cdot\mathbf{J}^{(1)}\right)^2}{\hbar^2}(\cos\theta - 1) - \frac{i\hat{\boldsymbol{\theta}}\cdot\mathbf{J}^{(1)}}{\hbar}\sin\theta \tag{47}$$

[I'm not sure why Shankar restricts this problem to the x axis, or, for that matter, why he expects us to use the matrix for J_x.]

PINGBACKS

Pingback: rotations in 3-d classical and quantum rotations compared
Pingback: rotations in 3-d euler angles
Pingback: spherical harmonics: rotation about the x axis
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Pingback: Spherical tensor operators; commutators
Pingback: Spherical tensor operators; a scalar operator

ROTATIONS IN 3-D CLASSICAL AND QUANTUM ROTATIONS COMPARED

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 12, Exercise 12.5.6.

Post date: 31 May 2017

[If some equations are too small to read easily, use your browser's magnifying option (Ctrl + on Chrome, probably something similar on other browsers).]

This is an example of how risky it can be to attempt to derive quantum behaviour by using logic based on classical mechanics. In classical mechanics, if we have a system with some total angular momentum with magnitude $|\mathbf{J}|$ and rotate this sytem through any angle, the magnitude of the angular momentum remains the same (although, of course, its direction changes). Based on this fact, we might think that if we start with a quantum state such as $|jm\rangle$ (where j is the total angular momentum number and m is the number for J_z), we should be able to obtain the other states with the same total angular momentum number j by rotating this state through various angles about the appropriate rotation axis. To see that this won't work, suppose we consider a state with $j = 1$ and $m = 1$, that is $|jm\rangle = |11\rangle$. Classically, such a system has its angular momentum aligned along the z axis, so we might think that if we rotate this system by $\frac{\pi}{2}$ about, say, the x axis, we should get a state with $m = 0$, since the angular momentum is now aligned along the $-y$ axis.

To see if this works, we can use the formula for a finite rotation for a $j = 1$ state. Since j remains constant, a rotation of a state $|jm\rangle$ is given by

$$D^{(1)}[R]\,|jm\rangle \tag{1}$$

where

$$D^{(1)}[R] = I^{(1)} + \frac{\left(\hat{\boldsymbol{\theta}}\cdot\mathbf{J}^{(1)}\right)^2}{\hbar^2}(\cos\theta - 1) - \frac{i\hat{\boldsymbol{\theta}}\cdot\mathbf{J}^{(1)}}{\hbar}\sin\theta \tag{2}$$

For a rotation by an angle θ about the x axis, this formula reduces to

$$D^{(1)}\left[R\left(\theta\hat{\mathbf{x}}\right)\right] = I^{(1)} + \frac{\left(J_x^{(1)}\right)^2}{\hbar^2}\left(\cos\theta - 1\right) - \frac{iJ_x^{(1)}}{\hbar}\sin\theta \tag{3}$$

We can copy the matrix $J_x^{(1)}$ from Shankar's equation 12.5.23:

$$J_x^{(1)} = \frac{\hbar}{\sqrt{2}}\begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \tag{4}$$

We therefore have

$$\left(J_x^{(1)}\right)^2 = \frac{\hbar^2}{2}\begin{bmatrix} 1 & 0 & 1 \\ 0 & 2 & 0 \\ 1 & 0 & 1 \end{bmatrix} \tag{5}$$

Plugging these into 3 we have

$$D^{(1)}\left[R\left(\theta\hat{\mathbf{x}}\right)\right] = \frac{1}{2}\begin{bmatrix} 1+\cos\theta & -\sqrt{2}i\sin\theta & \cos\theta - 1 \\ -\sqrt{2}i\sin\theta & 2\cos\theta & -\sqrt{2}i\sin\theta \\ \cos\theta - 1 & -\sqrt{2}i\sin\theta & 1+\cos\theta \end{bmatrix} \tag{6}$$

In the $|jm\rangle$ basis, the state $|11\rangle$ is represented by

$$|11\rangle = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \tag{7}$$

Thus a rotation about the x axis rotates this state into:

$$|\psi\rangle = D^{(1)}\left[R\left(\theta\hat{\mathbf{x}}\right)\right]|11\rangle \tag{8}$$

$$= \frac{1}{2}\begin{bmatrix} 1+\cos\theta & -\sqrt{2}i\sin\theta & \cos\theta - 1 \\ -\sqrt{2}i\sin\theta & 2\cos\theta & -\sqrt{2}i\sin\theta \\ \cos\theta - 1 & -\sqrt{2}i\sin\theta & 1+\cos\theta \end{bmatrix}\begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \tag{9}$$

$$= \frac{1}{2}\begin{bmatrix} 1+\cos\theta \\ -\sqrt{2}i\sin\theta \\ \cos\theta - 1 \end{bmatrix} \tag{10}$$

If rotation by some angle θ could change $|11\rangle$ into the state $|10\rangle$, this result would need to be a multiple of $\begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}$, so we'd need to find θ such that both of the following equations are true:

$$1+\cos\theta = 0 \quad (11)$$
$$\cos\theta-1 = 0 \quad (12)$$

This is impossible, so no rotation about the x axis can change $|11\rangle$ into the state $|10\rangle$.

However, there is still a correspondence between classical and quantum mechanics if we compare the *average* values of the components of **J**. That is, we want to find $\langle \mathbf{J} \rangle$ for the state 10. To do this, we need the other two matrix components $J_y^{(1)}$ and $J_z^{(1)}$. We can get $J_y^{(1)}$ from Shankar's equation 12.5.24:

$$J_y^{(1)} = \frac{i\hbar}{\sqrt{2}} \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & -1 \\ 0 & 1 & 0 \end{bmatrix} \quad (13)$$

$J_z^{(1)}$ is just the diagonal matrix:

$$J_z^{(1)} = \hbar \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix} \quad (14)$$

We can now calculate the averages for the state 10:

$$\left\langle J_x^{(1)} \right\rangle = \left\langle \psi \middle| J_x^{(1)} \middle| \psi \right\rangle \tag{15}$$

$$= \frac{\hbar}{4\sqrt{2}} \begin{bmatrix} 1+\cos\theta & \sqrt{2}i\sin\theta & \cos\theta-1 \end{bmatrix} \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} 1+\cos\theta \\ -\sqrt{2}i\sin\theta \\ \cos\theta-1 \end{bmatrix} \tag{16}$$

$$= \frac{\hbar}{4} \begin{bmatrix} i\sin\theta & \sqrt{2}\cos\theta & i\sin\theta \end{bmatrix} \begin{bmatrix} 1+\cos\theta \\ -\sqrt{2}i\sin\theta \\ \cos\theta-1 \end{bmatrix} \tag{17}$$

$$= 0 \tag{18}$$

$$\left\langle J_y^{(1)} \right\rangle = \left\langle \psi \middle| J_y^{(1)} \middle| \psi \right\rangle \tag{19}$$

$$= \frac{i\hbar}{4\sqrt{2}} \begin{bmatrix} 1+\cos\theta & \sqrt{2}i\sin\theta & \cos\theta-1 \end{bmatrix} \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & -1 \\ 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} 1+\cos\theta \\ -\sqrt{2}i\sin\theta \\ \cos\theta-1 \end{bmatrix} \tag{20}$$

$$= \frac{\hbar}{4} \begin{bmatrix} -\sin\theta & -i\sqrt{2} & \sin\theta \end{bmatrix} \begin{bmatrix} 1+\cos\theta \\ -\sqrt{2}i\sin\theta \\ \cos\theta-1 \end{bmatrix} \tag{21}$$

$$= -\hbar\sin\theta \tag{22}$$

$$\left\langle J_z^{(1)} \right\rangle = \left\langle \psi \middle| J_z^{(1)} \middle| \psi \right\rangle \tag{23}$$

$$= \frac{\hbar}{4} \begin{bmatrix} 1+\cos\theta & \sqrt{2}i\sin\theta & \cos\theta-1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix} \begin{bmatrix} 1+\cos\theta \\ -\sqrt{2}i\sin\theta \\ \cos\theta-1 \end{bmatrix} \tag{24}$$

$$= \frac{\hbar}{4} \begin{bmatrix} 1+\cos\theta & 0 & 1-\cos\theta \end{bmatrix} \begin{bmatrix} 1+\cos\theta \\ -\sqrt{2}i\sin\theta \\ \cos\theta-1 \end{bmatrix} \tag{25}$$

$$= \hbar\cos\theta \tag{26}$$

Thus for the average, we have

$$\langle \mathbf{J} \rangle = -\hbar\sin\theta\hat{\mathbf{y}} + \hbar\cos\theta\hat{\mathbf{z}} \tag{27}$$

In this case, a rotation by $\theta = \frac{\pi}{2}$ does indeed rotate $\langle \mathbf{J} \rangle$ so that it points along the $-y$ axis, just as it would in classical mechanics.

PINGBACKS

Pingback: rotations in 3-d euler angles

ROTATIONS IN 3-D EULER ANGLES

Link to: physicspages home page.

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Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 12, Exercise 12.5.7.

Post date: 31 May 2017

[If some equations are too small to read easily, use your browser's magnifying option (Ctrl + on Chrome, probably something similar on other browsers).]

Any 3-d rotation can be expressed in terms of the Euler angles. These angles specify a sequence of three successive rotations about the rectangular axes. There are various definitions of Euler angles involving different sets of rotations, but the set used by Shankar in this problem consists of (1) a rotation by γ about the z axis, followed by (2) a rotation by β about the y axis and concluding with (3) a rotation by α about the z axis. The proof that any rotation can be expressed this way would take us too far afield at this point, so we'll just accept this for now.

We can see how these work in quantum mechanics by considering the special case of $j = 1$, for which we derived the formula for a finite rotation here. A state $|\psi\rangle$ is transformed by a rotation $\boldsymbol{\theta}$ according to

$$\left|\psi'\right\rangle = D^{(1)}\left[R\right]|\psi\rangle \tag{1}$$

$$= \left[I^{(1)} + \frac{\left(\hat{\boldsymbol{\theta}}\cdot\mathbf{J}^{(1)}\right)^2}{\hbar^2}\left(\cos\theta - 1\right) - \frac{i\hat{\boldsymbol{\theta}}\cdot\mathbf{J}^{(1)}}{\hbar}\sin\theta \right]|\psi\rangle \tag{2}$$

For our purposes below, we'll need the three components of $\mathbf{J}^{(1)}$, which can be copied from Shankar's equations 12.5.23 and 12.5.24:

$$J_x^{(1)} = \frac{\hbar}{\sqrt{2}} \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \tag{3}$$

$$J_y^{(1)} = \frac{i\hbar}{\sqrt{2}} \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & -1 \\ 0 & 1 & 0 \end{bmatrix} \tag{4}$$

$$\left(J_y^{(1)}\right)^2 = \frac{\hbar^2}{2} \begin{bmatrix} 1 & 0 & -1 \\ 0 & 2 & 0 \\ -1 & 0 & 1 \end{bmatrix} \tag{5}$$

$$J_z^{(1)} = \hbar \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix} \tag{6}$$

$$\left(J_z^{(1)}\right)^2 = \hbar^2 \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \tag{7}$$

Evaluating 2 for the three Euler rotations, we have

$$D_\gamma = I^{(1)} + \frac{\left(J_z^{(1)}\right)^2}{\hbar^2}(\cos\gamma - 1) - \frac{iJ_z^{(1)}}{\hbar}\sin\gamma \tag{8}$$

$$= \begin{bmatrix} \cos\gamma - i\sin\gamma & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \cos\gamma + i\sin\gamma \end{bmatrix} \tag{9}$$

$$= \begin{bmatrix} e^{-i\gamma} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & e^{i\gamma} \end{bmatrix} \tag{10}$$

$$D_\beta = I^{(1)} + \frac{\left(J_y^{(1)}\right)^2}{\hbar^2}(\cos\beta - 1) - \frac{iJ_y^{(1)}}{\hbar}\sin\beta \tag{11}$$

$$= \frac{1}{2}\begin{bmatrix} 1+\cos\beta & -\sqrt{2}\sin\beta & 1-\cos\beta \\ \sqrt{2}\sin\beta & 2\cos\beta & -\sqrt{2}\sin\beta \\ 1-\cos\beta & \sqrt{2}\sin\beta & 1+\cos\beta \end{bmatrix} \tag{12}$$

$$D_\alpha = I^{(1)} + \frac{\left(J_z^{(1)}\right)^2}{\hbar^2}(\cos\alpha - 1) - \frac{iJ_z^{(1)}}{\hbar}\sin\alpha \tag{13}$$

$$= \begin{bmatrix} \cos\alpha - i\sin\alpha & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \cos\alpha + i\sin\alpha \end{bmatrix} \tag{14}$$

$$= \begin{bmatrix} e^{-i\alpha} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & e^{i\alpha} \end{bmatrix} \tag{15}$$

The complete rotation is the product of the three matrices:

$$D_{total} = D_\alpha D_\beta D_\gamma \tag{16}$$

$$= D_\alpha \frac{1}{2}\begin{bmatrix} (1+\cos\beta)\,e^{-i\gamma} & -\sqrt{2}\sin\beta & (1-\cos\beta)\,e^{i\gamma} \\ \sqrt{2}\sin\beta e^{-i\gamma} & 2\cos\beta & -\sqrt{2}\sin\beta e^{i\gamma} \\ (1-\cos\beta)\,e^{-i\gamma} & \sqrt{2}\sin\beta & (1+\cos\beta)\,e^{i\gamma} \end{bmatrix} \tag{17}$$

$$= \frac{1}{2}\begin{bmatrix} (1+\cos\beta)\,e^{-i\gamma}e^{-i\alpha} & -\sqrt{2}\sin\beta e^{-i\alpha} & (1-\cos\beta)\,e^{i\gamma}e^{-i\alpha} \\ \sqrt{2}\sin\beta e^{-i\gamma} & 2\cos\beta & -\sqrt{2}\sin\beta e^{i\gamma} \\ (1-\cos\beta)\,e^{-i\gamma}e^{i\alpha} & \sqrt{2}\sin\beta e^{i\alpha} & (1+\cos\beta)\,e^{i\gamma}e^{i\alpha} \end{bmatrix} \tag{18}$$

In the $|jm\rangle$ basis, the state $|11\rangle$ is represented by

$$|11\rangle = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \tag{19}$$

Applying the rotation 18 to this state, we get

$$\begin{aligned}
\left|11'\right\rangle &= D_{total}\,|11\rangle && (20)\\
&= \frac{1}{2}\begin{bmatrix} (1+\cos\beta)\,e^{-i\gamma}e^{-i\alpha} & -\sqrt{2}\sin\beta e^{-i\alpha} & (1-\cos\beta)\,e^{i\gamma}e^{-i\alpha} \\ \sqrt{2}\sin\beta e^{-i\gamma} & 2\cos\beta & -\sqrt{2}\sin\beta e^{i\gamma} \\ (1-\cos\beta)\,e^{-i\gamma}e^{i\alpha} & \sqrt{2}\sin\beta e^{i\alpha} & (1+\cos\beta)\,e^{i\gamma}e^{i\alpha} \end{bmatrix}\begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} && (21)\\
&= \frac{1}{2}\begin{bmatrix} (1+\cos\beta)\,e^{-i\gamma}e^{-i\alpha} \\ \sqrt{2}\sin\beta e^{-i\gamma} \\ (1-\cos\beta)\,e^{-i\gamma}e^{i\alpha} \end{bmatrix} && (22)\\
&= \frac{e^{-i\gamma}}{2}\begin{bmatrix} (1+\cos\beta)\,e^{-i\alpha} \\ \sqrt{2}\sin\beta \\ (1-\cos\beta)\,e^{i\alpha} \end{bmatrix} && (23)
\end{aligned}$$

We can work out the average values of the components of **J** in the rotated state in the same way as in the previous problem, by using 3, 4 and 6. Note that γ disappears from the matrix elements as it enters only in an overall phase factor. We get (I used Maple to do the tedious matrix multiplications):

$$\langle J_x \rangle = \langle 11' | J_x | 11' \rangle \tag{24}$$

$$= \frac{\hbar}{4\sqrt{2}} \begin{bmatrix} (1+\cos\beta)\, e^{i\alpha} & \sqrt{2}\sin\beta & (1-\cos\beta)\, e^{-i\alpha} \end{bmatrix} \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} (1+\cos\beta)\, e^{-i\alpha} \\ \sqrt{2}\sin\beta \\ (1-\cos\beta)\, e^{i\alpha} \end{bmatrix} \tag{25}$$

$$= \hbar \sin\beta \cos\alpha \tag{26}$$

$$\langle J_y \rangle = \langle 11' | J_y | 11' \rangle \tag{27}$$

$$= \frac{i\hbar}{4\sqrt{2}} \begin{bmatrix} (1+\cos\beta)\, e^{i\alpha} & \sqrt{2}\sin\beta & (1-\cos\beta)\, e^{-i\alpha} \end{bmatrix} \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & -1 \\ 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} (1+\cos\beta)\, e^{-i\alpha} \\ \sqrt{2}\sin\beta \\ (1-\cos\beta)\, e^{i\alpha} \end{bmatrix} \tag{28}$$

$$= \hbar \sin\beta \sin\alpha \tag{29}$$

$$\langle J_z \rangle = \langle 11' | J_z | 11' \rangle \tag{30}$$

$$= \frac{\hbar}{4} \begin{bmatrix} (1+\cos\beta)\, e^{i\alpha} & \sqrt{2}\sin\beta & (1-\cos\beta)\, e^{-i\alpha} \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix} \begin{bmatrix} (1+\cos\beta)\, e^{-i\alpha} \\ \sqrt{2}\sin\beta \\ (1-\cos\beta)\, e^{i\alpha} \end{bmatrix} \tag{31}$$

$$= \hbar \cos\beta \tag{32}$$

Going back to 23, we can confirm our earlier result that it is impossible to rotate the state $|11\rangle$ into just $|10\rangle$. To do so, the state in 23 would have to be a multiple of $\begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}$ which could happen only if both $1+\cos\beta$ and $1-\cos\beta$ were zero, which is impossible.

However, if we take $\beta = \pi$, then the rotated state 23 becomes

$$\left|11'\right\rangle = e^{i(\alpha-\gamma)} \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} = e^{i(\alpha-\gamma)} |1,-1\rangle \tag{33}$$

so apart from a phase factor, it is possible to rotate one eigenstate of J_z into another.

The only values of β that produce zero elements in 23 are $\beta = 0$ and $\beta = \pi$, (the values of α and γ produce only phase factors), so for any other value of β, all three elements of 23 are non-zero. Thus a general rotation from any starting state can always be made to produce a rotated state containing all three eigenstates of J_z: $|11\rangle$, $|10\rangle$ and $|1,-1\rangle$.

ANGULAR MOMENTUM RAISING AND LOWERING OPERATORS FROM RECTANGULAR COORDINATES

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Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 12, Exercise 12.5.8.

Post date: 3 Jun 2017

[If some equations are too small to read easily, use your browser's magnifying option (Ctrl + on Chrome, probably something similar on other browsers).]

To calculate the eigenfunctions of angular momentum, we will need expressions for the raising and lowering operators $L_\pm$ in spherical coordinates. We've seen one way of getting these by working with the gradient in spherical coordinates from the start, but it is also possible to convert the rectangular forms of $L_\pm$ to spherical coordinates by using the chain rule from calculus. This method is similar to one we used earlier in 2-d. To set the scene, we need the conversion formulas between rectangular and spherical coordinates:

$$
\begin{aligned}
x &= r\sin\theta\cos\phi && (1)\\
y &= r\sin\theta\sin\phi && (2)\\
z &= r\cos\theta && (3)\\
r &= \sqrt{x^2+y^2+z^2} && (4)\\
\theta &= \arctan\frac{\sqrt{x^2+y^2}}{z} && (5)\\
&= \arctan\frac{q}{z} && (6)\\
\phi &= \arctan\frac{y}{x} && (7)
\end{aligned}
$$

To simplify the notation, we've defined

$$q \equiv \sqrt{x^2+y^2} = r\sin\theta \tag{8}$$

We'll also use shorthand notation for sines and cosines so that

$$s_\theta \equiv \sin\theta \tag{9}$$
$$c_\theta \equiv \cos\theta \tag{10}$$

and similarly for ϕ. We'll also use the notation ∂_r to mean the partial derivative with respect to r, with a similar notation for other derivatives.

The required derivatives are

$$\partial_x = \partial_x r \cdot \partial_r + \partial_x \theta \cdot \partial_\theta + \partial_x \phi \cdot \partial_\phi \tag{11}$$
$$\partial_y = \partial_y r \cdot \partial_r + \partial_y \theta \cdot \partial_\theta + \partial_y \phi \cdot \partial_\phi \tag{12}$$
$$\partial_z = \partial_z r \cdot \partial_r + \partial_z \theta \cdot \partial_\theta \tag{13}$$

The required derivatives are

$$\partial_x r = \frac{x}{r} \tag{14}$$
$$\partial_y r = \frac{y}{r} \tag{15}$$
$$\partial_z r = \frac{z}{r} \tag{16}$$
$$\partial_x \theta = \frac{x/q}{z\left(1+\frac{q^2}{z^2}\right)} \tag{17}$$
$$= \frac{xz}{qr^2} \tag{18}$$
$$\partial_y \theta = \frac{yz}{qr^2} \tag{19}$$
$$\partial_z \theta = -\frac{q}{r^2} \tag{20}$$
$$\partial_x \phi = \frac{-y/x^2}{1+y^2/x^2} \tag{21}$$
$$= -\frac{y}{q^2} \tag{22}$$
$$\partial_y \phi = \frac{x}{q^2} \tag{23}$$
$$\partial_z \phi = 0 \tag{24}$$

Plugging all these into 11 to 13 we have

$$\partial_x = \frac{x}{r}\partial_r + \frac{xz}{qr^2}\partial_\theta - \frac{y}{q^2}\partial_\phi \tag{25}$$

$$\partial_y = \frac{y}{r}\partial_r + \frac{yz}{qr^2}\partial_\theta + \frac{x}{q^2}\partial_\phi \tag{26}$$

$$\partial_z = \frac{z}{r}\partial_r - \frac{q}{r^2}\partial_\theta \tag{27}$$

We can now calculate the components L_x and L_y:

$$L_x = -i\hbar\left(y\partial_z - z\partial_y\right) \tag{28}$$

$$= -i\hbar\left[\frac{yz}{r}\partial_r - \frac{yq}{r^2}\partial_\theta - \frac{yz}{r}\partial_r - \frac{yz^2}{qr^2}\partial_\theta - \frac{xz}{q^2}\partial_\phi\right] \tag{29}$$

$$= i\hbar\left[\left(\frac{yq}{r^2} + \frac{yz^2}{qr^2}\right)\partial_\theta + \frac{xz}{q^2}\partial_\phi\right] \tag{30}$$

$$= i\hbar\left[\left(s_\theta^2 s_\phi + \frac{s_\theta s_\phi c_\theta^2}{s_\theta}\right)\partial_\theta + \frac{s_\theta c_\theta c_\phi}{s_\theta^2}\partial_\phi\right] \tag{31}$$

$$= i\hbar\left(\sin\phi\frac{\partial}{\partial\theta} + \cos\phi\cot\theta\frac{\partial}{\partial\phi}\right) \tag{32}$$

$$L_y = -i\hbar\left(z\partial_x - x\partial_z\right) \tag{33}$$

$$= -i\hbar\left[\frac{xz}{r}\partial_r + \frac{xz^2}{qr^2}\partial_\theta - \frac{xz}{r}\partial_r + \frac{xq}{r^2}\partial_\theta - \frac{yz}{q^2}\partial_\phi\right] \tag{34}$$

$$= i\hbar\left[\left(-\frac{xz^2}{qr^2} - \frac{xq}{r^2}\right)\partial_\theta + \frac{yz}{q^2}\partial_\phi\right] \tag{35}$$

$$= i\hbar\left[\left(-\frac{s_\theta c_\phi c_\theta^2}{s_\theta} - s_\theta^2 c_\phi\right)\partial_\theta + \frac{s_\theta c_\theta s_\phi}{s_\theta^2}\partial_\phi\right] \tag{36}$$

$$= i\hbar\left(-\cos\phi\frac{\partial}{\partial\theta} + \sin\phi\cot\theta\frac{\partial}{\partial\phi}\right) \tag{37}$$

From this we get the raising and lowering operators

$$L_\pm = L_x \pm iL_y \tag{38}$$

$$= i\hbar\left(\sin\phi\frac{\partial}{\partial\theta} + \cos\phi\cot\theta\frac{\partial}{\partial\phi}\right) \mp \tag{39}$$

$$\hbar\left(-\cos\phi\frac{\partial}{\partial\theta} + \sin\phi\cot\theta\frac{\partial}{\partial\phi}\right) \tag{40}$$

$$= \hbar e^{\pm i\phi}\frac{\partial}{\partial\theta} \pm i\hbar e^{\pm i\phi}\cot\theta\frac{\partial}{\partial\phi} \tag{41}$$

$$= \hbar e^{\pm i\phi}\left(\frac{\partial}{\partial\theta} \pm i\cot\theta\frac{\partial}{\partial\phi}\right) \tag{42}$$

[Admittedly, it's probably easier and more elegant to use spherical coordinates from the start, but it's instructive to see how it's done starting with rectangular coordinates.]

TOTAL ANGULAR MOMENTUM IS HERMITIAN

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Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 12, Exercise 12.5.9.

Post date: 5 Jun 2017

[If some equations are too small to read easily, use your browser's magnifying option (Ctrl + on Chrome, probably something similar on other browsers).]

The total angular momentum operator L^2 can be written in spherical coordinates as

$$L^2 = -\hbar^2 \left[\frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \left(\sin\theta \frac{\partial}{\partial\theta} \right) + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\phi^2} \right] \tag{1}$$

As L^2 is an observable, it should be Hermitian. We can verify this by showing that

$$\left\langle \psi_2 \left| L^2 \right| \psi_1 \right\rangle = \left\langle \psi_1 \left| L^2 \right| \psi_2 \right\rangle^* \tag{2}$$

In spherical coordinates, this becomes

$$\int \psi_2^* \left(L^2 \psi_1 \right) d\Omega = \left[\int \psi_1^* \left(L^2 \psi_2 \right) d\Omega \right]^* \tag{3}$$

The element of solid angle $d\Omega = \sin\theta \, d\theta \, d\phi$, so the full integral is

$$\int \psi_2^* \left(L^2 \psi_1 \right) d\Omega = \int_0^{2\pi} \int_0^{\pi} \psi_2^* \left(L^2 \psi_1 \right) \sin\theta \, d\theta \, d\phi \tag{4}$$

We can verify 3 by showing that it is true for each of the two terms in 1 separately. As usual for these sorts of integrals, we need to use integration by parts. To simplify things, we'll consider $-L^2/\hbar^2$ so we can deal only with the terms in the brackets in 1. We'll also use the shorthand notation

$$s \equiv \sin\theta \tag{5}$$

$$c \equiv \cos\theta \tag{6}$$

Also, a prime indicates a derivative with respect to θ: $\psi_1' \equiv \frac{\partial \psi_1}{\partial \theta}$, etc.

For the first term, we have, considering only the integration over θ:

$$\int_0^\pi \psi_2^* \frac{1}{s}\frac{\partial}{\partial\theta}\left(s\frac{\partial\psi_1}{\partial\theta}\right) s\, d\theta = \int_0^\pi \left[\psi_2^* c\psi_1' + \psi_2^* s\psi_1''\right] d\theta \tag{7}$$

$$= \psi_2^* c\psi_1\big|_0^\pi + \psi_2^* s\psi_1'\big|_0^\pi - \tag{8}$$

$$\int_0^\pi \left[(\psi_2^*)' c\psi_1 - \psi_2^* s\psi_1\right] d\theta - \tag{9}$$

$$\int_0^\pi \left[(\psi_2^*)' s\psi_1' + \psi_2^* c\psi_1'\right] d\theta \tag{10}$$

The second term in 8 is zero since $\sin 0 = \sin\pi = 0$, but we can't ignore the first term, which is not, in general, zero. Thus we are left with

$$\int_0^\pi \psi_2^* \frac{\partial}{\partial\theta}\left(s\frac{\partial\psi_1}{\partial\theta}\right) d\theta = \psi_2^* c\psi_1\big|_0^\pi - \tag{11}$$

$$\int_0^\pi \left[(\psi_2^*)' c\psi_1 - \psi_2^* s\psi_1\right] d\theta - \tag{12}$$

$$\int_0^\pi \left[(\psi_2^*)' s\psi_1' + \psi_2^* c\psi_1'\right] d\theta \tag{13}$$

We can now integrate the last line by parts again to get rid of the derivatives of ψ_1:

$$-\int_0^\pi \left[(\psi_2^*)' s\psi_1' + \psi_2^* c\psi_1'\right] d\theta = -\left(\psi_2^*\right)' s\psi_1\big|_0^\pi - \psi_2^* c\psi_1\big|_0^\pi + \tag{14}$$

$$\int_0^\pi \left[\psi_1 (\psi_2^*)'' s + (\psi_2^*)' c\psi_1\right] d\theta + \tag{15}$$

$$\int_0^\pi \left[\psi_1 (\psi_2^*)' c - \psi_2^* s\psi_1\right] d\theta \tag{16}$$

$$= -\psi_2^* c\psi_1\big|_0^\pi + \tag{17}$$

$$\int_0^\pi \left[\psi_1 (\psi_2^*)'' s + (\psi_2^*)' c\psi_1\right] d\theta + \tag{18}$$

$$\int_0^\pi \left[\psi_1 (\psi_2^*)' c - \psi_2^* s\psi_1\right] d\theta \tag{19}$$

Inserting this back into 11 and cancelling terms, we have

$$\int_0^\pi \psi_2^* \frac{\partial}{\partial\theta}\left(s\frac{\partial\psi_1}{\partial\theta}\right) d\theta = \int_0^\pi \left[\psi_1 (\psi_2^*)'' s + (\psi_2^*)' c\psi_1\right] d\theta \tag{20}$$

Comparing this with 7, we see that

$$\int_0^\pi \psi_2^* \frac{\partial}{\partial\theta}\left(s\frac{\partial\psi_1}{\partial\theta}\right) d\theta = \left[\int_0^\pi \psi_1^* \frac{\partial}{\partial\theta}\left(s\frac{\partial\psi_2}{\partial\theta}\right) d\theta\right]^* \tag{21}$$

Thus the first term in 1 is Hermitian. (As this first term involves no derivatives with respect to ϕ, the integration over ϕ is automatically Hermitian.)

For the second term in 1, we need to consider only the integral over ϕ, so we have

$$\int_0^{2\pi} \psi_2^* \frac{1}{\sin^2\theta} \frac{\partial^2 \psi_1}{\partial \phi^2} \sin\theta \, d\phi = \frac{1}{s} \int_0^{2\pi} \psi_2^* \frac{\partial^2 \psi_1}{\partial \phi^2} \, d\phi \tag{22}$$

(As we're integrating over ϕ, terms in θ act as constants and can be taken outside the integral.) The first integration by parts gives (where a prime now indicates a derivative with respect to ϕ):

$$\int_0^{2\pi} \psi_2^* \psi_1'' \, d\phi = \psi_2^* \psi_1' \Big|_0^{2\pi} - \int_0^{2\pi} (\psi_2^*)' \psi_1' \, d\phi \tag{23}$$

$$= - \int_0^{2\pi} (\psi_2^*)' \psi_1' \, d\phi \tag{24}$$

This time, we're able to set the integrated term to zero, since $\phi = 0$ and $\phi = 2\pi$ refer to the same angle. A second integration by parts gives

$$- \int_0^{2\pi} (\psi_2^*)' \psi_1' \, d\phi = - (\psi_2^*)' \psi_1 \Big|_0^{2\pi} + \int_0^{2\pi} (\psi_2^*)'' \psi_1 \, d\phi \tag{25}$$

$$= \int_0^{2\pi} (\psi_2^*)'' \psi_1 \, d\phi \tag{26}$$

$$= \left[\int_0^{2\pi} \psi_1^* \psi_2'' \, d\phi \right]^* \tag{27}$$

Thus both terms in 1 are Hermitian, so the complete operator L^2 is also Hermitian.

SPHERICAL HARMONICS FROM POWER SERIES EXAMPLES FOR M=0

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To leave a comment or report an error, please use the auxiliary blog.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 12, Exercise 12.5.10.

Post date: 6 Jun 2017

[If some equations are too small to read easily, use your browser's magnifying option (Ctrl + on Chrome, probably something similar on other browsers).]

The total angular momentum operator L^2 can be written in spherical coordinates as

$$L^2 = -\hbar^2 \left[\frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \left(\sin\theta \frac{\partial}{\partial\theta} \right) + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\phi^2} \right] \tag{1}$$

Since $\left[L^2, L_z\right] = 0$, we can find a basis consisting of simultaneous eigenfunctions of L^2 and L_z. Suppose we call these states $|\alpha\beta\rangle$, where α is the eigenvalue of L^2 and β is the eigenvalue of L_z. In spherical coordinates, we know that

$$L_z = -i\hbar \frac{\partial}{\partial\phi} \tag{2}$$

and that its eigenvalues are $m\hbar$ for integer values of m. Thus we can separate the θ and ϕ dependence in the eigenstates and write

$$\psi_{\alpha m}(\theta, \phi) = P_\alpha^m(\theta)\, e^{im\phi} \tag{3}$$

We therefore have the eigenvalue equation

$$\begin{aligned} L^2 |\alpha m\rangle &= \alpha |\alpha m\rangle & (4) \\ L^2 \psi_{\alpha m}(\theta, \phi) &= \alpha \psi_{\alpha m}(\theta, \phi) & (5) \end{aligned}$$

Combining 3 with 1, we have

$$\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi_{\alpha m}}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2\psi_{\alpha m}}{\partial\phi^2}=\alpha\psi_{\alpha m} \tag{6}$$

$$\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial P_\alpha^m}{\partial\theta}\right)-\frac{m^2}{\sin^2\theta}P_\alpha^m+\frac{\alpha}{\hbar^2}P_\alpha^m=0 \tag{7}$$

We'd like to show that solutions of this equation require that (1)

$$\alpha = \hbar^2\ell(\ell+1) \tag{8}$$

$$|m| \leq \ell \tag{9}$$

for $\ell=0,1,2,\ldots$. In the problem given in Shankar, we tackle the less demanding case of $m=0$ and demonstrate only the result for α. We begin by transforming 7 using the variable substitution:

$$u\equiv\cos\theta \tag{10}$$

This gives us

$$du=-\sin\theta\,d\theta \tag{11}$$

so that 7 becomes

$$\frac{-\sin\theta}{\sin\theta}\frac{\partial}{\partial u}\left(-\sin^2\theta\frac{\partial P_\alpha^0}{\partial u}\right)+\frac{\alpha}{\hbar^2}P_\alpha^0=0 \tag{12}$$

$$\frac{\partial}{\partial u}\left(\left(1-u^2\right)\frac{\partial P_\alpha^0}{\partial u}\right)+\frac{\alpha}{\hbar^2}P_\alpha^0=0 \tag{13}$$

$$\left(1-u^2\right)\frac{\partial^2 P_\alpha^0}{\partial u^2}-2u\frac{\partial P_\alpha^0}{\partial u}+\frac{\alpha}{\hbar^2}P_\alpha^0=0 \tag{14}$$

We can use a power series to solve this by defining

$$P_\alpha^0(u) = \sum_{n=0}^{\infty}C_n u^n \tag{15}$$

$$\frac{\partial P_\alpha^0}{\partial u} = \sum_{n=0}^{\infty}C_n n u^{n-1} \tag{16}$$

$$\frac{\partial^2 P_\alpha^0}{\partial u^2} = \sum_{n=0}^{\infty}C_n n\left(n-1\right)u^{n-2} \tag{17}$$

$$= \sum_{n=0}^{\infty}C_{n+2}\left(n+2\right)\left(n+1\right)u^{n} \tag{18}$$

Plugging these into 14 and collecting terms, we get

$$P_\alpha^0(u) = \sum_{n=0}^{\infty} \left[C_{n+2}(n+2)(n+1) + C_n \left(-n(n-1) - 2n + \frac{\alpha}{\hbar^2} \right) \right] u^n = 0 \tag{19}$$

If a power series equals zero, the coefficient of each power of u must be zero (power series theorem from math), so we get the recurrence relation

$$C_{n+2} = \frac{n(n-1) + 2n - \frac{\alpha}{\hbar^2}}{(n+2)(n+1)} C_n \tag{20}$$

$$= \frac{n^2 + n - \frac{\alpha}{\hbar^2}}{n^2 + 3n + 2} C_n \tag{21}$$

For large n we have

$$C_{n+2} \to \frac{n^2}{n^2} C_n = C_n \tag{22}$$

Since $u = \cos\theta$, $u \in [-1, 1]$ and the series must converge for all these values. Although the power series $\sum_{n=0}^{\infty} u^n$ converges if $|u| < 1$ (that's the standard geometric series), it clearly diverges if $u = 1$. Thus we require the series to terminate, which imposes a condition on α:

$$\alpha = \ell(\ell+1)\hbar^2 \tag{23}$$

for some integer value $\ell = 0, 1, 2, \ldots$. Since choosing a value for ℓ can be done only once in any given series, and the recursion relation relates every *second* coefficient, this implies that either all even coefficients or all odd coefficients must be zero. Thus $P_\alpha^0(u)$ is either a sum of even powers (making it an even function) or of odd powers (making it an odd function) only.

The first few values of $P_\alpha^0(u)$ are found by choosing values for C_0 and C_1 and then generating all higher coefficients using 21. If we take

$$C_0 = 1 \tag{24}$$

$$C_1 = 0 \tag{25}$$

then if we choose $\ell = 0$ we get

$$P_0^0 = 1 \tag{26}$$

Taking

$$C_0 = 0 \tag{27}$$
$$C_1 = 1 \tag{28}$$

and $\ell = 1$ gives

$$P_1^0 = u = \cos\theta \tag{29}$$

Reverting to an even series and taking $\ell = 2$ we have from 21

$$C_2 = -\frac{\alpha}{2\hbar^2} C_0 = -\frac{\ell(\ell+1)}{2}(1) = -3 \tag{30}$$
$$P_2^0 = 1 - 3u^2 = 1 - 3\cos^2\theta \tag{31}$$

These values for P_ℓ^0 agree with the spherical harmonics Y_ℓ^0 apart from the constant scaling factors in each case. See Shankar's equation 12.5.39 for comparison.

PINGBACKS

Pingback: angular momentum and parity

SPHERICAL HARMONICS USING THE LOWERING OPERATOR

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 12, Exercise 12.5.11.

Post date: 7 Jun 2017

[If some equations are too small to read easily, use your browser's magnifying option (Ctrl + on Chrome, probably something similar on other browsers).]

The raising and lowering operators for angular momentum are

$$L_{\pm} \equiv L_x \pm iL_y \tag{1}$$

On a state $|\ell m\rangle$ in the basis of eigenstates of L^2 and L_z, they have the effect:

$$L_{\pm}|\ell m\rangle = \hbar\sqrt{(\ell \mp m)(\ell \pm m + 1)}\,|\ell, m \pm 1\rangle \tag{2}$$

This means that, if we can find the top state $|\ell\ell\rangle$, we can find the state for all lower values of m by applying L_- successively. To illustrate the process we'll derive the 3 states for $\ell = 1$. The top state $|11\rangle$ can be obtained by following the derivation given in Shankar from his equation 12.5.28 onwards. In spherical coordinates, the raising and lowering operators have the form

$$L_{\pm} = \pm\hbar e^{\pm i\phi}\left[\frac{\partial}{\partial\theta} \pm i\cot\theta\frac{\partial}{\partial\phi}\right] \tag{3}$$

Applying L_+ to the top state $|11\rangle$ must give zero, so if ψ_1^1 is the representation of this state in spherical coordinates, we must solve the differential equation

$$\left[\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\phi}\right]\psi_1^1 = 0 \tag{4}$$

Since ψ_1^1 is also an eigenfunction of L_z with eigenvalue $\hbar$, we know that

$$\psi_1^1 = U_1^1(r,\theta)\,e^{i\phi} \tag{5}$$

Thus 4 becomes

$$\left(\frac{\partial}{\partial\theta}-\cot\theta\right)U_1^1=0 \tag{6}$$

This can be solved by writing it in the form

$$\frac{dU_1^1}{U_1^1} = \frac{d(\sin\theta)}{\sin\theta} \tag{7}$$

$$\ln U_1^1 = \ln(\sin\theta)+\ln R(r)+\ln A \tag{8}$$

where R is some unspecified function of r, and A is a constant. We therefore have

$$U_1^1(r,\theta) = R(r)(A\sin\theta) \tag{9}$$

If we ignore R for now, we can normalize over the angular coordinates by requiring

$$\int |A\sin\theta|^2\, d\Omega = 1 \tag{10}$$

The element $d\Omega$ of solid angle is

$$d\Omega = \sin\theta\; d\phi\; d\theta \tag{11}$$

so we have

$$|A|^2\int_0^{\pi}\int_0^{2\pi}\sin^3\theta\; d\phi\; d\theta = 2\pi\,|A|^2\int_0^{\pi}\sin\theta\left(1-\cos^2\theta\right)d\theta \tag{12}$$

$$= \frac{8\pi}{3}\,|A|^2 \tag{13}$$

$$A = \sqrt{\frac{3}{8\pi}} \tag{14}$$

Thus the spherical harmonic Y_1^1 is (using Shankar's normalization convention of multiplying by $(-1)^{\ell}$):

$$Y_1^1 = -\sqrt{\frac{3}{8\pi}}\sin\theta e^{i\phi} \tag{15}$$

We can now get Y_1^0 by applying L_- to Y_1^1. From 2 we have

$$L_-Y_1^1 = \hbar\sqrt{(1+1)(1-1+1)}Y_1^0 \tag{16}$$

$$= \sqrt{2}\hbar Y_1^0 \tag{17}$$

From 3 we have

$$L_- Y_1^1 = -\hbar e^{-i\phi}\left[\frac{\partial}{\partial\theta} - i\cot\theta\frac{\partial}{\partial\phi}\right]Y_1^1 \tag{18}$$

$$= -\hbar e^{-i\phi}\left(-\sqrt{\frac{3}{8\pi}}\right)\left[\cos\theta - i\cot\theta\,(i\sin\theta)\right]e^{i\phi} \tag{19}$$

$$= 2\hbar\sqrt{\frac{3}{8\pi}}\cos\theta \tag{20}$$

Comparing the last two results gives

$$\sqrt{2}\hbar Y_1^0 = 2\sqrt{\frac{3}{8\pi}}\cos\theta \tag{21}$$

$$Y_1^0 = \sqrt{\frac{3}{4\pi}}\cos\theta \tag{22}$$

Repeating the process, we get

$$L_- Y_1^0 = \hbar\sqrt{(1+0)\,(1-0+1)}Y_1^{-1} \tag{23}$$

$$= \sqrt{2}\hbar Y_1^{-1} \tag{24}$$

Also

$$L_- Y_1^0 = -\hbar e^{-i\phi}\left[\frac{\partial}{\partial\theta} - i\cot\theta\frac{\partial}{\partial\phi}\right]Y_1^0 \tag{25}$$

$$= -\hbar e^{-i\phi}\sqrt{\frac{3}{4\pi}}\,(-\sin\theta - 0) \tag{26}$$

$$= \hbar\sqrt{\frac{3}{4\pi}}\sin\theta e^{-i\phi} \tag{27}$$

Thus

$$\sqrt{2}\hbar Y_1^{-1} = \hbar\sqrt{\frac{3}{4\pi}}\sin\theta e^{-i\phi} \tag{28}$$

$$Y_1^{-1} = \sqrt{\frac{3}{8\pi}}\sin\theta e^{-i\phi} \tag{29}$$

Comparing these results with Shankar's equation 12.5.39 we see that they match. [This exercise is similar to one we did earlier, where we used the raising operator to generate spherical harmonics with higher values of m.]

PINGBACKS

Pingback: angular momentum and parity

ANGULAR MOMENTUM AND PARITY

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 12, Exercise 12.5.12.

Post date: 9 Jun 2017

[If some equations are too small to read easily, use your browser's magnifying option (Ctrl + on Chrome, probably something similar on other browsers).]

The parity operator in 3-d reflects every point directly through the origin, so that a position vector $\mathbf{r} \rightarrow -\mathbf{r}$. In rectangular coordinates this means replacing each coordinate by its negative. In spherical coordinates, the angular coordinates change according to

$$\theta \rightarrow \pi - \theta \tag{1}$$

$$\phi \rightarrow \pi + \phi \tag{2}$$

If this isn't obvious, picture reflecting a vector $\mathbf{r}$ through the origin. If the original vector makes an angle θ with the z (vertical) axis, then the reflected vector makes an angle θ with the $-z$ axis, which is equivalent to an angle of $\pi - \theta$ with the $+z$ axis. The azimuthal angle ϕ just gets rotated by π to lie on the other side of the z axis.

Using this, we can see that the parity operator Π commutes with both L^2 and L_z, as follows. Since neither of these operators involves the radial coordinate, we can consider their effect on a function $f(\theta, \phi)$. Under parity, we have

$$\Pi f(\theta, \phi) \rightarrow f(\pi - \theta, \pi + \phi) \tag{3}$$

Thus the derivatives transform under parity according to

$$\frac{\partial f(\theta, \phi)}{\partial \theta} \rightarrow -\frac{\partial f(\pi - \theta, \pi + \phi)}{\partial \theta} \tag{4}$$

$$\frac{\partial f(\theta, \phi)}{\partial \phi} \rightarrow \frac{\partial f(\pi - \theta, \pi + \phi)}{\partial \phi} \tag{5}$$

The angular momentum operators are

$$L^2 = -\hbar^2 \left[\frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \left(\sin\theta \frac{\partial}{\partial\theta} \right) + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\phi^2} \right] \tag{6}$$

$$L_z = -i\hbar \frac{\partial}{\partial\phi} \tag{7}$$

Thus the combined operation gives

$$L^2 \Pi f(\theta,\phi) \to -\hbar^2 \left[\frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \left(\sin\theta \frac{\partial}{\partial\theta} \right) + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\phi^2} \right] f(\pi-\theta,\pi+\phi) \tag{8}$$

$$= -\hbar^2 \left[\frac{1}{\sin\theta} \left(-\frac{\partial}{\partial\theta} \right) \left(\sin\theta \left(-\frac{\partial}{\partial\theta} \right) \right) + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\phi^2} \right] f(\pi-\theta,\pi+\phi) \tag{9}$$

$$= -\hbar^2 \left[\frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \left(\sin\theta \frac{\partial}{\partial\theta} \right) + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\phi^2} \right] f(\pi-\theta,\pi+\phi) \tag{10}$$

$$= L^2 f(\pi-\theta,\pi+\phi) \tag{11}$$

If we apply Π to L^2, we have

$$\Pi \left[L^2 f(\theta,\phi) \right] = -\hbar^2 \left[\frac{1}{\sin(\pi-\theta)} \left(-\frac{\partial}{\partial\theta} \right) \left(\sin(\pi-\theta) \left(-\frac{\partial}{\partial\theta} \right) \right) + \frac{1}{\sin^2(\pi-\theta)} \frac{\partial^2}{\partial\phi^2} \right] f(\pi-\theta,\pi+\phi) \tag{12}$$

$$= -\hbar^2 \left[\frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \left(\sin\theta \frac{\partial}{\partial\theta} \right) + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\phi^2} \right] f(\pi-\theta,\pi+\phi) \tag{13}$$

$$= L^2 f(\pi-\theta,\pi+\phi) \tag{14}$$

Thus

$$\left[\Pi, L^2 \right] = 0 \tag{15}$$

where in the first line we used $\sin(\pi-\theta) = \sin\theta$.

Since L_z involves only a derivative with respect to ϕ which doesn't change under parity, we have

$$[\Pi, L_z] = 0 \tag{16}$$

Since Π commutes with both L^2 and L_z it is possible to find a set of functions that are simultaneous eigenfunctions of all three operators. These

functions turn out to be the same spherical harmonics that we've been using all along. We can show this by starting with the top spherical harmonic

$$Y_l^l = (-1)^l \sqrt{\frac{(2l+1)!}{4\pi}} \frac{1}{2^l l!} e^{il\phi} \sin^l \theta \tag{17}$$

where we've included the $(-1)^l$ to be consistent with Shankar's equation 12.5.32. Under parity, this transforms as

$$\Pi Y_l^l = (-1)^l \sqrt{\frac{(2l+1)!}{4\pi}} \frac{1}{2^l l!} e^{il(\pi+\phi)} \sin^l (\pi - \theta) \tag{18}$$

$$= (-1)^l e^{il\pi} \sqrt{\frac{(2l+1)!}{4\pi}} \frac{1}{2^l l!} e^{il\phi} \sin^l \theta \tag{19}$$

$$= (-1)^l Y_l^l \tag{20}$$

where we used $e^{il\pi} = (-1)^l$ in the second line. Thus Y_l^l is an eigenfunction of Π with eigenvalue $(-1)^l$.

To show that the other spherical harmonics are also eigenfunctions, we can use the lowering operator L_-. In spherical coordinates, we have

$$L_- Y_l^m = \hbar \sqrt{(\ell+m)(\ell-m+1)} Y_l^{m-1} \tag{21}$$

The operator can be expressed as

$$L_- = -\hbar e^{-i\phi} \left[\frac{\partial}{\partial \theta} - i \cot\theta \frac{\partial}{\partial \phi} \right] \tag{22}$$

Under parity, we can transform 22 using $\sin(\pi - \theta) = \sin\theta$ and $\cos(\pi - \theta) = -\cos\theta$, so that $\cot(\pi - \theta) = -\cot\theta$. We therefore have

$$\Pi L_- = -\hbar e^{-i(\pi+\phi)} \left[-\frac{\partial}{\partial \theta} + i \cot\theta \frac{\partial}{\partial \phi} \right] \tag{23}$$

$$= -\hbar e^{-i\phi} \left[\frac{\partial}{\partial \theta} - i \cot\theta \frac{\partial}{\partial \phi} \right] \tag{24}$$

$$= L_- \tag{25}$$

Thus L_- is unchanged by parity, which means that from 21, Y_l^{m-1} has the same parity as Y_l^m. Starting with Y_l^l and using the lowering operator successively to reduce the superscript index, we have therefore

$$\Pi Y_l^m = (-1)^l Y_l^m \tag{26}$$

Thus all spherical harmonics are also eigenfunctions of parity.

LINEAR COMBINATIONS OF SPHERICAL HARMONICS - PROBABILITIES

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 12, Exercise 12.5.13.

Post date: 13 Jun 2017

[If some equations are too small to read easily, use your browser's magnifying option (Ctrl + on Chrome, probably something similar on other browsers).]

If we can express a 3-d quantum state in terms of the spherical harmonics, we can calculate directly the probabilities of L_z having one of its eigenvalues. That is, if we can write a state ψ as

$$\psi(r,\theta,\phi) = f(r)\sum_m C_l^m Y_l^m \tag{1}$$

for some constant coefficients C_l^m and f is some function of r alone, then

$$P(l_z = m\hbar) = \frac{\left|C_l^m\right|^2}{\sum_n \left|C_l^n\right|^2} \tag{2}$$

As an example, suppose we have

$$\psi = N(x+y+2z)e^{-\alpha r} \tag{3}$$

where N is a normalization constant. We start by expressing x, y and z in terms of Y_1^m. We have

$$Y_1^{\pm 1} = \mp\sqrt{\frac{3}{8\pi}}\sin\theta e^{\pm i\phi} \tag{4}$$

$$Y_1^0 = \sqrt{\frac{3}{4\pi}}\cos\theta \tag{5}$$

Using standard spherical-to-rectangular conversions

$$x = r\sin\theta\cos\phi \tag{6}$$

$$y = r\sin\theta\sin\phi \tag{7}$$

$$z = r\cos\theta \tag{8}$$

Therefore

$$\cos\phi = \frac{x}{r\sin\theta} \tag{9}$$

$$\sin\phi = \frac{y}{r\sin\theta} \tag{10}$$

$$\cos\theta = \frac{z}{r} \tag{11}$$

Plugging these into 4 we have

$$Y_1^{\pm 1} = \mp\sqrt{\frac{3}{8\pi}}\sin\theta\left(\cos\phi \pm i\sin\phi\right) \tag{12}$$

$$= \mp\sqrt{\frac{3}{8\pi}}\frac{x \pm iy}{r} \tag{13}$$

$$Y_1^0 = \sqrt{\frac{3}{4\pi}}\frac{z}{r} \tag{14}$$

$$= \sqrt{2}\sqrt{\frac{3}{8\pi}}\frac{z}{r} \tag{15}$$

Inverting these, we have

$$x = \frac{1}{2}\sqrt{\frac{8\pi}{3}}r\left(Y_1^{-1} - Y_1^1\right) \tag{16}$$

$$y = -\frac{1}{2i}\sqrt{\frac{8\pi}{3}}r\left(Y_1^{-1} + Y_1^1\right) \tag{17}$$

$$z = \frac{1}{\sqrt{2}}\sqrt{\frac{8\pi}{3}}rY_1^0 \tag{18}$$

Thus 3 becomes

$$\psi = \sqrt{\frac{8\pi}{3}}Nre^{-\alpha r}\left[Y_1^1\left(-\frac{1}{2} - \frac{1}{2i}\right) + Y_1^{-1}\left(\frac{1}{2} - \frac{1}{2i}\right) + Y_1^0\sqrt{2}\right] \tag{19}$$

Comparing with 1 we find

$$C_1^1 = -\frac{1}{2} - \frac{1}{2i} \tag{20}$$

$$C_1^{-1} = \frac{1}{2} - \frac{1}{2i} \tag{21}$$

$$C_1^0 = \sqrt{2} \tag{22}$$

We have

$$\sum_n |C_1^n|^2 = \frac{1}{2} + \frac{1}{2} + 2 = 3 \tag{23}$$

$$P(l_z = 0) = \frac{\left|C_l^0\right|^2}{\sum_n \left|C_l^n\right|^2} = \frac{2}{3} \tag{24}$$

$$P(l_z = \hbar) = \frac{\left|C_l^1\right|^2}{\sum_n \left|C_l^n\right|^2} = \frac{1}{6} \tag{25}$$

$$P(l_z = -\hbar) = \frac{\left|C_l^{-1}\right|^2}{\sum_n \left|C_l^n\right|^2} = \frac{1}{6} \tag{26}$$

PINGBACKS

Pingback: spherical harmonics: rotation about the x axis
Pingback: Wigner-Eckart Theorem

SPHERICAL HARMONICS: ROTATION ABOUT THE X AXIS

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 12, Exercise 12.5.14.

Post date: 18 Jun 2017

[If some equations are too small to read easily, use your browser's magnifying option (Ctrl + on Chrome, probably something similar on other browsers).]

Here's another example of using spherical harmonics to study the behaviour of wave functions in 3-d. Under a rotation by θ_x about the x axis, the coordinates transform using the rotation matrix

$$R(\theta_x \hat{\mathbf{x}}) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos\theta_x & -\sin\theta_x \\ 0 & \sin\theta_x & \cos\theta_x \end{bmatrix} \tag{1}$$

This results in the coordinate transformations

$$x \rightarrow x \tag{2}$$

$$y \rightarrow y\cos\theta_x - z\sin\theta_x \tag{3}$$

$$z \rightarrow z\cos\theta_x + y\sin\theta_x \tag{4}$$

Using similar techniques to those for translations, it is found that the wave function $\psi(x,y,z)$ transforms into the wave function at the position obtained by rotating by $-\theta_x$ (that is, by rotating by θ_x in the opposite direction):

$$\psi(x,y,z) \rightarrow \psi_R = \psi(x, y\cos\theta_x + z\sin\theta_x, z\cos\theta_x - y\sin\theta_x) \tag{5}$$

Suppose we have a wave function given by

$$\psi = Aze^{-r^2/a^2} \tag{6}$$

for some constants a and A. Under this rotation, using 5 it transforms to

$$\psi_R = A(z\cos\theta_x - y\sin\theta_x)\, e^{-r^2/a^2} \tag{7}$$

[Note that r^2 remains invariant under rotations about the origin, since the distance of a point from the origin is not affected by a rotation. You can

verify this directly if you like by working out $r^2 = x^2 + y^2 + z^2$ after the rotation.]

Equatioin 7 differs from the equation given in Shankar, which is

$$\psi_R = A\,(z\cos\theta_x + y\sin\theta_x)\,e^{-r^2/a^2} \tag{8}$$

Curiously, in the errata for Shankar's book (2006 edition) 7 is listed as the incorrect version, which is 'corrected' to 8. In my copy of the book (which doesn't have a date on the title page), 8 is printed, but I don't think this is right. In any case, we'll proceed with the problem.

First, we write 6 in terms of spherical harmonics, using

$$x = \frac{1}{2}\sqrt{\frac{8\pi}{3}}r\left(Y_1^{-1} - Y_1^1\right) \tag{9}$$

$$y = -\frac{1}{2i}\sqrt{\frac{8\pi}{3}}r\left(Y_1^{-1} + Y_1^1\right) \tag{10}$$

$$z = \sqrt{\frac{4\pi}{3}}rY_1^0 \tag{11}$$

We have

$$\psi = A\sqrt{\frac{4\pi}{3}}rY_1^0 e^{-r^2/a^2} \tag{12}$$

With the three spherical harmonics Y_1^1, Y_1^0 and Y_1^{-1} as the basis, we can write this in vector notation as

$$\psi = A\sqrt{\frac{4\pi}{3}}re^{-r^2/a^2}\begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} \tag{13}$$

A rotation in 3-d for $\ell = 1$ is given by

$$D^{(1)}[R] = I^{(1)} + \frac{\left(\hat{\boldsymbol{\theta}}\cdot\mathbf{J}^{(1)}\right)^2}{\hbar^2}(\cos\theta - 1) - \frac{i\hat{\boldsymbol{\theta}}\cdot\mathbf{J}^{(1)}}{\hbar}\sin\theta \tag{14}$$

For $\hat{\boldsymbol{\theta}} = \theta_x\hat{\mathbf{x}}$, this works out to

$$D^{(1)}[R(\theta_x\hat{\mathbf{x}})] = \frac{1}{2}\begin{bmatrix} 1+\cos\theta_x & -\sqrt{2}i\sin\theta_x & \cos\theta_x - 1 \\ -\sqrt{2}i\sin\theta_x & 2\cos\theta_x & -\sqrt{2}i\sin\theta_x \\ \cos\theta_x - 1 & -\sqrt{2}i\sin\theta_x & 1+\cos\theta_x \end{bmatrix} \tag{15}$$

We can use this to transform 13 to get

$$\psi_R = D^{(1)}\left[R\left(\theta_x \hat{\mathbf{x}}\right)\right]\psi \tag{16}$$

$$= A\sqrt{\frac{4\pi}{3}} r e^{-r^2/a^2} \frac{1}{2} \begin{bmatrix} 1+\cos\theta_x & -\sqrt{2}i\sin\theta_x & \cos\theta_x - 1 \\ -\sqrt{2}i\sin\theta_x & 2\cos\theta_x & -\sqrt{2}i\sin\theta_x \\ \cos\theta_x - 1 & -\sqrt{2}i\sin\theta_x & 1+\cos\theta_x \end{bmatrix} \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} \tag{17}$$

$$= A\sqrt{\frac{\pi}{3}} r e^{-r^2/a^2} \begin{bmatrix} -\sqrt{2}i\sin\theta_x \\ 2\cos\theta_x \\ -\sqrt{2}i\sin\theta_x \end{bmatrix} \tag{18}$$

$$= Ae^{-r^2/a^2} \left\{ \sqrt{\frac{4\pi}{3}} r \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} \cos\theta_x - \sqrt{\frac{2\pi}{3}} r i \sin\theta_x \left(\begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \right) \right\} \tag{19}$$

$$= Ae^{-r^2/a^2} \left\{ \sqrt{\frac{4\pi}{3}} r Y_1^0 \cos\theta_x + \frac{1}{2i}\sqrt{\frac{8\pi}{3}} r \left(Y_1^1 + Y_1^{-1}\right) \sin\theta_x \right\} \tag{20}$$

$$= Ae^{-r^2/a^2} \left(z\cos\theta_x - y\sin\theta_x\right) \tag{21}$$

where we used 10 to get the last line. This result agrees with 7 and not with the equation 8 given in Shankar, so (provided I got the signs right) it looks like Shankar's equation is wrong.

FREE PARTICLE IN SPHERICAL COORDINATES

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 12, Section 12.6.

Post date: 29 Jun 2017

[If some equations are too small to read easily, use your browser's magnifying option (Ctrl + on Chrome, probably something similar on other browsers).]

In solving the Schrödinger equation for spherically symmetric potentials, we found that we could reduce the problem to the equation

$$\left[-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}+V(r)+\frac{l(l+1)\hbar^2}{2\mu r^2}\right]U_{El}=EU_{El} \tag{1}$$

where $U_{El}(r)$ is related to the radial function by

$$R_{El}(r)=\frac{U_{El}(r)}{r} \tag{2}$$

For a free particle, $V=0$ and $E>0$, so we have

$$\left[-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}+\frac{l(l+1)\hbar^2}{2\mu r^2}\right]U_{El}=EU_{El} \tag{3}$$

Defining

$$k^2 \equiv \frac{2\mu E}{\hbar^2} \tag{4}$$

$$\rho \equiv kr \tag{5}$$

we convert the equation to

$$\left(-\frac{d^2}{d\rho^2}+\frac{l(l+1)}{\rho^2}\right)U_l=U_l \tag{6}$$

This equation can be solved by a method similar to that for the harmonic oscillator and its raising and lowering operators. The entire solution is fairly involved, so we'll start out here by showing how the new raising and lowering operators are defined.

We define

$$d_l \equiv \frac{d}{d\rho} + \frac{l+1}{\rho} \tag{7}$$

The adjoint is

$$d_l^\dagger = -\frac{d}{d\rho} + \frac{l+1}{\rho} \tag{8}$$

To see where the minus sign comes from on the RHS, we need to recall that the momentum operator is defined in one dimension as

$$P = -i\hbar\frac{\partial}{\partial x} \tag{9}$$

Since P is an observable, it is hermitian, so that $P^\dagger = P$. Under the hermitian operation $i \to -i$, so we must also have $\frac{\partial}{\partial x} \to -\frac{\partial}{\partial x}$. Thus the first derivative with respect to a position variable is anti-hermitian. If this doesn't convince you, you can also work out the integral:

$$\int_0^\infty \psi_2^* \frac{d}{d\rho}\psi_1 d\rho = \psi_2^*\psi_1|_0^\infty - \int_0^\infty \psi_1 \frac{d}{d\rho}\psi_2^* d\rho \tag{10}$$

Under the usual assumption that $\psi \to 0$ at the limits, the integrated term is zero and we have

$$\begin{aligned} \int_0^\infty \psi_2^* \frac{d}{d\rho}\psi_1 d\rho &= -\int_0^\infty \psi_1 \frac{d}{d\rho}\psi_2^* d\rho & (11)\\ &= -\left[\int_0^\infty \psi_1^* \frac{d}{d\rho}\psi_2 d\rho\right]^* & (12) \end{aligned}$$

In bracket notation, this is

$$\left\langle \psi_2 \middle| \frac{d}{d\rho}\psi_1 \right\rangle = -\left\langle \frac{d}{d\rho}\psi_2 \middle| \psi_1 \right\rangle \tag{13}$$

which shows that $\frac{d}{d\rho}$ is an anti-hermitian operator.
Returning to 7 and 8, we have

$$
\begin{aligned}
d_l d_l^\dagger U_l &= \left(\frac{d}{d\rho}+\frac{l+1}{\rho}\right)\left(-\frac{d}{d\rho}+\frac{l+1}{\rho}\right)U_l && (14)\\
&= \left(\frac{d}{d\rho}+\frac{l+1}{\rho}\right)\left(-U_l'+\frac{l+1}{\rho}U_l\right) && (15)\\
&= -U_l''-\frac{l+1}{\rho^2}U_l+\frac{l+1}{\rho}U_l'-\frac{l+1}{\rho}U_l'+\frac{(l+1)^2}{\rho^2}U_l && (16)\\
&= -U_l''+\frac{l(l+1)}{\rho^2}U_l && (17)
\end{aligned}
$$

Comparing with 6 we see that

$$d_l d_l^\dagger U_l = U_l \tag{18}$$

We can also show that

$$
\begin{aligned}
d_l^\dagger d_l U_l &= \left(-\frac{d}{d\rho}+\frac{l+1}{\rho}\right)\left(\frac{d}{d\rho}+\frac{l+1}{\rho}\right)U_l && (19)\\
&= \left(-\frac{d}{d\rho}+\frac{l+1}{\rho}\right)\left(U_l'+\frac{l+1}{\rho}U_l\right) && (20)\\
&= -U_l''+\frac{l+1}{\rho^2}U_l-\frac{l+1}{\rho}U_l'+\frac{l+1}{\rho}U_l'+\frac{(l+1)^2}{\rho^2}U_l && (21)\\
&= -U_l''+\frac{(l+1)^2+l+1}{\rho^2}U_l && (22)\\
&= -U_l''+\frac{(l+1)(l+2)}{\rho^2}U_l && (23)\\
&= d_{l+1}d_{l+1}^\dagger U_l && (24)
\end{aligned}
$$

Starting from 18 we multiply on the left by $d_l^\dagger$ to get

$$d_l^\dagger d_l\left(d_l^\dagger U_l\right) = d_l^\dagger U_l \tag{25}$$

Comparing this with 24 we see that

$$d_l^\dagger U_l = c_l U_{l+1} \tag{26}$$

where c_l is a constant.

Thus $d_l^\dagger$ is a raising operator, in that it raises the angular momentum number l by 1 when it acts on U_l. By convention, $c_l = 1$ (any adjustments to the constant can be made when normalizing).

We can start the process by looking at 6 with $l = 0$ which is

$$\frac{d^2}{d\rho^2}U_l = -U_l \tag{27}$$

This has the two solutions

$$\begin{aligned} U_0^A(\rho) &= \sin\rho & (28)\\ U_0^B(\rho) &= -\cos\rho & (29)\end{aligned}$$

The minus sign in front of $\cos\rho$ is just conventional. Since we require $U_0(0) = 0$, U_0^B is unacceptable if the region we're considering include $\rho = 0$, so we have

$$U_0(\rho) = \sin\rho \tag{30}$$

For the general case that excludes $\rho = 0$, we must include the cosine term as well.

From here, we can generate solutions for higher values of l by applying 26. Actually, the radial function that appears in the wave function is given by 2, so it is R_l that we really want. That is, we want

$$R_l = \frac{U_l}{r} = k\frac{U_l}{\rho} \tag{31}$$

As with the constant c_l in 26, we can absorb k into normalization to be done later, so we can generate functions

$$R_l = \frac{U_l}{\rho} \tag{32}$$

Applying 26 we have

$$\begin{aligned} \rho R_{l+1} &= d_l^\dagger(\rho R_l) & (33)\\ &= \left(-\frac{d}{d\rho} + \frac{l+1}{\rho}\right)(\rho R_l) & (34)\\ &= -R_l - \rho R_l' + (l+1)R_l & (35)\\ &= -\rho R_l' + lR_l & (36)\\ R_{l+1} &= \left(-\frac{d}{d\rho} + \frac{l}{\rho}\right)R_l & (37)\\ &= -\rho^l \frac{d}{d\rho}\left(\frac{R_l}{\rho^l}\right) & (38)\end{aligned}$$

We can convert this into a general formula by writing

$$\frac{R_{l+1}}{\rho^{l+1}} = \left(-\frac{1}{\rho}\frac{d}{d\rho}\right)\frac{R_l}{\rho^l} \tag{39}$$

Starting at $l = 0$, we have

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For the next step, we have

$$\begin{aligned}
\frac{R_2}{\rho^2} &= \left(-\frac{1}{\rho}\frac{d}{d\rho}\right)\frac{R_1}{\rho^1} && (41)\\
&= \left(-\frac{1}{\rho}\frac{d}{d\rho}\right)\left(-\frac{1}{\rho}\frac{d}{d\rho}\right)\frac{R_0}{\rho^0} && (42)\\
&= \left(-\frac{1}{\rho}\frac{d}{d\rho}\right)^2\frac{R_0}{\rho^0} && (43)
\end{aligned}$$

Thus in general

$$\frac{R_{l+1}}{\rho^{l+1}} = \left(-\frac{1}{\rho}\frac{d}{d\rho}\right)^{l+1}\frac{R_0}{\rho^0} \tag{44}$$

Note that

$$\left(-\frac{1}{\rho}\frac{d}{d\rho}\right)^{l+1} \neq \left(-\frac{1}{\rho}\right)^{l+1}\frac{d^{l+1}}{d\rho^{l+1}} \tag{45}$$

since the factor of $\frac{1}{\rho}$ has to be included when taking the derivative.
We'll explore the nature of these solutions in the next post.

SPHERICALLY SYMMETRIC POTENTIALS: A SIMPLE EXAMPLE

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Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 12, Exercise 12.6.1.

Post date: 27 Jun 2017

[If some equations are too small to read easily, use your browser's magnifying option (Ctrl + on Chrome, probably something similar on other browsers).]

The Schrödinger equation in 3-d for a potential that depends only on r is

$$-\frac{\hbar^2}{2\mu}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right)+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right)+\frac{1}{r^2\sin^2\theta}\left(\frac{\partial^2\psi}{\partial\phi^2}\right)\right]+V\psi=E\psi \tag{1}$$

The angular part of the operator on the LHS is essentially the angular momentum operator L^2 (times $1/2\mu r^2$):

$$L^2=-\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right] \tag{2}$$

, so we can write this as

$$-\frac{\hbar^2}{2\mu}\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right)+V\psi+\frac{L^2}{2\mu r^2}\psi=E\psi \tag{3}$$

Eigenfunctions in this equation satisfy

$$\psi=R_{Elm}(r)\,Y_l^m(\theta,\phi) \tag{4}$$

where the subscript Elm refers to the energy E and the angular momentum quantum numbers l and m. Y_l^m is a spherical harmonic and R_{Elm} is the radial function which depends on the potential V. The eigenvalues of L^2 are $l(l+1)\hbar^2$ so 3 becomes

$$-\frac{\hbar^2}{2\mu}\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial R_{El}}{\partial r}\right)+\frac{l(l+1)\hbar^2}{2\mu r^2}R_{El}+VR_{El}=ER_{El} \tag{5}$$

We've dropped the m from R_{Elm} since, for a spherically symmetric potential, the radial function is independent of m.

Example. Suppose a particle is described by the wave function

$$\psi_E(r,\theta,\phi) = Ae^{-r/a_0} \tag{6}$$

where A and a_0 are constants. What can we deduce about the system? First, since ψ_E is independent of θ and ϕ we see from 2 that

$$L^2\psi_E = 0 \tag{7}$$

so the eigenvalue is $l = 0$ and the state has no angular momentum. From 3 we therefore have

$$-\frac{\hbar^2}{2\mu}\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right) + V\psi = E\psi \tag{8}$$

Working out the derivatives, we have

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right) = -\frac{A}{r^2}\frac{d}{dr}\left(\frac{r^2}{a_0}e^{-r/a_0}\right) \tag{9}$$

$$= Ae^{-r/a_0}\left(-\frac{2}{ra_0} + \frac{1}{a_0^2}\right) \tag{10}$$

Plugging this back into 8 and cancelling terms gives

$$-\frac{2}{ra_0} + \frac{1}{a_0^2} = \frac{2\mu}{\hbar^2}(V - E) \tag{11}$$

If $V(r) \to 0$ as $r \to \infty$ we have, in this limit

$$E = -\frac{\hbar^2}{2\mu a_0^2} \tag{12}$$

The energy is constant at all values of r so we can now find V from 11

$$-\frac{2}{ra_0} + \frac{1}{a_0^2} = \frac{2\mu}{\hbar^2}\left(V(r) + \frac{\hbar^2}{2\mu a_0^2}\right) \tag{13}$$

$$V(r) = -\frac{\hbar^2}{\mu a_0 r} \tag{14}$$

SPHERICALLY SYMMETRIC POTENTIALS: HERMITICITY OF THE RADIAL FUNCTION

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To leave a comment or report an error, please use the auxiliary blog.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 12, Exercise 12.6.3.

Post date: 27 Jun 2017

[If some equations are too small to read easily, use your browser's magnifying option (Ctrl + on Chrome, probably something similar on other browsers).]

The Schrödinger equation in 3-d for a potential that depends only on r is

$$-\frac{\hbar^2}{2\mu}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right)+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right)+\frac{1}{r^2\sin^2\theta}\left(\frac{\partial^2\psi}{\partial\phi^2}\right)\right]+V\psi=E\psi \tag{1}$$

Eigenfunctions in this equation satisfy

$$\psi=R_{Elm}(r)\,Y_l^m(\theta,\phi) \tag{2}$$

where the subscript Elm refers to the energy E and the angular momentum quantum numbers l and m. Y_l^m is a spherical harmonic and R_{Elm} is the radial function which depends on the potential V. With the substitution

$$R_{El}(r)=\frac{U_{El}(r)}{r} \tag{3}$$

the differential equation reduces to

$$\left[-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}+V(r)+\frac{l(l+1)\hbar^2}{2\mu r^2}\right]U_{El}=EU_{El} \tag{4}$$

The quantity in the square brackets is an operator which will call $D_l(r)$:

$$D_l(r)\equiv-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}+V(r)+\frac{l(l+1)\hbar^2}{2\mu r^2} \tag{5}$$

Equation 4 is similar to the 1-d Schrödinger equation except that the variable r goes from 0 to ∞ rather than from $-\infty$ to ∞, and the potential is modified by the 'centrifugal term' $\frac{l(l+1)\hbar^2}{2\mu r^2}$. Because r begins at 0 rather than $-\infty$, the usual boundary conditions on U (that it tend to zero at $\pm\infty$) must

also be modified. We can get the new boundary conditions by imposing the hermiticity condition, which says that

$$\int_0^\infty U_1^* \left(D_l U_2\right) dr = \left[\int_0^\infty U_2^* \left(D_l U_1\right) dr\right]^* \tag{6}$$

$$= \int_0^\infty \left(D_l U_1\right)^* U_2 dr \tag{7}$$

The two terms $V(r) + \frac{l(l+1)\hbar^2}{2\mu r^2}$ in 5 are real and multiplicative, so the hermiticity condition is automatically satisfied for them. For the derivative term, we can use the usual integration by parts.

$$\int_0^\infty U_1^* \left(\frac{d^2}{dr^2} U_2\right) dr = U_1^* \frac{dU_2}{dr}\bigg|_0^\infty - \int_0^\infty \frac{dU_1^*}{dr}\frac{dU_2}{dr} dr \tag{8}$$

$$= U_1^* \frac{dU_2}{dr}\bigg|_0^\infty - U_2 \frac{dU_1^*}{dr}\bigg|_0^\infty + \int_0^\infty U_2 \left(\frac{d^2}{dr^2} U_1^*\right) dr \tag{9}$$

If we require

$$U_1^* \frac{dU_2}{dr}\bigg|_0^\infty - U_2 \frac{dU_1^*}{dr}\bigg|_0^\infty = 0 \tag{10}$$

then we have

$$\int_0^\infty U_1^* \left(\frac{d^2}{dr^2} U_2\right) dr = \int_0^\infty U_2 \left(\frac{d^2}{dr^2} U_1^*\right) dr \tag{11}$$

$$= \left[\int_0^\infty U_2^* \left(\frac{d^2}{dr^2} U_1\right) dr\right]^* \tag{12}$$

and the hermiticity condition 6 is satisfied.

PINGBACKS

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NONDEGENERATE STATES IN 3-D: SPHERICALLY SYMMETRIC SYSTEMS

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Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 12, Exercise 12.6.5.

Post date: 28 Jun 2017

[If some equations are too small to read easily, use your browser's magnifying option (Ctrl + on Chrome, probably something similar on other browsers).]

In solving the Schrödinger equation for spherically symmetric potentials, we found that we could reduce the problem to the equation

$$\left[-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}+V(r)+\frac{l(l+1)\hbar^2}{2\mu r^2}\right]U_{El}=EU_{El} \tag{1}$$

where $U_{El}(r)$ is related to the radial function by

$$R_{El}(r)=\frac{U_{El}(r)}{r} \tag{2}$$

We can write 1 as an eigenvalue equation for the operator D_l in the form

$$D_l(r)U_{El}=EU_{El} \tag{3}$$

with

$$D_l(r)\equiv-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}+V(r)+\frac{l(l+1)\hbar^2}{2\mu r^2} \tag{4}$$

We can show that, provided $U_{El}(r)\to 0$ as $r\to 0$, there are no degenerate eigenstates (that is, any state U_{El} that is an eigenstate with energy E is unique up to a scaling factor). The proof is similar to that in 1-d quantum mechanics, and goes by contradiction.

We suppose that there are two different functions U_1 and U_2 that satisfy 1 for the same energy E (and same angular momentum number l). We then have

$$\left[-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}+V(r)+\frac{l(l+1)\hbar^2}{2\mu r^2}\right]U_1=EU_1 \tag{5}$$

$$\left[-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}+V(r)+\frac{l(l+1)\hbar^2}{2\mu r^2}\right]U_2=EU_2 \tag{6}$$

Multiply the first by U_2 and the second by U_1 and subtract to get

$$U_2U_1''-U_1U_2''=0 \tag{7}$$

This expression is

$$U_2U_1''-U_1U_2''=\frac{d}{dr}\left(U_2U_1'-U_1U_2'\right)=0 \tag{8}$$

which we can integrate to get

$$U_2U_1'-U_1U_2'=C \tag{9}$$

for some constant C. This relation is valid for all r, so we can choose $r=0$ where $U_2(0)=U_1(0)=0$, which shows that $C=0$. Therefore

$$\frac{U_1'}{U_1}=\frac{U_2'}{U_2} \tag{10}$$

Integrating gives us

$$\ln U_1=\ln U_2+K \tag{11}$$

for some other constant K, so

$$U_1=e^KU_2 \tag{12}$$

That is, any two eigenfunctions with the same eigenvalue E are multiples of each other, so represent the same state, which is nondegenerate.

Note that the derivation didn't rely on the value of U anywhere except at $r=0$, so there is no requirement that, for example, $U\to 0$ as $r\to\infty$. Also, the derivation is valid whatever the sign of E.

FREE PARTICLE IN SPHERICAL COORDINATES: FINDING THE SOLUTIONS

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Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 12, Exercise 12.6.6.

Post date: 29 Jun 2017

[If some equations are too small to read easily, use your browser's magnifying option (Ctrl + on Chrome, probably something similar on other browsers).]

In solving the Schrödinger equation for spherically symmetric potentials, we found that we could reduce the problem to the equation

$$\left[-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}+V(r)+\frac{l(l+1)\hbar^2}{2\mu r^2}\right]U_{El}=EU_{El} \tag{1}$$

where $U_{El}(r)$ is related to the radial function by

$$R_{El}(r)=\frac{U_{El}(r)}{r} \tag{2}$$

For a free particle, $V=0$ and $E>0$, so we have

$$\left[-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}+\frac{l(l+1)\hbar^2}{2\mu r^2}\right]U_{El}=EU_{El} \tag{3}$$

Defining

$$k^2 \equiv \frac{2\mu E}{\hbar^2} \tag{4}$$

$$\rho \equiv kr \tag{5}$$

we convert the equation to

$$\left(-\frac{d^2}{d\rho^2}+\frac{l(l+1)}{\rho^2}\right)U_l=U_l \tag{6}$$

This equation can be solved by a method similar to that for the harmonic oscillator and its raising and lowering operators. The entire solution is fairly involved, so we'll start out here by showing how the new raising and lowering operators are defined.

We define

$$d_l \equiv \frac{d}{d\rho} + \frac{l+1}{\rho} \tag{7}$$

The adjoint is

$$d_l^\dagger = -\frac{d}{d\rho} + \frac{l+1}{\rho} \tag{8}$$

To see where the minus sign comes from on the RHS, we need to recall that the momentum operator is defined in one dimension as

$$P = -i\hbar\frac{\partial}{\partial x} \tag{9}$$

Since P is an observable, it is hermitian, so that $P^\dagger = P$. Under the hermitian operation $i \to -i$, so we must also have $\frac{\partial}{\partial x} \to -\frac{\partial}{\partial x}$. Thus the first derivative with respect to a position variable is anti-hermitian. If this doesn't convince you, you can also work out the integral:

$$\int_0^\infty \psi_2^* \frac{d}{d\rho}\psi_1 d\rho = \psi_2^*\psi_1|_0^\infty - \int_0^\infty \psi_1 \frac{d}{d\rho}\psi_2^* d\rho \tag{10}$$

Under the usual assumption that $\psi \to 0$ at the limits, the integrated term is zero and we have

$$\int_0^\infty \psi_2^* \frac{d}{d\rho}\psi_1 d\rho = -\int_0^\infty \psi_1 \frac{d}{d\rho}\psi_2^* d\rho \tag{11}$$

$$= -\left[\int_0^\infty \psi_1^* \frac{d}{d\rho}\psi_2 d\rho\right]^* \tag{12}$$

In bracket notation, this is

$$\left\langle \psi_2 \middle| \frac{d}{d\rho}\psi_1 \right\rangle = -\left\langle \frac{d}{d\rho}\psi_2 \middle| \psi_1 \right\rangle \tag{13}$$

which shows that $\frac{d}{d\rho}$ is an anti-hermitian operator.
Returning to 7 and 8, we have

$$d_l d_l^\dagger U_l = \left(\frac{d}{d\rho} + \frac{l+1}{\rho}\right)\left(-\frac{d}{d\rho} + \frac{l+1}{\rho}\right) U_l \tag{14}$$

$$= \left(\frac{d}{d\rho} + \frac{l+1}{\rho}\right)\left(-U_l' + \frac{l+1}{\rho} U_l\right) \tag{15}$$

$$= -U_l'' - \frac{l+1}{\rho^2} U_l + \frac{l+1}{\rho} U_l' - \frac{l+1}{\rho} U_l' + \frac{(l+1)^2}{\rho^2} U_l \tag{16}$$

$$= -U_l'' + \frac{l\,(l+1)}{\rho^2} U_l \tag{17}$$

Comparing with 6 we see that

$$d_l d_l^\dagger U_l = U_l \tag{18}$$

We can also show that

$$d_l^\dagger d_l U_l = \left(-\frac{d}{d\rho} + \frac{l+1}{\rho}\right)\left(\frac{d}{d\rho} + \frac{l+1}{\rho}\right) U_l \tag{19}$$

$$= \left(-\frac{d}{d\rho} + \frac{l+1}{\rho}\right)\left(U_l' + \frac{l+1}{\rho} U_l\right) \tag{20}$$

$$= -U_l'' + \frac{l+1}{\rho^2} U_l - \frac{l+1}{\rho} U_l' + \frac{l+1}{\rho} U_l' + \frac{(l+1)^2}{\rho^2} U_l \tag{21}$$

$$= -U_l'' + \frac{(l+1)^2 + l + 1}{\rho^2} U_l \tag{22}$$

$$= -U_l'' + \frac{(l+1)\,(l+2)}{\rho^2} U_l \tag{23}$$

$$= d_{l+1} d_{l+1}^\dagger U_l \tag{24}$$

Starting from 18 we multiply on the left by $d_l^\dagger$ to get

$$d_l^\dagger d_l \left(d_l^\dagger U_l\right) = d_l^\dagger U_l \tag{25}$$

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$$U_0^A(\rho) = \sin\rho \tag{28}$$
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From here, we can generate solutions for higher values of l by applying 26. Actually, the radial function that appears in the wave function is given by 2, so it is R_l that we really want. That is, we want

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$$R_l = \frac{U_l}{\rho} \tag{32}$$

Applying 26 we have

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$$= \left(-\frac{d}{d\rho} + \frac{l+1}{\rho}\right)(\rho R_l) \tag{34}$$
$$= -R_l - \rho R_l' + (l+1)R_l \tag{35}$$
$$= -\rho R_l' + lR_l \tag{36}$$
$$R_{l+1} = \left(-\frac{d}{d\rho} + \frac{l}{\rho}\right)R_l \tag{37}$$
$$= -\rho^l \frac{d}{d\rho}\left(\frac{R_l}{\rho^l}\right) \tag{38}$$

We can convert this into a general formula by writing

$$\frac{R_{l+1}}{\rho^{l+1}} = \left(-\frac{1}{\rho}\frac{d}{d\rho}\right)\frac{R_l}{\rho^l} \tag{39}$$

Starting at $l = 0$, we have

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For the next step, we have

$$\frac{R_2}{\rho^2} = \left(-\frac{1}{\rho}\frac{d}{d\rho}\right)\frac{R_1}{\rho^1} \tag{41}$$

$$= \left(-\frac{1}{\rho}\frac{d}{d\rho}\right)\left(-\frac{1}{\rho}\frac{d}{d\rho}\right)\frac{R_0}{\rho^0} \tag{42}$$

$$= \left(-\frac{1}{\rho}\frac{d}{d\rho}\right)^2\frac{R_0}{\rho^0} \tag{43}$$

Thus in general

$$\frac{R_{l+1}}{\rho^{l+1}} = \left(-\frac{1}{\rho}\frac{d}{d\rho}\right)^{l+1}\frac{R_0}{\rho^0} \tag{44}$$

Note that

$$\left(-\frac{1}{\rho}\frac{d}{d\rho}\right)^{l+1} \neq \left(-\frac{1}{\rho}\right)^{l+1}\frac{d^{l+1}}{d\rho^{l+1}} \tag{45}$$

since the factor of $\frac{1}{\rho}$ has to be included when taking the derivative.
We'll explore the nature of these solutions in the next post.

PINGBACKS

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Pingback: spherical bessel functions: behaviour for small arguments
Pingback: Free particle in spherical coordinates

SPHERICAL BESSEL FUNCTIONS: BEHAVIOUR FOR SMALL ARGUMENTS

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Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 12, Exercise 12.6.7.

Post date: 30 Jun 2017

[If some equations are too small to read easily, use your browser's magnifying option (Ctrl + on Chrome, probably something similar on other browsers).]

The general solution for a free particle in spherical coordinates involves the radial function, which turns out to be

$$\frac{R_{l+1}}{\rho^{l+1}} = \left(-\frac{1}{\rho}\frac{d}{d\rho}\right)^{l+1}\frac{R_0}{\rho^0} \tag{1}$$

where l is the total angular momentum quantum number and

$$k^2 \equiv \frac{2\mu E}{\hbar^2} \tag{2}$$

$$\rho \equiv kr \tag{3}$$

We can rewrite this as

$$R_l = (-\rho)^l\left(\frac{1}{\rho}\frac{d}{d\rho}\right)^l R_0 \tag{4}$$

We saw earlier that the solutions for $l = 0$ are, with $U_l = \rho R_l$

$$U_0^A(\rho) = \sin\rho \tag{5}$$

$$U_0^B(\rho) = -\cos\rho \tag{6}$$

Thus the two solutions for $l = 0$ are

$$R_0^A = \frac{\sin\rho}{\rho} \tag{7}$$

$$R_0^B = -\frac{\cos\rho}{\rho} \tag{8}$$

From these starting points, we can generate all the solutions for higher values of l using 4. These functions are

$$j_l(\rho) = (-\rho)^l \left(\frac{1}{\rho}\frac{d}{d\rho}\right)^l \frac{\sin\rho}{\rho} \tag{9}$$

$$n_l(\rho) = -(-\rho)^l \left(\frac{1}{\rho}\frac{d}{d\rho}\right)^l \frac{\cos\rho}{\rho} \tag{10}$$

and are known as spherical Bessel functions j_l and spherical Neumann functions n_l.

The asymptotic behaviour is given by

$$j_l \underset{\rho\to\infty}{\longrightarrow} \frac{1}{\rho}\sin\left(\rho - \frac{l\pi}{2}\right) \tag{11}$$

$$n_l \underset{\rho\to\infty}{\longrightarrow} -\frac{1}{\rho}\cos\left(\rho - \frac{l\pi}{2}\right) \tag{12}$$

For $\rho \to 0$, we have

$$j_l \underset{\rho\to 0}{\longrightarrow} \frac{\rho^l}{(2l+1)!!} \tag{13}$$

$$n_l \underset{\rho\to 0}{\longrightarrow} -\frac{(2l-1)!!}{\rho^{l+1}} \tag{14}$$

We can verify the latter equation for j_l for a couple of cases with small l. From 9, we can generate a couple of j_ls:

$$j_0 = \frac{\sin\rho}{\rho} \tag{15}$$

$$j_1 = -\rho\frac{1}{\rho}\frac{d}{dr}\left(\frac{\sin\rho}{\rho}\right) \tag{16}$$

$$= -\rho\frac{1}{\rho}\left(\frac{\cos\rho}{\rho} - \frac{\sin\rho}{\rho^2}\right) \tag{17}$$

$$= \frac{\sin\rho}{\rho^2} - \frac{\cos\rho}{\rho} \tag{18}$$

$$j_2 = (-\rho)^2\frac{1}{\rho}\frac{d}{d\rho}\left[\frac{1}{\rho}\frac{d}{dr}\left(\frac{\sin\rho}{\rho}\right)\right] \tag{19}$$

$$(-\rho)^2\frac{1}{\rho}\frac{d}{d\rho}\left[\frac{1}{\rho}\left(\frac{\cos\rho}{\rho} - \frac{\sin\rho}{\rho^2}\right)\right] \tag{20}$$

$$= \left(\frac{3}{\rho^3} - \frac{1}{\rho}\right)\sin\rho - \frac{3\cos\rho}{\rho^2} \tag{21}$$

We can get the limits for $\rho \to 0$ by expanding the sine and cosine. That is, we use the limiting forms

$$\sin\rho \quad \to \quad \rho - \frac{\rho^3}{3!} + \ldots \tag{22}$$

$$\cos\rho \quad \to \quad 1 - \frac{1}{2}\rho^2 + \ldots \tag{23}$$

We need to retain enough terms for j_l so that we get all the terms up to the first power of ρ that doesn't cancel out when we do the algebra. We get

$$j_0 \to 1 = \frac{\rho^0}{1!!} \tag{24}$$

$$j_1 \to \frac{1}{\rho} - \frac{\rho}{6} - \frac{1}{\rho}\left(1 - \frac{1}{2}\rho^2\right) \tag{25}$$

$$= \frac{\rho}{3} = \frac{\rho^1}{3!!} \tag{26}$$

$$j_2 \to \left(\frac{3}{\rho^3} - \frac{1}{\rho}\right)\left(\rho - \frac{\rho^3}{6} + \frac{\rho^5}{120}\right) - \frac{3}{\rho^2}\left(1 - \frac{1}{2}\rho^2 + \frac{1}{24}\rho^4\right) \tag{27}$$

$$\to \left(\frac{1}{6} + \frac{1}{40} - \frac{1}{8}\right)\rho^2 \tag{28}$$

$$= \frac{20+3-15}{120}\rho^2 \tag{29}$$

$$= \frac{\rho^2}{15} = \frac{\rho^2}{5!!} \tag{30}$$

PINGBACKS

Pingback: free particle moving in the z direction

FREE PARTICLE MOVING IN THE Z DIRECTION

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 12, Exercise 12.6.10.

Post date: 3 Jul 2017

[If some equations are too small to read easily, use your browser's magnifying option (Ctrl + on Chrome, probably something similar on other browsers).]

The radial function for a free particle can be either a spherical Bessel function j_l or a spherical Neumann function n_l. If the solution space includes the origin, then only j_l is acceptable since the n_l functions diverge as $r \to 0$.

In rectangular coordinates, a free particle wave function has the form

$$\psi_E(x,y,z) = \frac{1}{(2\pi\hbar)^{3/2}} e^{i\mathbf{p}\cdot\mathbf{r}/\hbar} \tag{1}$$

where the energy E is

$$E = \frac{p^2}{2\mu} = \frac{\hbar^2 k^2}{2\mu} \tag{2}$$

For a free particle travelling in the z direction, this becomes

$$\psi_E(r,\theta,\phi) = \frac{1}{(2\pi\hbar)^{3/2}} e^{ikr\cos\theta} \tag{3}$$

since $z = r\cos\theta$.

Since the solutions of the free-particle Schrödinger equation in spherical coordinations form a complete set, we must be able to express this wave function as a linear combination of these solutions, so that

$$e^{ikr\cos\theta} = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} C_l^m j_l(kr) Y_l^m(\theta,\phi) \tag{4}$$

where the C_l^m are constants. Because we're looking at motion in the z direction, there is no angular momentum about the z axis, which is reflected in the fact that ψ_E does not depend on ϕ. Thus $L_z = m\hbar = 0$ and $m = 0$. We therefore have

$$e^{ikr\cos\theta} = \sum_{l=0}^{\infty} C_l^0 j_l(kr) Y_l^0(\theta,\phi) \tag{5}$$

$$= \sum_{l=0}^{\infty} \sqrt{\frac{2l+1}{4\pi}} C_l^0 j_l(kr) P_l(\cos\theta) \tag{6}$$

$$= \sum_{l=0}^{\infty} C_l j_l(kr) P_l(\cos\theta) \tag{7}$$

where

$$C_l \equiv \sqrt{\frac{2l+1}{4\pi}} C_l^0 \tag{8}$$

The problem, of course, is to find these constants. We can do this using the identities given by Shankar in his problem 12.6.10, which are

$$\int_{-1}^{1} P_l(x) P_{l'}(x)\, dx = \frac{2\delta_{ll'}}{2l+1} \tag{9}$$

$$P_l(x) = \frac{1}{2^l l!} \frac{d^l \left(x^2-1\right)^l}{dx^l} \tag{10}$$

$$= \frac{(-1)^l}{2^l l!} \frac{d^l \left(1-x^2\right)^l}{dx^l} \tag{11}$$

$$\int_0^1 \left(1-x^2\right)^m dx = \frac{(2m)!!}{(2m+1)!!} \tag{12}$$

$$\int_{-1}^1 \left(1-x^2\right)^m dx = \frac{2(2m)!!}{(2m+1)!!} \tag{13}$$

The last line follows because $\left(1-x^2\right)^m$ is an even function and is therefore symmetric about $x = 0$.

We can use the standard procedure for isolating C_l by multiplying both sides by C_a and using 9.

$$\int_{-1}^{1} P_a(x) e^{ikrx} dx = \sum_{l=0}^{\infty} C_l j_l(kr) \int_{-1}^{1} P_a(x) P_l(x)\, dx \tag{14}$$

$$= \frac{2}{2a+1} C_a j_a(kr) \tag{15}$$

This relation must be true for all values of r, so we can look at the limit of small (but not zero, since both sides are then zero) r. We have the asymptotic relation for the spherical Bessel functions

$$j_l \underset{\rho\to 0}{\longrightarrow} \frac{\rho^l}{(2l+1)!!} \tag{16}$$

We thus have

$$\int_{-1}^{1} P_a(x)\, e^{ikrx} dx \underset{r\to 0}{\longrightarrow} \frac{2}{2a+1}\frac{k^a r^a}{(2a+1)!!} C_a \tag{17}$$

We can then look at the integral on the LHS and hope that, when we expand the exponential, that the terms in $(kr)^n$ for $n < a$ vanish. We can then match the coefficients of $(kr)^a$ on both sides to find C_a.

We can see that this will work because the Legendre polynomials P_l are a complete set of functions, and the polynomial P_l has degree l. This means that *any* polynomial of degree $a-1$ can be written as a linear combination of the P_l, where $l = 0, \ldots, a-1$. Because of 9, this means that

$$\int_{-1}^{1} x^l P_a(x)\, dx = 0 \text{ if } l < a \tag{18}$$

Therefore, when we expand e^{ikrx} in a power series, we have

$$\int_{-1}^{1} P_a(x)\, e^{ikrx} dx = \int_{-1}^{1} P_a(x) \left(1 + ikrx + \frac{(ikrx)^2}{2!} + \ldots\right) dx \tag{19}$$

$$= \int_{-1}^{1} P_a(x) \left(\frac{(ikrx)^a}{a!} + \ldots\right) dx \tag{20}$$

In the limit of small r, higher order terms in the sum on the RHS can be ignored, so we get

$$\frac{(ikr)^a}{a!}\int_{-1}^{1} x^a P_a(x)\, dx = \frac{2}{2a+1}\frac{k^a r^a}{(2a+1)!!} C_a \tag{21}$$

$$C_a = \frac{i^a (2a+1)(2a+1)!!}{2a!}\int_{-1}^{1} x^a P_a(x)\, dx \tag{22}$$

Now consider the integral in the last line. Using 11 we have

$$\int_{-1}^{1} x^a P_a(x)\, dx = \frac{(-1)^a}{2^a a!}\int_{-1}^{1} x^a \frac{d^a\left(1-x^2\right)^a}{dx^a} dx \tag{23}$$

We can integrate by parts repeatedly until the derivative in the integrand disappears. Note that the nth derivative of $\left(1-x^2\right)^a$ will always contain a factor of $\left(1-x^2\right)$ to some power for any $n < a$, and thus is zero at both limits of integration. Since the integrated term in the integration by parts always contains such a derivative, all integrated terms are zero at both limits.

We therefore integrate $\frac{d^a\left(1-x^2\right)^a}{dx^a}$ (a times) and differentiate x^a (a times) and keep only the residual integral after each iteration. The differentiation of x^a (a times) introduces a factor of $a!$. Since the sign of the residual integral alternates as we perform each integration by parts, the final result is

$$\int_{-1}^{1} x^a P_a(x)\,dx = \frac{(-1)^{2a}}{2^a a!} a! \int_{-1}^{1} \left(1-x^2\right)^a dx \tag{24}$$

$$= \frac{1}{2^a}\frac{2\,(2a)!!}{(2a+1)!!} \tag{25}$$

where we used 13 in the last line. The double factorial in the numerator can be written as

$$\begin{aligned}(2a)!! &= (2a)(2a-2)\ldots(4)(2) &(26)\\ &= 2^a a(a-1)\ldots(2)(1) &(27)\\ &= 2^a a! &(28)\end{aligned}$$

We therefore have

$$\begin{aligned}\int_{-1}^{1} x^a P_a(x)\,dx &= \frac{1}{2^a}\frac{2\times 2^a a!}{(2a+1)!!} &(29)\\ &= \frac{2a!}{(2a+1)!!} &(30)\end{aligned}$$

Plugging this back into 22 we have

$$C_a = i^a(2a+1) \tag{31}$$

The wave function for a free particle moving in the z direction is therefore

$$\psi_E(r,\theta,\phi) = \frac{1}{(2\pi\hbar)^{3/2}}\sum_{l=0}^{\infty} i^a(2a+1)\,j_l(kr)\,P_l(\cos\theta) \tag{32}$$

ISOTROPIC HARMONIC OSCILLATOR IN 3-D: USE OF SPHERICAL HARMONICS

Link to: physicspages home page.

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Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 12, Exercise 12.6.11.

Post date: 4 Jul 2017

[If some equations are too small to read easily, use your browser's magnifying option (Ctrl + on Chrome, probably something similar on other browsers).]

We've solved the 3-d isotropic harmonic oscillator before, so we've already solved most of Shankar's exercise 12.6.11. We can quote the results here. The solution has the form

$$\psi_{Elm} = \frac{U_{El}(r)}{r} Y_l^m(\theta, \phi) \tag{1}$$

The earlier solution uses notation from Griffiths's book, but as the end result is the same, it's not worth going through the derivation again using Shankar's notation.

The potential is

$$V(r) = \frac{1}{2} m\omega^2 r^2 \tag{2}$$

The radial equation to be solved is

$$\frac{d^2u}{d\rho^2} = \left(-1 + \frac{l(l+1)}{\rho^2} + \rho_0^2 \rho^2 \right) u \tag{3}$$

If we define

$$\kappa^2 \equiv \frac{2\mu E}{\hbar^2} \tag{4}$$

$$\rho \equiv \kappa r \tag{5}$$

$$\rho_0 \equiv \frac{\mu\omega}{\hbar\kappa^2} = \frac{\hbar\omega}{2E} \tag{6}$$

Taking the asymptotic behaviour of the radial function for small and large r into account leads us to a solution of form

$$u(\rho) = \rho^{l+1} e^{-\rho_0 \rho^2/2} v(\rho) \tag{7}$$

Note that Griffiths's v is not the same as Shankar's v, the latter of which is defined by Shankar's equation 12.6.49.

This gives a differential equation for Griffiths's v

$$\rho\frac{d^2v}{d\rho^2}+2\left(l+1-\rho_0\rho^2\right)\frac{dv}{d\rho}+\rho(1-\rho_0(2l+3))v=0 \tag{8}$$

The function v can be solved as a power series, giving

$$v(\rho)=\sum c_j\rho^j \tag{9}$$

Substituting into 8 leads to the recursion relation

$$c_{q+2}=\frac{\rho_0(2q+2l+3)-1}{(q+2)(q+2l+3)}c_q \tag{10}$$

with $c_1=0$, so that $c_q=0$ for all odd q. The requirement that the series terminates at some finite value of j leads to the quantization condition on E:

$$E = \hbar\omega\left(q_{max}+l+\frac{3}{2}\right) \tag{11}$$

or, defining $n=q_{max}+l$,

$$E_n=\hbar\omega\left(n+\frac{3}{2}\right) \tag{12}$$

We worked out the degeneracies in the earlier post as well, so that the degeneracy of E_n is

$$d(n)=\frac{1}{2}(n+1)(n+2) \tag{13}$$

To complete Shankar's exercise, we need to work out the eigenfunctions for $n=0$ and $n=1$. For $n=0$, $q_{max}=l=0$, so only $c_0\neq 0$ and we have

$$\begin{aligned} v(\rho) &= c_0 && (14)\\ u(\rho) &= c_0\rho e^{-\rho_0\rho^2/2} && (15)\\ \psi_{000} &= \frac{u}{r}Y_0^0 && (16)\\ &= c_0\kappa e^{-\rho_0\rho^2/2}Y_0^0 && (17)\\ &= c_0\sqrt{\frac{2\mu 3\omega}{4\pi\hbar}}e^{-\mu\omega r^2/2\hbar} && (18)\end{aligned}$$

where in the fourth line we used

$$\kappa = \frac{\sqrt{2\mu E}}{\hbar} = \frac{\sqrt{2\mu \frac{3}{2}\hbar\omega}}{\hbar} = \sqrt{\frac{3\mu\omega}{\hbar}} \tag{19}$$

$$Y_0^0 = \frac{1}{\sqrt{4\pi}} \tag{20}$$

Normalizing this requires that

$$\int_0^{2\pi}\int_0^{\pi}\int_0^{\infty} \psi_{000}^2 r^2 \sin\theta dr\, d\theta\, d\phi = c_0^2 \frac{6\mu\omega}{\hbar}\int_0^{\infty} e^{-\mu\omega r^2/\hbar} r^2 dr \tag{21}$$

$$= 1 \tag{22}$$

This is a standard Gaussian integral and can be done using software or tables so we get

$$c_0 = \frac{\sqrt{6}}{3}\left(\frac{\mu\omega}{\pi\hbar}\right)^{1/4} \tag{23}$$

This gives a wave function of

$$\psi_{000} = \left(\frac{\mu\omega}{\pi\hbar}\right)^{3/4} e^{-\mu\omega r^2/2\hbar} \tag{24}$$

which agrees with the earlier result.
For $n = 1$, the degeneracy is, from 13

$$d(1) = 3 \tag{25}$$

The three possibilities are $m = 0, \pm 1$ which are reflected in the three spherical harmonics $Y_1^{0,\pm 1}$. The radial function is the same in all cases, and is obtained from $q_{max} = 0$, $l = 1$. From 7, this gives

$$v(\rho) = c_0 \tag{26}$$

$$u(\rho) = c_0 \rho^2 e^{-\rho_0\rho^2/2} \tag{27}$$

$$\psi_{11m} = \frac{u}{r} Y_1^m \tag{28}$$

$$= c_0 \kappa^2 r e^{-\rho_0\rho^2/2} Y_1^m \tag{29}$$

$$= c_0 \frac{5\mu\omega}{\hbar} r e^{-\mu\omega r^2/2\hbar} Y_1^m \tag{30}$$

Again, we work out c_0 by imposing normalization. For example

$$\psi_{111} = c_0 \frac{5\mu\omega}{\hbar} r e^{-\mu\omega r^2/2\hbar} Y_1^1 \tag{31}$$

$$= -c_0 \frac{5\mu\omega}{\hbar} r e^{-\mu\omega r^2/2\hbar} \sqrt{\frac{3}{8\pi}} \sin\theta e^{i\phi} \tag{32}$$

The normalization integral is

$$\int_0^{2\pi}\int_0^{\pi}\int_0^{\infty} \psi_{111}^2 r^2 \sin\theta dr\, d\theta\, d\phi = c_0^2 \left(\frac{5\mu\omega}{\hbar}\right)^2 \frac{3}{8\pi} 2\pi \int_0^{\pi}\int_0^{\infty} e^{-\mu\omega r^2/\hbar} r^4 \sin^3\theta dr\, d\theta \tag{33}$$

$$= c_0^2 \frac{75}{8} \sqrt{\frac{\pi\hbar}{\mu\omega}} = 1 \tag{34}$$

$$c_0 = \frac{2\sqrt{6}}{15} \left(\frac{\mu\omega}{\pi\hbar}\right)^{1/4} \tag{35}$$

I used Maple to do the integrals. This gives a wave function of

$$\psi_{111} = -\sqrt{\frac{\mu\omega}{\hbar}} \left(\frac{\mu\omega}{\pi\hbar}\right)^{3/4} r e^{-\mu\omega r^2/2\hbar} \sin\theta e^{i\phi} \tag{36}$$

We can work out the other two wave functions the same way (I used Maple, so I won't go into the details):

$$\psi_{11-1} = \sqrt{\frac{\mu\omega}{\hbar}} \left(\frac{\mu\omega}{\pi\hbar}\right)^{3/4} r e^{-\mu\omega r^2/2\hbar} \sin\theta e^{-i\phi} \tag{37}$$

$$\psi_{110} = \sqrt{\frac{2\mu\omega}{\hbar}} \left(\frac{\mu\omega}{\pi\hbar}\right)^{3/4} r e^{-\mu\omega r^2/2\hbar} \cos\theta \tag{38}$$

The ψ_{110} here is the same as ψ_{001} in our rectangular solution set. The other two are linear combinations of ψ_{100} and ψ_{010} from our rectangular set, which were (the suffixes in these 2 equations stand for x, y and z, and not n, l and m):

$$\psi_{100} = \sqrt{\frac{2m\omega}{\hbar}} \left(\frac{m\omega}{\pi\hbar}\right)^{3/4} e^{-m\omega r^2/2\hbar} r \sin\theta\cos\phi \tag{39}$$

$$\psi_{010} = \sqrt{\frac{2m\omega}{\hbar}} \left(\frac{m\omega}{\pi\hbar}\right)^{3/4} e^{-m\omega r^2/2\hbar} r \sin\theta\sin\phi \tag{40}$$

We have

$$\psi_{111} = \frac{1}{\sqrt{2}}(\psi_{100} + i\psi_{010}) \tag{41}$$

$$\psi_{11-1} = \frac{1}{\sqrt{2}}(\psi_{100} - i\psi_{010}) \tag{42}$$

RADIAL FUNCTION FOR LARGE R

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Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 12, Section 12.6.

Post date: 18 Jul 2017

[If some equations are too small to read easily, use your browser's magnifying option (Ctrl + on Chrome, probably something similar on other browsers).]

In solving the Schrödinger equation for spherically symmetric potentials, we found that we could reduce the problem to the equation

$$\left[-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}+V(r)+\frac{l(l+1)\hbar^2}{2\mu r^2}\right]U_{El}=EU_{El} \tag{1}$$

where $U_{El}(r)$ is related to the radial function by

$$R_{El}(r)=\frac{U_{El}(r)}{r} \tag{2}$$

We've looked at some properties of U_{El} (which Griffiths calls u) for the hydrogen atom, but we can also try to extract some information about U_{El} in the more general case where we don't need to specify the potential V precisely. Here we'll examine what happens as $r\to\infty$.

By looking at 1, we can see that the centrifugal barrier term (the last term in the square brackets) disappears for large r, so the behaviour is determined by the nature of the potential V. We might think that, provided $V\underset{r\to\infty}{\longrightarrow}0$, we can just ignore the potential and solve the reduced equation

$$\frac{d^2U_E}{dr^2}=-\frac{2\mu E}{\hbar^2}U_E \tag{3}$$

where we've dropped the subscript l since we're ignoring the centrifugal barrier, which is the only term in which l appears. In fact, this assumption proves to be faulty, in that the analysis is valid only if $V\to\frac{1}{r^a}$ where $a>1$, or in other words, if $rV(r)\to 0$. To see why, we need to consider two cases: $E>0$ (so that the particle can escape to infinity, since we're assuming $V\leq 0$ everywhere, and thus that E can take on any positive value); $E<0$, so that the particle is bound, and there are discrete energy levels. Shakar treats the

$E > 0$ case so we'll look at the $E < 0$ case. In this case, 3 has the general solution

$$U_E = Ae^{-\kappa r} + Be^{\kappa r} \tag{4}$$

where

$$\kappa = \sqrt{-\frac{2\mu E}{\hbar^2}} = \sqrt{\frac{2\mu |E|}{\hbar^2}} \tag{5}$$

In the most general case, the constants A and B can be anything, subject to the usual constraint that the overall wave function is normalized. However, in order for this normalization to occur, we can't have the $e^{\kappa r}$ term, since that terms blows up as $r \to \infty$. As we've seen in the specific example of the hydrogen atom, when we express the radial function as a series in powers of r, the series must terminate after a finite number of terms in order to keep the wave function finite, and it is this that results in the quantized energy levels. Although a direct link between the series solution and the form 4 isn't obvious, the net effect is that, when the energy has one of the allowed discrete values, the term $Be^{\kappa r}$ disappears from the asymptotic solution.

The form 4 is valid only under the restriction that $rV(r) \to 0$ for large r. To see why, suppose we write

$$U_E = f(r)\, e^{\pm \kappa r} \tag{6}$$

for some function f. If 4 is valid, then f should tend to a constant for large r. We can plug 6 into 1 and ignore the centrifugal term since we're looking only at large r. This gives

$$\frac{d^2U_E}{dr^2} - \frac{2\mu}{\hbar^2} V U_E - \kappa^2 U_E = 0 \tag{7}$$

Calculating the derivative, we have

$$\frac{dU_E}{dr} = \left(f' \pm \kappa f\right) e^{\pm \kappa r} \tag{8}$$

$$\frac{d^2U_E}{dr^2} = \left(f'' \pm \kappa f' \pm \kappa f' + \kappa^2 f\right) e^{\pm \kappa r} \tag{9}$$

$$= \left(f'' \pm 2\kappa f' + \kappa^2 f\right) e^{\pm \kappa r} \tag{10}$$

Plugging this into 7 we get

$$f'' \pm 2\kappa f' - \frac{2\mu}{\hbar^2} V f = 0 \tag{11}$$

At this point, Shankar assumes that f is slowly varying for large r, which seems reasonable, so we can disregard the second derivative, to get

$$f' = \mp \frac{\mu}{\kappa \hbar^2} V f \tag{12}$$

or

$$\frac{df}{f} = \mp \frac{\mu}{\kappa \hbar^2} V(r)\, dr \tag{13}$$

If we integrate this from some constant lower value r_0 up to an arbitrary large value r, we have

$$f(r) = f(r_0) \exp\left[\mp \frac{\mu}{\kappa \hbar^2} \int_{r_0}^{r} V\left(r'\right) dr' \right] \tag{14}$$

The point now is that if $V(r) \to \frac{1}{r^a}$ with $a > 1$, then the integral of V will be an inverse power of r, and thus will go to zero as $r \to \infty$. In that case, the RHS of 14 does indeed tend to a constant as $r \to \infty$, and the asymptotic solution 4 is valid. However, if $V = -\frac{e^2}{r}$ (the Coulomb potential, as found in the hydrogen atom), then the integral of V is a logarithm and does not tend to zero for large r. In this case, we get

$$f(r) = f(r_0) \exp\left[\pm \frac{\mu e^2}{\kappa \hbar^2} \ln \frac{r}{r_0} \right] \tag{15}$$

$$= \left[r_0^{\mp \mu e^2 / \kappa \hbar^2} f(r_0) \right] r^{\pm \mu e^2 / \kappa \hbar^2} \tag{16}$$

The quantity in square brackets is a constant, but the last factor is a power of r which, for the positive exponent, continues to grow as $r \to \infty$. Thus the asymptotic solution 4 is valid only for potentials that fall off faster than $\frac{1}{r}$ for large r.

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RADIAL FUNCTION FOR SMALL R

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Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 12, Section 12.6.

Post date: 18 Jul 2017

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where $U_{El}(r)$ is related to the radial function by

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We've looked at some properties of U_{El} (which Griffiths calls u) for the hydrogen atom, but we can also try to extract some information about U_{El} in the more general case where we don't need to specify the potential V precisely. Here we'll examine what happens as $r \to 0$.

The quantity in the square brackets in 1 is an operator which will call $D_l(r)$:

$$D_l(r)\equiv-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}+V(r)+\frac{l(l+1)\hbar^2}{2\mu r^2} \tag{3}$$

If we require D_L to be hermitian, this results in the condition that, for two functions U_1 and U_2,

$$U_1^*\frac{dU_2}{dr}\bigg|_0^\infty-U_2\frac{dU_1^*}{dr}\bigg|_0^\infty=0 \tag{4}$$

If we require U_{El} to be normalizable then it must satisfy either

$$U_{El}\underset{r\to\infty}{\longrightarrow}0 \tag{5}$$

which is valid for bound states where $E > V$ as $r \to \infty$, or

$$U_{El} \underset{r\to\infty}{\longrightarrow} e^{ikr} \tag{6}$$

where

$$k = \sqrt{\frac{2\mu E}{\hbar^2}} \tag{7}$$

if $E > V$ as $r \to \infty$. In the latter case, we're using the definition of normalization for an oscillating function. If $U_{El} \underset{r\to\infty}{\longrightarrow} 0$ then 4 is 0 at the upper limit. Using the normalization condition for oscillating functions, if $U_{El} \underset{r\to\infty}{\longrightarrow} e^{ikr}$ then 4 is also zero (on average) at the upper limit. Thus in order for D_l to be Hermitian, we must have

$$U_1^* \frac{dU_2}{dr}\bigg|_0 - U_2 \frac{dU_1^*}{dr}\bigg|_0 = 0 \tag{8}$$

at the lower limit as well.

One way of satisfying this condition is if

$$U_{El} \underset{r\to 0}{\longrightarrow} c \tag{9}$$

Because the actual radial function is given by 2, a value of $c \neq 0$ would give

$$R \sim \frac{U}{r} \sim \frac{c}{r} \tag{10}$$

Such a function is still square integrable because an integral over all space introduces a factor of r^2 in the volume element:

$$\int R^2 r^2 \sin\theta dr\, d\theta\, d\phi \tag{11}$$

Thus the integrand is still finite at $r = 0$ so the integral itself can be finite.

The problem with $c \neq 0$ is that the Laplacian of $\frac{1}{r}$ gives a delta function:

$$\nabla^2 \frac{1}{r} = -4\pi\delta^3(\mathbf{r}) \tag{12}$$

Unless the potential V has a delta function at the origin (which would be quite unusual), the ∇^2 in the Schrödinger equation can't be allowed to generate a delta function there, so we must have $c = 0$.

So far, everything is true for any potential. If we now assume that V is less singular than $\frac{1}{r^2}$ (that is, $V \underset{r\to 0}{\longrightarrow} \frac{1}{r^a}$ where $a < 2$), the centrifugal barrier term in 1 will dominate as $r \to 0$, so for small r, 1 reduces to the differential equation

$$U_l'' \simeq \frac{l\,(l+1)}{r^2} U_l \tag{13}$$

The E in the suffix of U has been dropped because the term involving E in 1 is negligible compared to the centrifugal barrier for $r \to 0$. This equation has solutions

$$U_l \sim r^{\alpha} \tag{14}$$

Plugging this into 13 we get

$$\alpha\,(\alpha-1) = l\,(l+1) \tag{15}$$

This is a quadratic equation in α which has the two solutions

$$\alpha = -l, l+1 \tag{16}$$

If we are to have $U_{El} \to 0$ as $r \to 0$, then we must discard the solution $U_l \sim r^{-l}$, so we have that

$$U_{El} \sim r^{l+1} \tag{17}$$

All of this works only if $l \neq 0$ since in the case where $l = 0$ (zero angular momentum), there is no centrifugal barrier and we must look at the form of the potential. Shankar notes that the problems he considers in his book are such that 17 is also valid for $l = 0$.

INFINITE SPHERICAL WELL - NUMERICAL SOLUTIONS

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

References: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Section 4.1.3 & Problem 4.8.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 12, Exercise 12.6.8.

Post date: 7 Jan 2013.

In the radial equation for the infinite spherical well, we found the solutions to involve the spherical Bessel functions j_l and the spherical Neumann functions n_l. We saw in the last post that the general solution was

$$u(r) = Arj_l(kr) + Brn_l(kr) \tag{1}$$

We can verify this explicity for $l = 1$ and $u(r) = rj_1(r)$ by using the derivative formula

$$\begin{aligned} j_1(x) &= -x\frac{1}{x}\frac{d}{dx}\left(\frac{\sin x}{x}\right) && (2)\\ &= \frac{\sin x}{x^2} - \frac{\cos x}{x} && (3)\\ rj_1(kr) &= \frac{\sin kr}{k^2 r} - \frac{\cos kr}{k} && (4) \end{aligned}$$

The radial equation for $l = 1$ is

$$\frac{d^2u}{dr^2} - \left(\frac{2}{r^2} - k^2\right)u = 0 \tag{5}$$

So we get (using Maple)

$$\begin{aligned} \frac{d^2u}{dr^2} &= \frac{1}{k^2r^3}\left[\sin kr\left(2 - k^2r^2\right) + \cos kr\left(k^3r^3 - 2\right)\right] && (6)\\ -\left(\frac{2}{r^2} - k^2\right)u &= -\frac{1}{k^2r^3}\left(k^2r^2 - 2\right)(kr\cos kr - \sin kr) && (7) \end{aligned}$$

Thus the first term cancels the second and the equation is satisfied.

For $l = 0$, the equation actually has a simple solution. We could either solve the original ODE in this case, or use the formula for j_0. From the latter, we get

$$u(r) = Arj_0(kr) \tag{8}$$
$$= \frac{A}{k}\sin kr \tag{9}$$

One of the properties of the spherical Neumann functions is that they all become infinite as $x \to 0$, so they have to be excluded from our general solution. From the continuity of the wave function at the boundary $r = a$, we must have

$$u(a) = 0 \tag{10}$$
$$\sin ka = 0 \tag{11}$$

from which we get

$$k = \frac{n\pi}{a} \tag{12}$$
$$\frac{\sqrt{2mE}}{\hbar} = \frac{n\pi}{a} \tag{13}$$
$$E = \frac{n^2\pi^2\hbar^2}{2ma^2} \tag{14}$$

This is the same set of energies as in the one dimensional infinite square well.

For higher values of l, as before, we have to exclude the n_l as they become infinite, so the general solution is

$$u(r) = Arj_l(kr) \tag{15}$$

To find the energies requires finding the zeroes of j_l, which has to be done numerically, since the condition $j_l(kr) = 0$ gives rise to transcendental equations (involving both r and a trigonometric function of r). Rough solutions can be found graphically, but a more accurate solution can be found using software such as Maple.

Maple has a BesselJZeros function which will find the zeroes of the Bessel functions of the first kind J_l (that's a capital J). As noted in the last post, these are *not* the same as the spherical Bessel functions we are using here. However, the two functions are related by a simple formula:

$$j_l(x) = \sqrt{\frac{\pi}{2x}}J_{l+\frac{1}{2}}(x) \tag{16}$$

This means that the zeroes of $j_1(x)$ are also the zeroes of $J_{n+1/2}(x)$. With this proviso, the first few zeroes can be found by calling Maple's BesselJZeroes(index, number), where 'index' is $l+\frac{1}{2}$ and 'number' is the ordinal number of the required zero (first, second, third, etc). The first three zeroes of $J_{\frac{3}{2}}$ are at $ka = 4.493, 7.725, 10.904$. If we denote the n^{th} zero as z_{1n}, then $ka = z_n$; $E_{1n} = \hbar^2 z_{1n}^2/2ma^2$. Thus the energies are $E_{11} = 20.187\frac{\hbar^2}{2ma^2}$; $E_{12} = 59.676\frac{\hbar^2}{2ma^2}$; $E_{13} = 118.897\frac{\hbar^2}{2ma^2}$. The same method can obviously be used to find the energy levels for larger l, where the graphical method becomes a lot more difficult due to the complexity of the equations.

The function for which we are finding the zeroes is

$$j_1(x) = \frac{\sin x}{x^2} - \frac{\cos x}{x} \tag{17}$$

where $x \equiv ka$. Thus the zeroes are at

$$\frac{\sin x}{x} - \cos x = 0 \tag{18}$$

$$\tan x = x \tag{19}$$

For large n, we are looking at large x, so the first term becomes negligible, and we are essentially looking for the zeroes of $\cos x$, which occur at $ka = (2n+1)\pi/2 = \pi(n+\frac{1}{2})$. Thus the energies are approximately $E_{1n} \approx \hbar^2\pi^2(n+1/2)^2/2ma^2$.

FINITE SPHERICAL WELL

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

References: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Problem 4.9.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 12, Exercise 12.6.9.

Post date: 7 Jan 2013.

A variant on the infinite spherical well is the finite spherical well, with potential

$$V(r) = \begin{cases} -V_0 & r < a \\ 0 & r > a \end{cases} \tag{1}$$

This problem is superficially like that of the finite square well in one dimension, but there is a crucial difference, which is that the variable r starts at 0 rather than $-a$, so we can't use the argument that the wave function is even or odd. However, we have worked out a similar one-dimensional problem with the hybrid square well, and we can adapt that solution to this problem.

The wave function must be found in the two regions separately, and then boundary conditions used to determine the energies.

For $r < a$, the radial equation is (with $l = 0$)

$$\begin{aligned} -\frac{\hbar^2}{2m}\frac{d^2u}{dr^2} - V_0 u &= Eu & (2) \\ \frac{d^2u}{dr^2} &= -\frac{2m}{\hbar^2}(V_0 + E)u & (3) \\ &\equiv -\mu^2 u & (4) \end{aligned}$$

where

$$\mu = \sqrt{\frac{2m(V_0 + E)}{\hbar^2}} \tag{5}$$

This has the general solution

$$u(r) = C\sin\mu r + D\cos\mu r \tag{6}$$

As with the infinite square well, we note that the actual radial function is $u(r)/r$, so we must eliminate the cosine term to keep the radial function finite at $r = 0$. Therefore

$$u(r) = C\sin\mu r \tag{7}$$

For $r > a$, the equation is

$$\frac{d^2u}{dr^2} = k^2u \tag{8}$$

where

$$k \equiv \sqrt{-\frac{2mE}{\hbar^2}} \tag{9}$$

Note that for a bound state, E is negative, so k is real. This equation has a general solution

$$u(r) = Ae^{kr} + Be^{-kr} \tag{10}$$

and in order for the function to remain finite at infinity, we must set $A = 0$ so we have:

$$u(r) = Be^{-kr} \tag{11}$$

Now for the boundary conditions. We have only one boundary, at $r = a$, so as with the square well in the one-dimensional case, we require the function and its first derivative to be continuous at the boundary. These conditions give us

$$C\sin\mu a = Be^{-ka} \tag{12}$$

$$\mu C\cos\mu a = -kBe^{-ka} \tag{13}$$

Eliminating the exponential by dividing these two equations gives us a condition similar to that in the square well case:

$$-\frac{\mu}{k} = \tan\mu a \tag{14}$$

We can look for solutions graphically. As before we introduce two variables

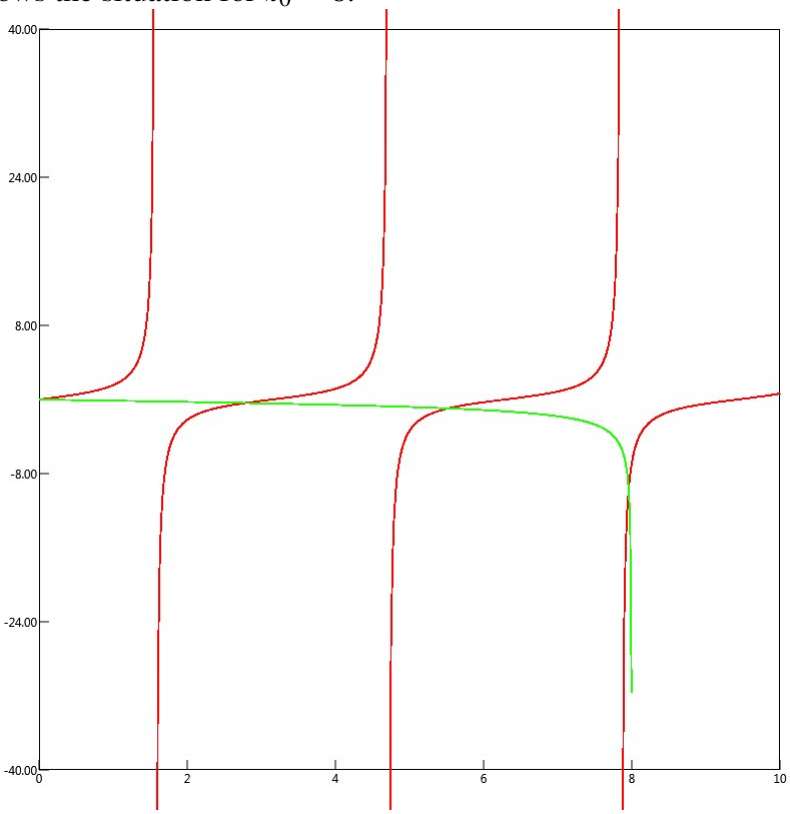
$$z \equiv \mu a \tag{15}$$

$$z_0 \equiv \frac{a}{\hbar}\sqrt{2mV_0} \tag{16}$$

Then $ka = \sqrt{z_0^2 - z^2}$ and the equation to solve is

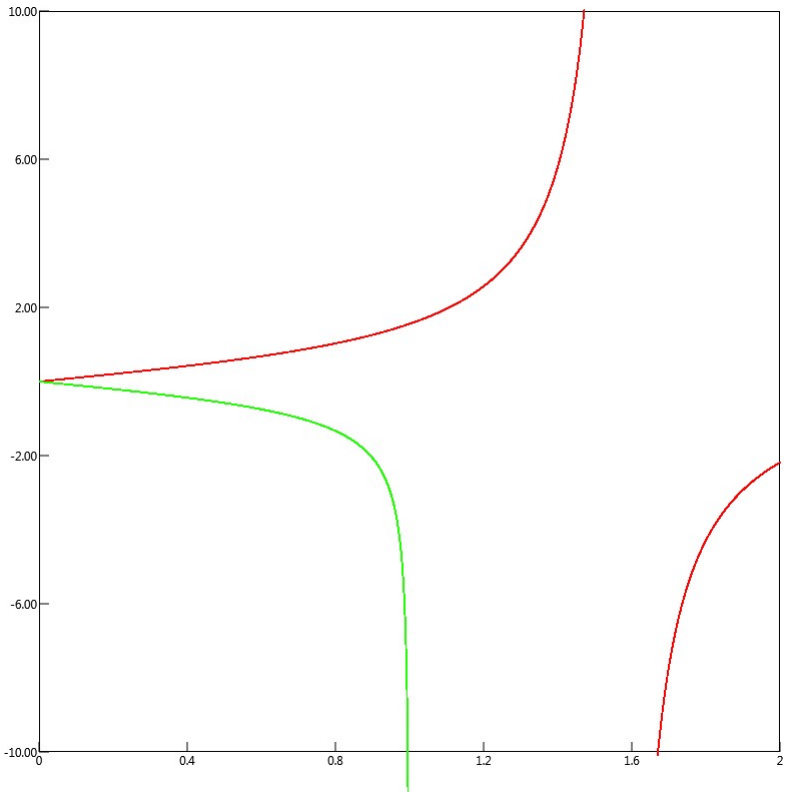
$$\tan z = \frac{-1}{\sqrt{z_0^2/z^2 - 1}} \tag{17}$$

The number of solutions depends on the value chosen for z_0. The plot shows the situation for $z_0 = 8$.



The green curve is $\frac{-1}{\sqrt{z_0^2/z^2-1}}$ and the red curve is $\tan z$. In this case we can see there are 3 intersections, so here there are 3 bound states. The precise values of the energies can be found by solving the equation numerically using software such as Maple's fsolve command.

The asymptote of $\frac{-1}{\sqrt{z_0^2/z^2-1}}$ is at $z = z_0$ so since the first asymptote for the tangent is at $z = \pi/2$, clearly if $z_0 < \pi/2$ the two curves will not intersect. The following plot shows the situation for $z_0 = 1$:



The condition $z_0 < \pi/2$ translates into

$$V_0 a^2 < \frac{\hbar^2 \pi^2}{8m} \tag{18}$$

Incidentally, the intersection at $z = 0$ isn't a physical solution, since it implies $E = -V_0$, which in turn means $d^2u/dr^2 = 0$ and $\mu = 0$, giving $u = Cr + D$, $R = u/r = C + D/r$. To avoid infinity at the origin, we must have $B = 0$, and to satisfy continuity of the wave function and its derivative at $r = a$ (see above) gives $C = Be^{-ka}$ for the wave function and $-kBe^{-ka} = 0$ for its derivative. The latter condition means $B = 0$ and hence $C = 0$, meaning the wave function is zero everywhere and not normalizable.

SCHRÖDINGER EQUATION IN THREE DIMENSIONS - THE RADIAL EQUATION

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

Reference: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Sec 4.1.3.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 12, Exercise 12.6.2.

Post date: 28 Mar 2011.

[If some equations are too small to read easily, use your browser's magnifying option (Ctrl + on Chrome, probably something similar on other browsers).]

When we considered the solution of the Schrödinger equation in three dimensions, we found that the general solution separated neatly into a product of three functions, one for each variable in spherical coordinates.

The Schrödinger equation in three dimensions can be written as

$$-\frac{\hbar^2}{2m}\nabla^2\Psi + V\Psi = i\hbar\frac{\partial\Psi}{\partial t} \tag{1}$$

If we assume that the potential $V = V(x, y, z)$ is independent of time, we can use the same separation of variables method that we used in one dimension to split off the time part of the solution to get

$$\Psi(x, y, z, t) = \psi(x, y, z)e^{-iEt/\hbar} \tag{2}$$

where, as before, the energy E takes on a set of discrete values for the bound states and a set of continuous values for the scattering, or unbound, states. The spatial wave function ψ satisfies the time-independent Schrödinger equation:

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = E\psi \tag{3}$$

So far, the analysis is the same as that for one dimension.

Using separation of variables in the form $\psi(r, \theta, \phi) = R(r)Y(\theta, \phi)$ we got two separated equations:

$$\frac{1}{R}\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right)-\frac{2mr^2}{\hbar^2}(V-E) = l(l+1) \quad (4)$$

$$\frac{1}{Y\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right)+\frac{1}{Y\sin^2\theta}\left(\frac{\partial^2 Y}{\partial\phi^2}\right) = -l(l+1) \quad (5)$$

where $l(l+1)$ is a constant term.

We found that the angular equation could be solved and that the solutions were the spherical harmonics:

$$Y_l^m(\theta,\phi)=\left[\frac{2l+1}{4\pi}\frac{(p-m)!}{(p+m)!}\right]^{1/2}e^{im\phi}P_l^m(\cos\theta) \quad (6)$$

They obey the normalization condition

$$\int_0^{2\pi}\int_0^{\pi}(Y_l^m)^*Y_{l'}^{m'}\sin\theta d\theta d\phi=\delta_{ll'}\delta_{mm'} \quad (7)$$

Returning to the radial function we find that we can actually make one further transformation of the equation that makes it a bit easier to solve in some cases. We can rewrite the equation using total derivatives, since $R(r)$ depends only on r:

$$\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)-\frac{2mr^2}{\hbar^2}(V-E)R=l(l+1)R \quad (8)$$

We can now make the substitution

$$u(r) \equiv rR \quad (9)$$

$$R = \frac{u}{r} \quad (10)$$

$$\frac{dR}{dr} = -\frac{u}{r^2}+\frac{u'}{r} \quad (11)$$

$$= \frac{1}{r^2}(ru'-u) \quad (12)$$

$$\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) = u'+ru''-u' \quad (13)$$

$$= ru'' \quad (14)$$

The radial equation then becomes

$$r\frac{d^2u}{dr^2} - \frac{2mr}{\hbar^2}(V-E)u = l(l+1)\frac{u}{r} \tag{15}$$

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dr^2} + \left(V + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}\right)u = Eu \tag{16}$$

In this form, the equation looks like the original one-dimensional Schrödinger equation with the wave function given by u and the potential given by

$$V_{rad} = V + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2} \tag{17}$$

The extra term $\frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}$ is called the centrifugal term. Classically, the force due to this term is:

$$F_{cent} = -\frac{d}{dr}\frac{\hbar^2}{2m}\frac{l(l+1)}{r^2} \tag{18}$$

$$= \frac{\hbar^2}{m}\frac{l(l+1)}{r^3} \tag{19}$$

which is a force that tends to repel the particle from the origin (the force gets larger the closer to the origin we are). Thus it is analogous to the pseudo-force known as the centrifugal force in classical physics.

PINGBACKS

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DIRAC DELTA FUNCTION IN THREE DIMENSIONS

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

Reference: Griffiths, David J. (2007) Introduction to Electrodynamics, 3rd Edition; Prentice Hall - Sec. 1.5.3, Problem 2.46.

Post date: 14 Nov 2011.

We've seen that we can define a curious function called the Dirac delta function in one dimension. Here we examine how this can be extended to three dimensions, and how this extension is relevant to electrostatics.

The easiest way to define a three-dimensional delta function is just to take the product of three one-dimensional functions:

$$\delta_3(\mathbf{r}) \equiv \delta(x)\delta(y)\delta(z) \tag{1}$$

The integral of this function over any volume containing the origin is again 1, and the integral of any function of $\mathbf{r}$ is a simple extension of the one-dimensional case:

$$\int f(\mathbf{r})\delta_3(\mathbf{r}-\mathbf{a})d^3\mathbf{r} = f(\mathbf{a}) \tag{2}$$

In electrostatics, there is one situation where the delta function is needed to explain an apparent inconsistency involving the divergence theorem. If we have a point charge q at the origin, the electric field of that charge is

$$\mathbf{E} = \frac{1}{4\pi\epsilon_0}\frac{q}{r^2}\hat{\mathbf{r}} \tag{3}$$

According to the divergence theorem, the surface integral of the field is equal to the volume integral of the divergence of that field:

$$\oint \mathbf{E}\cdot d\mathbf{a} = \int_V \nabla\cdot\mathbf{E}d^3\mathbf{r} \tag{4}$$

where the integral on the left is over some closed surface, and that on the right is over the volume enclosed by the surface. In electrostatics, the integral on the right evaluates to the total charge contained in the volume divided by ϵ_0

$$\int_V \nabla\cdot\mathbf{E}d^3\mathbf{r} = \frac{q}{\epsilon_0} \tag{5}$$

Now for the catch. If we calculate $\nabla \cdot \mathbf{E}$ (in spherical coordinates) for the point charge, we get, since only the radial component of the field is non-zero:

$$\begin{aligned} \nabla \cdot \mathbf{E} &= \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 E_r\right) && (6) \\ &= \frac{q}{4\pi\epsilon_0}\frac{1}{r^2}\frac{\partial(1)}{\partial r} && (7) \end{aligned}$$

At this stage, we might be tempted to say that the derivative is zero (since the derivative of any constant is zero), but the problem is that at $r = 0$ we also have a zero in the denominator, so we have the indeterminate fraction of zero-over-zero. Thus although it is true that $\nabla \cdot \mathbf{E} = 0$ everywhere *except* the origin, we know from the divergence theorem that $\int_V \nabla \cdot \mathbf{E} d^3\mathbf{r} = \frac{q}{\epsilon_0}$ so we must have

$$\int_V \nabla \cdot \left(\frac{1}{r^2}\hat{\mathbf{r}}\right) d^3\mathbf{r} = 4\pi \tag{8}$$

and

$$\nabla \cdot \left(\frac{1}{r^2}\hat{\mathbf{r}}\right) = 0 \qquad \text{if} \quad r \neq 0 \tag{9}$$

These two conditions can be satisfied if

$$\nabla \cdot \left(\frac{1}{r^2}\hat{\mathbf{r}}\right) = 4\pi\delta_3(\mathbf{r}) \tag{10}$$

Another useful formula is

$$\begin{aligned} \nabla\frac{1}{r} &= \nabla\frac{1}{\sqrt{x^2+y^2+z^2}} && (11) \\ &= -\frac{1}{\left(x^2+y^2+z^2\right)^{3/2}}\left[x\hat{\mathbf{x}} + y\hat{\mathbf{y}} + z\hat{\mathbf{z}}\right] && (12) \\ &= -\frac{r\hat{\mathbf{r}}}{r^3} && (13) \\ &= -\frac{\hat{\mathbf{r}}}{r^2} && (14) \end{aligned}$$

Therefore, the Laplacian of $\frac{1}{r}$ gives a delta function:

$$\nabla^2\frac{1}{r} = -4\pi\delta_3\left(\mathbf{r}\right) \tag{15}$$

Example. Suppose we have some distribution of charge that gives a potential function

$$V(\mathbf{r}) = A\frac{e^{-\lambda r}}{r} \tag{16}$$

We can find the field by taking the gradient

$$\begin{aligned} \mathbf{E} &= -\nabla V & (17)\\ &= A\frac{e^{-\lambda r}}{r^2}(1+\lambda r)\,\hat{\mathbf{r}} & (18)\end{aligned}$$

We can now find the charge distribution by taking the divergence, remembering what we've discussed above. Applying the divergence formula in spherical coordinates directly gives

$$\rho = -\epsilon_0 A\left(\frac{\lambda^2 e^{-\lambda r}}{r}\right) \tag{19}$$

but this formula is valid only for $r \neq 0$. To get the full charge distribution we need to incorporate the delta function. Using the product rule for the divergence ($\nabla\cdot(f\mathbf{A}) = f\nabla\cdot\mathbf{A} + \mathbf{A}\cdot\nabla f$):

$$\begin{aligned} \nabla\cdot\mathbf{E} &= \nabla\cdot\left[\frac{\hat{\mathbf{r}}}{r^2}Ae^{-\lambda r}(1+\lambda r)\right] & (20)\\ &= Ae^{-\lambda r}(1+\lambda r)\,\nabla\cdot\left(\frac{1}{r^2}\hat{\mathbf{r}}\right) + \frac{\hat{\mathbf{r}}}{r^2}\cdot\nabla\left(Ae^{-\lambda r}(1+\lambda r)\right) & (21)\\ &= Ae^{-\lambda r}(1+\lambda r)\,(4\pi\delta_3(\mathbf{r})) - A\left(\frac{\lambda^2 e^{-\lambda r}}{r}\right) & (22)\\ &= 4\pi A\delta_3(\mathbf{r}) - A\left(\frac{\lambda^2 e^{-\lambda r}}{r}\right) & (23)\\ \rho &= A\epsilon_0\left[4\pi\delta_3(\mathbf{r}) - \frac{\lambda^2 e^{-\lambda r}}{r}\right] & (24)\end{aligned}$$

In the fourth line, we used the fact that $f(\mathbf{r})\delta_3(\mathbf{r}) = f(0)\delta_3(\mathbf{r})$, since the delta function is zero everywhere except at $\mathbf{r} = 0$.

From this, we can find the total net charge by integrating ρ:

$$
\begin{aligned}
Q &= \int_V \rho d^3\mathbf{r} && (25)\\
&= A\epsilon_0 \int_V 4\pi\delta_3(\mathbf{r}) d^3\mathbf{r} - A\epsilon_0 \int_V \frac{\lambda^2 e^{-\lambda r}}{r} d^3\mathbf{r} && (26)\\
&= 4\pi A\epsilon_0 - 4\pi A\epsilon_0 \lambda^2 \int_0^\infty \frac{e^{-\lambda r}}{r} r^2 dr && (27)\\
&= 4\pi A\epsilon_0 \left(1 - \frac{\lambda^2}{\lambda^2}\right) && (28)\\
&= 0 && (29)
\end{aligned}
$$

That is, the delta function contributes a point charge of $+4\pi A\epsilon_0$ at the origin, and the second term contributes a continuous charge distribution smeared out over all space that sums up to $-4\pi A\epsilon_0$.

PINGBACKS

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HYDROGEN ATOM: A SAMPLE WAVE FUNCTION

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Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 13, Exercise 13.1.3.

Post date: 10 Jul 2017

[If some equations are too small to read easily, use your browser's magnifying option (Ctrl + on Chrome, probably something similar on other browsers).]

The wave function for the hydrogen atom can be obtained by a series solution of the differential equation, leading to the result (which I've rewritten in Shankar's notation, although my original post used Griffiths's notation):

$$\psi_{nlm}(r,\theta,\phi) = \frac{U_{El}(r)}{r} Y_l^m(\theta,\phi) \tag{1}$$

Here, we have

$$\begin{aligned} U_{El} &= e^{-\rho} v_{El} && (2)\\ v_{El} &= \rho^{l+1} \sum_{k=0}^{\infty} C_k \rho^k && (3)\\ \rho &= \sqrt{\frac{-2mE}{\hbar^2}}\, r && (4) \end{aligned}$$

The energy levels of the hydrogen atom are

$$E = -\frac{me^4}{2\hbar^2 n^2} \tag{5}$$

where $n = 1, 2, 3, \ldots$. The coefficients C_k in 3 are given by a recursion relation

$$C_{k+1} = \frac{-e^2\lambda + 2(k+l+1)}{(k+l+2)(k+l+1) - l(l+1)} C_k \tag{6}$$

$$\lambda = \sqrt{-\frac{2m}{\hbar^2 E}} \tag{7}$$

Combining λ and E, the formula becomes, for a given n

$$C_{k+1} = \frac{2(k+l+1)-2n}{(k+l+2)(k+l+1)-l(l+1)}C_k$$

The coefficient C_0 which starts everything off is determined by normalization.

As an example, we can find the wave function ψ_{210}. In this case $n=2$ and $l=1$ so the first term in the recursion, with $k=0$ gives $k+l+1=2$ and $C_1=0$. The full wave function is then

$$\psi_{210} = \frac{1}{r}\rho^2 e^{-\rho} C_0 Y_1^0 \tag{8}$$

To evaluate ρ we use the energy for $n=2$:

$$E_2 = -\frac{me^4}{8\hbar^2} \tag{9}$$

This gives

$$\rho = \sqrt{\frac{2m^2e^4}{8\hbar^4}}r = \frac{me^2}{2\hbar^2}r = \frac{r}{2a_0} \tag{10}$$

where a_0 is the Bohr radius

$$a_0 \equiv \frac{\hbar^2}{me^2} \tag{11}$$

Plugging everything into 8, using $Y_1^0 = \sqrt{\frac{3}{4\pi}}\cos\theta$, we have

$$\psi_{210} = \sqrt{\frac{3}{4\pi}}\frac{C_0}{4a_0^2} r e^{-r/2a_0}\cos\theta \tag{12}$$

Normalizing gives the condition

$$\int_0^{2\pi}\int_0^{\pi}\int_0^{\infty} \psi_{210}^2 r^2 \sin\theta dr\, d\theta\, d\phi = 1 \tag{13}$$

Working out the integral (using software or tables) gives

$$\frac{3}{2}a_0 C_0^2 = 1 \tag{14}$$

$$C_0 = \sqrt{\frac{2}{3a_0}} \tag{15}$$

So the final wave function is

$$\psi_{210} = \frac{1}{\sqrt{32\pi a_0^3}} \frac{r}{a_0} e^{-r/2a_0} \cos\theta \tag{16}$$

which agrees with Shankar's equation 13.1.27.

HYDROGEN ATOM: RADIAL FUNCTION AT LARGE R

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 13, Exercise 13.1.4.

Post date: 19 Jul 2017

[If some equations are too small to read easily, use your browser's magnifying option (Ctrl + on Chrome, probably something similar on other browsers).]

When solving the 3-d Schrödinger equation for a spherically symmetric potential, the radial function has the asymptotic form for large r, and for the energy $E < 0$:

$$U_{El}(r) \underset{r\to\infty}{\longrightarrow} Ar^{\pm me^2/\kappa\hbar^2} e^{-\kappa r} \tag{1}$$

where

$$\kappa \equiv \sqrt{\frac{2m|E|}{\hbar^2}} \tag{2}$$

For the hydrogen atom, the function U_{El} is obtained from a series solution of the differential equation with the result

$$\begin{aligned} U_{El} &= e^{-\rho} v_{El} && (3)\\ v_{El} &= \rho^{l+1} \sum_{k=0}^{\infty} C_k \rho^k && (4)\\ \rho &= \sqrt{\frac{-2mE}{\hbar^2}} r && (5)\\ &= \kappa r && (6) \end{aligned}$$

To keep the wave function finite at large r, we require the series to terminate, which leads to the quantized energy levels, given by

$$E_n = -\frac{me^4}{2\hbar^2 n^2} \tag{7}$$

The series in 4 terminates at a value of $k = n - l - 1$, so the function v_{El} is a polynomial in ρ, and thus in r, of degree n. Since the actual radial function is

$$R_{nl} = \frac{U_{El}}{r} \tag{8}$$

we have that R_{nl} is a polynomial of degree $n-1$ in r multiplied by the exponential $e^{-\rho} = e^{-\kappa r}$. That is, for large r

$$R_{nl} \sim r^{n-1} e^{-\kappa r} \tag{9}$$

To show that this is consistent with 1, we use 7 and 2.

$$n = \sqrt{\frac{me^4}{2\hbar^2 |E_n|}} \tag{10}$$

$$= \sqrt{\frac{me^4}{2\hbar^2}} \sqrt{\frac{2m}{\hbar^2}} \frac{1}{\kappa} \tag{11}$$

$$= \frac{me^2}{\kappa\hbar^2} \tag{12}$$

Comparing this with 1, we see that

$$r^n = r^{me^2/\kappa\hbar^2} \tag{13}$$

so the condition is satisfied.

RUNGE LENZ VECTOR AND CLOSED ORBITS

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 13, Exercise 13.2.1.

Post date: 25 Jul 2017

[If some equations are too small to read easily, use your browser's magnifying option (Ctrl + on Chrome, probably something similar on other browsers).]

The energy levels of hydrogen, when calculated from the Coulomb potential alone (ignoring various perturbations) depend only on the principal quantum number n according to

$$E = -\frac{1}{n^2}\frac{\mu e^4}{2\hbar^2} \tag{1}$$

The quantization arises entirely from the requirement that the radial function remain finite for large r, and makes no mention of the angular quantum numbers l and m. Thus each energy level (each value of n) has a degeneracy of n^2, with $2l+1$ degenerate states for each l. Each symmetry is associated with the conservation of some dynamical quantity, with the degeneracy in m due to conservation of angular momentum.

Shankar points out that, in classical mechanics, any potential with a $\frac{1}{r}$ dependence conserves the Runge-Lenz vector, defined for the hydregen atom potential as

$$\mathbf{n} = \frac{\mathbf{p}\times\boldsymbol{\ell}}{\mu} - \frac{e^2}{r}\mathbf{r} \tag{2}$$

where I've used μ for the electron mass to avoid confusion with the L_z quantum number m.

Although it doesn't make sense to talk about the orbit of the electron in quantum mechanics, classically we can see that the conservation of $\mathbf{n}$ implies that the orbit is closed. We can see this as follows.

First, using

$$\boldsymbol{\ell} = \mathbf{r}\times\mathbf{p} \tag{3}$$

we have

$$\mathbf{n} = \frac{1}{\mu}\mathbf{p}\times(\mathbf{r}\times\mathbf{p}) - \frac{e^2}{r}\mathbf{r} \tag{4}$$

$$= \frac{1}{\mu}\mathbf{r}\times(\mathbf{p}\cdot\mathbf{p}) - \mathbf{p}(\mathbf{r}\cdot\mathbf{p}) - \frac{e^2}{r}\mathbf{r} \tag{5}$$

$$= \left(\frac{p^2}{\mu} - \frac{e^2}{r}\right)\mathbf{r} - \mathbf{p}(\mathbf{r}\cdot\mathbf{p}) \tag{6}$$

In the second line, we used the vector identity

$$\mathbf{A}\times(\mathbf{B}\times\mathbf{C}) = \mathbf{B}(\mathbf{A}\cdot\mathbf{C}) - \mathbf{C}(\mathbf{A}\cdot\mathbf{B}) \tag{7}$$

Since we're dealing with a bound state, r must always remain finite, so it must have a maximum value. At this point $\frac{dr}{dt} = 0$, which means that there is no radial motion, which in turn means that all motion at that point must be perpendicular to $\mathbf{r}$. In other words

$$\mathbf{p}\cdot\mathbf{r}_{max} = 0 \tag{8}$$

Also, from conservation of energy, we have

$$E = \frac{p^2}{2\mu} - \frac{e^2}{r} \tag{9}$$

so at r_{max} we have

$$p^2 = 2\mu\left(E + \frac{e^2}{r_{max}}\right) \tag{10}$$

Plugging these into 6, we get

$$\mathbf{n} = \left(2E + \frac{2e^2}{r_{max}} - \frac{e^2}{r_{max}}\right)\mathbf{r}_{max} \tag{11}$$

$$= \left(2E + \frac{e^2}{r_{max}}\right)\mathbf{r}_{max} \tag{12}$$

Exactly the same argument applies to the case where r is a minimum: again $\frac{dr}{dt} = 0$ so $\mathbf{r}\cdot\mathbf{p} = 0$ and we end up with

$$\mathbf{n} = \left(2E + \frac{e^2}{r_{min}}\right)\mathbf{r}_{min} \tag{13}$$

If $\mathbf{n}$ is conserved (constant), then it must be parallel or anti-parallel to both $\mathbf{r}_{max}$ and $\mathbf{r}_{min}$, and the latter two vectors must therefore always have the same direction. In other words, the particle reaches its maximum (and

minimum) distance always at the same point in its orbit, meaning that the orbit is closed.

In a general (elliptical) orbit, $r_{max} > r_{min}$ so $\frac{e^2}{r_{max}} < \frac{e^2}{r_{min}}$. Since $E < 0$ for a bound orbit, we therefore must have

$$2E + \frac{e^2}{r_{max}} < 0 \tag{14}$$

$$2E + \frac{e^2}{r_{min}} > 0 \tag{15}$$

This in turn implies that $\mathbf{n}$ is anti-parallel to $\mathbf{r}_{max}$ and parallel to $\mathbf{r}_{min}$.

For a circular orbit, both r and p are constant, so both the kinetic and potential energies are also constant. From the virial theorem, we know that, for $V \propto \frac{1}{r}$

$$\langle T \rangle = -\frac{1}{2} \langle V \rangle \tag{16}$$

Thus

$$E = T + V \tag{17}$$

$$= \frac{V}{2} \tag{18}$$

$$= -\frac{e^2}{2r} \tag{19}$$

Thus from 12, we see that $\mathbf{n} = 0$ for a circular orbit.

SIZES OF ELEMENTARY PARTICLES

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 13, Exercises 13.3.1 - 13.3.2.

Post date: 28 Jul 2017

[If some equations are too small to read easily, use your browser's magnifying option (Ctrl + on Chrome, probably something similar on other browsers).]

Due to the position-momentum uncertainty principle, if we wish to determine the location of a particle to within a distance ΔX, the momentum of the photon used to detect the particle must satisfy

$$\Delta P \Delta X \geq \frac{\hbar}{2} \tag{1}$$

This relation is valid in non-relativistic quantum mechanics, where we are using position eigenkets $|X\rangle$ which define a particle's position exactly. To do this, however, would require a photon of infinite energy. In relativistic quantum theory, if the energy of the photon is large enough, it is possible to convert the energy into mass by creating a particle-antiparticle pair. If we're trying to determine the location of an electron, then if the energy of the bombarding photon is around twice the rest energy of an electron, this pair creation process can occur. Thus for practical purposes, the maximum photon energy that we can use to detect the electron is finite, which means that the electron's position can be determined only approximately.

To get an idea of the 'radius' of an electron using these ideas (I put 'radius' in quotes because an electron doesn't have a rigid boundary in quantum theory), we can proceed as follows. We'll work only to orders of magnitude, rather than precise quantities.

From the uncertaintly relation, the photon's momentum is about

$$\Delta P \sim \frac{\hbar}{\Delta X} \tag{2}$$

For a photon, the relativistic energy is related to the momentum by

$$\Delta E = \Delta P c \tag{3}$$

where c is the speed of light. Therefore, the energy of the incident photon is

$$\Delta E \sim \frac{\hbar c}{\Delta X} \tag{4}$$

We therefore want to restrict this energy to less than twice the electron's rest energy, so

$$\Delta E \lesssim 2mc^2 \tag{5}$$

which leads to

$$\frac{\hbar c}{\Delta X} \lesssim 2mc^2 \tag{6}$$

$$\Delta X \gtrsim \frac{\hbar}{2mc} \sim \frac{\hbar}{mc} \tag{7}$$

The latter quantity is the Compton wavelength of the electron. [When we originally encountered the Compton wavelength is Carroll & Ostlie's book on astrophysics, they defined it as h/mc, so Shankar's Compton wavelength is $\frac{1}{2\pi}$ times that of Carroll & Ostlie. However, since we're working with orders of magnitude, this won't matter much.]

Thus the Compton wavelength can be taken as a rough size of the electron. We can write this as a fraction of the Bohr radius a_0 using

$$a_0 \equiv \frac{\hbar^2}{me^2} \tag{8}$$

so that

$$\frac{\hbar/mc}{a_0} = \frac{\hbar}{mc}\frac{me^2}{\hbar^2} = \frac{e^2}{\hbar c} = \alpha \approx \frac{1}{137} \tag{9}$$

where α is the famous fine structure constant. Since a_0 is roughly the radius of a ground-state hydrogen atom, the electron is about 100 times smaller than this.

We can use similar arguments to do some rough calculations on other particles.

Example 1. For example, the pion has a range of about 10^{-15} m as a mediator of the nuclear force, so if we take this as ΔX then

$$2m_\pi c^2 \sim \frac{\hbar c}{\Delta X} \tag{10}$$

The rest energy of an electron is about 0.5 MeV, so we can get an estimate of the rest energy of the pion as follows.

$$\frac{m_\pi c^2}{m_e c^2} = \frac{\Delta X_e}{\Delta X_\pi} = \frac{a_0/137}{10^{-15}} \tag{11}$$

The Bohr radius is about

$$a_0 \approx 5 \times 10^{-11} \text{ m} \tag{12}$$

so

$$m_\pi c^2 \approx (0.5 \text{ MeV}) \frac{5 \times 10^{-11}}{137 \times 10^{-15}} = 182 \text{ MeV} \tag{13}$$

The actual rest mass of a pion is around 140 MeV, so this estimate isn't too bad.

Example 2. The de Broglie wavelength of a particle is defined by

$$\lambda = \frac{h}{p} \tag{14}$$

For an electron with kinetic energy 200 eV, we need to find its momentum to calculate λ. The relativistic kinetic energy is

$$K = mc^2 (\gamma - 1) \tag{15}$$

where

$$\gamma = \frac{1}{\sqrt{1 - v^2/c^2}} \tag{16}$$

We have

$$\gamma = \frac{K}{mc^2} + 1 = \frac{200 \text{ eV}}{0.5 \times 10^6 \text{ eV}} + 1 = 1.0004 \tag{17}$$

Thus the electron is travelling at a non-relativistic speed, so to a good approximation we can use Newtonian formulas. The speed is

$$v = c\sqrt{\frac{2K}{mc^2}} = c\sqrt{\frac{2\,(200)}{0.5 \times 10^6}} \approx 0.03c \tag{18}$$

$$p = mv = \left(9.1 \times 10^{-31}\right)(0.03)\left(3 \times 10^8\right) = 7.7 \times 10^{-24} \text{ kg m s}^{-1} \tag{19}$$

$$\lambda = \frac{h}{p} = \frac{6.6 \times 10^{-34}}{7.7 \times 10^{-24}} \approx 10^{-10} \text{ m} \tag{20}$$

VIRIAL THEOREM IN 3-D

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

Reference: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Problem 4.40.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 13, Exercise 13.1.5.

Post date: 18 Jan 2013.

[If some equations are too small to read easily, use your browser's magnifying option (Ctrl + on Chrome, probably something similar on other browsers).]

We've seen the virial theorem in one dimension, which states:

$$2\langle T\rangle = \left\langle x\frac{dV}{dx}\right\rangle \tag{1}$$

where T is the kinetic energy.

We can derive the 3-d version of the virial theorem using a similar method. From the formula for the rate of change of an observable, we have,

$$\frac{d}{dt}\langle \mathbf{r}\cdot\mathbf{p}\rangle = \frac{i}{\hbar}\langle[\hat{H},\mathbf{r}\cdot\mathbf{p}]\rangle \tag{2}$$

assuming that the potential is time-independent. (This is what Shankar refers to as Ehrenfest's theorem.) In three dimensions, we have

$$\begin{aligned}
\mathbf{r}\cdot\mathbf{p} &= -i\hbar x\frac{\partial}{\partial x} - i\hbar y\frac{\partial}{\partial y} - i\hbar z\frac{\partial}{\partial z} && (3)\\
\hat{H} &= T+V && (4)\\
&= -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)+V && (5)
\end{aligned}$$

Since each term in the commutator (except for the potential V) contains only one of the three spatial coordinates, any derivative term commutes with any other derivative term that contains a different variable. The remaining three non-zero commutators, one for each coordinate, can be calculated in the same way as in one dimension. We are therefore left with a simple generalization of the result for one dimension.

$$\frac{i}{\hbar}[\hat{H}, \mathbf{r}\cdot\mathbf{p}] = -\frac{\hbar^2}{m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right) - x\frac{\partial V}{\partial x} - y\frac{\partial V}{\partial y} - z\frac{\partial V}{\partial z} \tag{6}$$

$$\frac{d}{dt}\langle \mathbf{r}\cdot\mathbf{p}\rangle = 2\langle T\rangle - \langle \mathbf{r}\cdot\nabla V\rangle \tag{7}$$

For stationary states the time derivative is zero, so

$$2\langle T\rangle = \langle \mathbf{r}\cdot\nabla V\rangle \tag{8}$$

For hydrogen,

$$V = -\frac{e^2}{4\pi\epsilon_0}\frac{1}{r} \tag{9}$$

so since $r = \sqrt{x^2+y^2+z^2}$,

$$\frac{\partial V}{\partial x} = \frac{e^2}{4\pi\epsilon_0}\frac{x}{r^3} \tag{10}$$

$$\frac{\partial V}{\partial y} = \frac{e^2}{4\pi\epsilon_0}\frac{y}{r^3} \tag{11}$$

$$\frac{\partial V}{\partial z} = \frac{e^2}{4\pi\epsilon_0}\frac{z}{r^3} \tag{12}$$

$$\mathbf{r}\cdot\nabla V = \frac{e^2}{4\pi\epsilon_0}\frac{x^2+y^2+z^2}{r^3} \tag{13}$$

$$= \frac{e^2}{4\pi\epsilon_0}\frac{1}{r} \tag{14}$$

$$= -V \tag{15}$$

Thus we have

$$2\langle T\rangle = -\langle V\rangle$$

But we know that the total energy for the hydrogen atom in quantum state n is $E_n = \langle T\rangle + \langle V\rangle = \langle T\rangle - 2\langle T\rangle = -\langle T\rangle$ so we get $\langle T\rangle = -E_n$ and $\langle V\rangle = 2E_n$.

For the 3-d harmonic oscillator

$$V = \frac{1}{2}m\omega^2 r^2 \tag{16}$$

so

$$\nabla V = m\omega^2 \mathbf{r} \tag{17}$$
$$\mathbf{r} \cdot \nabla V = m\omega^2 r^2 \tag{18}$$
$$= 2V \tag{19}$$

The total energy in state n is $E_n = \langle T \rangle + \langle V \rangle = \frac{1}{2}(2\langle V \rangle) + \langle V \rangle = 2\langle V \rangle$ so $\langle V \rangle = E_n/2 = \langle T \rangle$.

PINGBACKS

Pingback: Momentum space in 3-d
Pingback: Fine structure of hydrogen: relativistic correction
Pingback: runge lenz vector and closed orbits

HYDROGEN ATOM - SERIES SOLUTION AND BOHR ENERGY LEVELS

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

Reference: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Sec 4.2.1.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 13, Exercises 13.1.1 - 13.1.2.

Post date: 7 Jun 2011.

[This page follows the derivation given in Griffiths. The discussion in Shankar's chapter 13 is similar, but he uses Gaussian units, so the answer looks different. However, I can't be bothered going through the whole derivation again with different units, since the steps are essentially the same.]

We saw in an earlier post that the radial part of the three-dimensional Schrödinger equation for the hydrogen atom can be reduced to the differential equation

$$\rho\frac{d^2v}{d\rho^2}+2(l+1-\rho)\frac{dv}{d\rho}+(\rho_0-2l-2)v=0 \tag{1}$$

where

$$\begin{aligned} u(\rho) &= \rho^{l+1}e^{-\rho}v(\rho) && (2)\\ u(r) &\equiv rR(r) && (3)\\ \rho &= \kappa r && (4)\\ \rho_0 &= \frac{me^2}{2\pi\epsilon_0\hbar^2\kappa} && (5)\\ \kappa &= \frac{\sqrt{-2mE}}{\hbar} && (6) \end{aligned}$$

and $R(r)$ is the radial part of the three-dimensional wave function.

Our task here is to solve 1 by using the same method as for the harmonic oscillator. We propose a solution of the form

$$v(\rho)=\sum_{j=0}^{\infty}c_j\rho^j \tag{7}$$

and attempt to determine the coefficients c_j. The two derivatives needed in the equation are

$$\frac{dv}{d\rho} = \sum_{j=0}^{\infty} j c_j \rho^{j-1} \tag{8}$$

$$\frac{d^2v}{d\rho^2} = \sum_{j=0}^{\infty} j(j-1) c_j \rho^{j-2} \tag{9}$$

We now plug these back into 1 and fiddle with the summation indexes so that every term in every sum is a multiple of ρ^j.

$$\sum_{j=0}^{\infty} j(j-1)c_j\rho^{j-1} + 2(l+1)\sum_{j=0}^{\infty} j c_j \rho^{j-1} - 2\sum_{j=0}^{\infty} j c_j \rho^j + (\rho_0 - 2l - 2)\sum_{j=0}^{\infty} c_j \rho^j = 0 \tag{10}$$

The two terms containing ρ^{j-1} can be converted to sums over ρ^j by shifting the summation index from j to $j+1$. This means that the sum becomes

$$\sum_{j=-1}^{\infty} (j+1)j c_{j+1}\rho^j + 2(l+1)\sum_{j=-1}^{\infty} (j+1)c_{j+1}\rho^j - 2\sum_{j=0}^{\infty} j c_j \rho^j + (\rho_0 - 2l - 2)\sum_{j=0}^{\infty} c_j \rho^j = 0 \tag{11}$$

Note that the term with $j = -1$ in the first two sums is zero because of the $(j+1)$ factor, so we can start the sum at $j = 0$. Since ρ^j is now a common factor in all sums we can write the overall sum as

$$\sum_{j=0}^{\infty} \left[(j+1)j c_{j+1} + 2(l+1)(j+1)c_{j+1} - 2j c_j + (\rho_0 - 2l - 2)c_j\right]\rho^j = 0 \tag{12}$$

Because each power series is unique (a mathematical theorem), the only way this sum can be valid for all values of ρ is if all the coefficients are zero. That is

$$(j+1)j c_{j+1} + 2(l+1)(j+1)c_{j+1} - 2j c_j + (\rho_0 - 2l - 2)c_j = 0 \tag{13}$$

This can be rewritten as a recursion relation:

$$c_{j+1} = \frac{2(j+l+1) - \rho_0}{(j+1)(j+2(l+1))} c_j \tag{14}$$

[This equation is essentially the same as Shankar's 13.1.11 if you replace $j \to k$ and use Gaussian units in ρ_0.]

The argument at this point is again similar to that for the harmonic oscillator: we examine the behaviour for large j. In that case, we can ignore the $l+1$ and ρ_0 terms and write

$$\begin{aligned} c_{j+1} &\sim \frac{2j}{j(j+1)}c_j && (15)\\ &= \frac{2}{j+1}c_j && (16)\end{aligned}$$

(We could also ignore the 1 in the denominator, but keeping it makes the argument easier, as we will see.) If we took this as an exact recursion relation, then starting with some initial constant c_0, we get

$$\begin{aligned} c_1 &= \frac{2}{1}c_0 && (17)\\ c_2 &= \frac{2^2}{2\times 1}c_0 && (18)\\ c_3 &= \frac{2^3}{3\times 2\times 1}c_0 && (19)\\ c_j &= \frac{2^j}{j!}c_0 && (20)\\ v(\rho) &= c_0\sum_{j=0}^{\infty}\frac{2^j}{j!}\rho^j && (21)\\ &= c_0 e^{2\rho} && (22)\end{aligned}$$

In the last line we used the series expansion for the exponential function. Returning for a moment to the original definition of $v(\rho)$, we get

$$\begin{aligned} u(\rho) &= \rho^{l+1}e^{-\rho}v(\rho) && (23)\\ &= c_0\rho^{l+1}e^{\rho} && (24)\end{aligned}$$

Thus the infinite series solution gives a value for u that increases exponentially for large ρ, which isn't normalizable, so isn't a valid solution. The only way to resolve this problem is again the same as in the harmonic oscillator case, which is to require the series to terminate after a finite number of terms. That is, we must have, for some value of j,

$$2(j+l+1) = \rho_0 \qquad (25)$$

That is, ρ_0 must be an even integer, which we can define as $2n$. Recalling the definition of ρ_0 from above, we therefore have the condition which quantizes the energy levels in the hydrogen atom:

$$\begin{aligned} \rho_0 &= \frac{me^2}{2\pi\epsilon_0\hbar^2\kappa} && (26)\\ &= 2n && (27) \end{aligned}$$

so

$$\kappa = \frac{me^2}{4\pi\epsilon_0\hbar^2 n} \tag{28}$$

But $\kappa = \frac{\sqrt{-2mE}}{\hbar}$, so for the energy levels, we get

$$E = -\frac{1}{n^2}\frac{me^4}{2\hbar^2(4\pi\epsilon_0)^2} \tag{29}$$

This is the Bohr formula (although Bohr got the formula without using the Schrödinger equation) for the energy levels of hydrogen. [Again, this is equivalent to Shankar's 13.1.16 if you use Gaussian units, so that the $(4\pi\epsilon_0)^2$ factor becomes 1.]

The degeneracy of each energy level is found by noting that for a given value of n, any value of l is possible such that $j+l+1=n$. Since j is just the index on the series coefficient c_j, this means that l can be any value from 0 up to $n-1$. For each l, the z component of angular momentum can have any value from $m=-l$ up to $m=+l$, which gives $2l+1$ possibilities for each l. Thus the degeneracy for energy state E_n is

$$\begin{aligned} d(n) &= \sum_{l=0}^{n-1}(2l+1) && (30)\\ &= 2\frac{1}{2}(n-1)n+n && (31)\\ &= n^2 && (32) \end{aligned}$$

where we've used the formula

$$\sum_{l=1}^{N} l = \frac{1}{2}N(N+1) \tag{33}$$

Before leaving the series solution, we need to point out that the polynomials produced by 14, with the constraint that $\rho_0 = 2n$, are known mathematically as the *associated Laguerre polynomials*. They can be written as derivatives. First we define the ordinary Laguerre polynomials L_q:

$$L_q(x) = e^x \frac{d^q}{dx^q}(e^{-x}x^q) \tag{34}$$

Now the associated Laguerre polynomials L^p_{q-p} which depend on two parameters can be defined in terms of the ordinary Laguerre polynomials:

$$L^p_{q-p}(x) = (-1)^p \frac{d^p}{dx^p}(L_q(x)) \tag{35}$$

A more useful formula for the associated Laguerre polynomials is

$$L^k_n(x) = \sum_{j=0}^{n} \frac{(-1)^j(n+k)!}{(n-j)!(k+j)!j!}x^j \tag{36}$$

In terms of associated Laguerre polynomials, the solution of 1 is (apart from normalization)

$$v(\rho) = L^{2l+1}_{n-l-1}(2\rho) \tag{37}$$

We can verify that this is the solution of 1 by direct substitution. First, we plug in the correct indexes into 36:

$$L^{2l+1}_{n-l-1}(2\rho) = \sum_{j=0}^{n-l-1} \frac{(-1)^j 2^j(n+l)!}{(n-l-j-1)!(2l+j+1)!j!}\rho^j \tag{38}$$

Now we define the coefficients in the polynomial and show that the recurrence relation 14 is valid:

$$c_j = \frac{(-1)^j 2^j(n+l)!}{(n-l-j-1)!(2l+j+1)!j!} \tag{39}$$

$$\frac{c_{j+1}}{c_j} = \frac{-2(n-l-1-j)}{(j+1)(2l+j+2)} \tag{40}$$

This is the same recurrence relation provided $\rho_0 = 2n$. However, this isn't enough to verify the solution since other definitions of c_j would give the same relation (for example, we could leave out the $(n+l)!$ factor in the numerator and still get the same recurrence relation). To verify that the polynomials are in fact solutions, we can work out their derivatives and plug them into 1 directly.

We get

$$\sum_{j=0}^{n-l-1}\left[c_j(j-1)j\rho^{j-1}+2(l+1-\rho)c_jj\rho^{j-1}+2(n-l-1)c_j\rho^j\right]= \tag{41}$$

$$\sum_{j=0}^{n-l-1}\left[c_j(j-1)j\rho^{j-1}+2(l+1)c_jj\rho^{j-1}+-2jc_j\rho^j+2(n-l-1)c_j\rho^j\right] \tag{42}$$

We can now shift the summation index for the first two terms so that we sum over $j+1$ instead of j. This results in

$$\sum_{j=-1}^{n-l-2}\left[c_{j+1}j(j+1)+2(l+1)(j+1)c_{j+1}\right]\rho^j+\sum_{j=0}^{n-l-1}\left[-2jc_j+2(n-l-1)c_j\right]\rho^j \tag{43}$$

In the first sum, the $j=-1$ term is zero due to the $(j+1)$ factor, so we can start both sums from $j=0$. Thus for all values of j from 0 to $n-l-2$, we can examine the coefficient of ρ^j:

$$c_{j+1}(j+1)(j+2l+2)+c_j(-2j+2n-2l-2) \tag{44}$$

Using the relation between c_j and c_{j+1} above, we get

$$\frac{c_{j+1}}{c_j}(j+1)(j+2l+2)+(-2j+2n-2l-2)=2(j+l+1-n)+2(-j+n-l-1) \tag{45}$$

$$=0 \tag{46}$$

For the one remaining term in the second sum where $j=n-l-1$ we note that this term is zero on its own, since $(-j+n-l-1)=0$ in this case. Thus the overall sum satisfies the original differential equation 1.

PINGBACKS

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KINEMATICS OF SPIN: HILBERT SPACE FOR AN ELECTRON

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To leave a comment or report an error, please use the auxiliary blog.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 14.3.

Post date: 30 Jul 2017

[If some equations are too small to read easily, use your browser's magnifying option (Ctrl + on Chrome, probably something similar on other browsers).]

We've looked at quantum mechanical spin before but Shankar's treatment is quite different to that of Griffiths, so it's worth another look. Shankar begins with a thought experiment in which an electron is prepared (don't ask how!) in a state with zero momentum. Since its momentum is known precisely, its position is completely uncertain, so we can take the wave function in position space to be a constant, independent of position. Since the angular momentum operator $\mathbf{L}$ that we've met before is defined by replacing classical quantities by quantum operators in the classical relation $\mathbf{L} = \mathbf{r} \times \mathbf{p}$, an electron in this state must have $\mathbf{L} = 0$. (We can see this also from the relation $L_z = -i\hbar \frac{\partial}{\partial \phi}$ which gives zero since the wave function is independent of position.) However, if we measure the angular momentum along some direction such as z of an electron in such a state, we find that it always has the values $\pm \frac{\hbar}{2}$.

If we want to construct a wave function that describes the electron, we therefore need to consider a function that has a component that is independent of position, but which has eigenvalues $\pm \frac{\hbar}{2}$ when operated on by some operator with the properties of an angular momentum operator. The key to finding such a wave function is given by our example of a vector wave function. In that example, which considered the behaviour of a 2-d vector valued function under an infinitesimal rotation, we found that there were two effects of such a rotation. (It might help the reader to refer back to our earlier discussion at this point.) First, the rotation carries a vector $\mathbf{V}$ from its initial location A to some other point B. Second, the original vector $\mathbf{V}$ also gets rotated through the infinitesimal angle so that it now points in a slightly different direction, giving the rotated vector $\mathbf{V}'$. The components of $\mathbf{V}'$ are linear combinations of the components of the unrotated vector $\mathbf{V}$.

The first effect (that of rotating the function at A into the new position B) is generated by the original angular momentum operator $\mathbf{L}$. This rotation

depends on the position coordinates, since we must know the coordinates of the two points A and B to calculate the effect of the rotation. The second effect (that of rotating the vector so it points in a different direction) does not depend on the positions; rather, it depends only on the angle of rotation. As we showed in the previous example (working in 2-d), the second effect is generated by a 2×2 matrix S_z. We need a matrix rather than just a single number since we need to form a linear combination of the two components of the original vector to get the rotated vector.

In the special case of the 2-d rotation, the combined effect of these two types of rotation are given by

$$J_z = L_z + S_z \tag{1}$$

$$= \begin{bmatrix} L_z & 0 \\ 0 & L_z \end{bmatrix} + \begin{bmatrix} 0 & -i\hbar \\ i\hbar & 0 \end{bmatrix} \tag{2}$$

The transformation then becomes

$$\begin{bmatrix} V_1' \\ V_2' \end{bmatrix} = \left[I - \frac{i\varepsilon_z}{\hbar} J_z \right] \begin{bmatrix} V_1 \\ V_2 \end{bmatrix} \tag{3}$$

This equation is valid for the rotation of a vector wave function with two components through an angle ε_z about the z axis, in two dimensions.

At this point, we can generalize this result to 3-d, and also to a wave function with some arbitrary number n components. The dimension of the matrix is determined by n, so if we again consider a rotation about the z axis by some angle ε, we get

$$\begin{bmatrix} \psi_1' \\ \vdots \\ \psi_n' \end{bmatrix} = \left[I - \frac{i\varepsilon_z}{\hbar} J_z \right] \begin{bmatrix} \psi_1 \\ \vdots \\ \psi_n \end{bmatrix} \tag{4}$$

$$= \left(\begin{bmatrix} 1 & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & 1 \end{bmatrix} - \frac{i\varepsilon_z}{\hbar} \begin{bmatrix} -i\hbar\frac{\partial}{\partial\phi} & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & -i\hbar\frac{\partial}{\partial\phi} \end{bmatrix} - \frac{i\varepsilon_z}{\hbar} S_z \right) \begin{bmatrix} \psi_1 \\ \vdots \\ \psi_n \end{bmatrix} \tag{5}$$

Here, the actual form of S_z is yet to be determined.

Although we worked out this for the special case of a rotation about the z axis, we can generalize it to a rotation about an arbitrary axis, and thus get a vector operator:

$$\mathbf{J} = \mathbf{L} + \mathbf{S} \tag{6}$$

The orbital angular momentum operator $\mathbf{L}$ operates on spatial coordinates (and is the same operator on each of the n components), while the spin operator $\mathbf{S}$ mixes the n components of the wave function (and not on the spatial coordinates). As these two operators operate on different quantities, they commute, which leads to the commutation relation

$$[J_i, J_j] = i\hbar \sum_k \varepsilon_{ijk} J_k \tag{7}$$

which separates into the same commutation relations for each component of $\mathbf{J}$ so we have

$$[L_i, L_j] = i\hbar \sum_k \varepsilon_{ijk} L_k \tag{8}$$

$$[S_i, S_j] = i\hbar \sum_k \varepsilon_{ijk} S_k \tag{9}$$

Shankar worked out the matrices that satisfy 7 in his equations 12.5.22 to 12.5.24 so we won't go through that again here. What's important to remember is that these matrices are block diagonal matrices consisting of a series of blocks of dimension $(2j+1) \times (2j+1)$ for $j = 0, \frac{1}{2}, 1, \frac{3}{2}, \ldots$. Each of these blocks satisfies 7 on its own, so we can pick the block with the right dimension to satisfy the experimental result that the electron has two spin states: $\pm\frac{\hbar}{2}$. That is, for the electron, we have the number of components in the wave $n = 2$, so we choose $j = \frac{1}{2}$ for the spin operators, which turn out to be the familiar ones we've met before:

$$S_x = \frac{\hbar}{2} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \tag{10}$$

$$S_y = \frac{\hbar}{2} \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \tag{11}$$

$$S_z = \frac{\hbar}{2} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \tag{12}$$

The complete wave function of an electron is therefore the product of a function of position with a two-component vector, called a *spinor*, which represents the spin state. That is, we can write, in the position-spin basis

$$|\psi\rangle = \psi_+(\mathbf{r}) \begin{bmatrix} 1 \\ 0 \end{bmatrix} + \psi_-(\mathbf{r}) \begin{bmatrix} 0 \\ 1 \end{bmatrix} \tag{13}$$

In terms of Hilbert space, the spatial components are essentially the infinite-dimensional vectors ψ_+ and ψ_- which have values defined at each point in

3-d space, while the spinor components are 2-d vectors. Thus the complete Hilbert space $\mathbb{V}_e$ of an electron is defined as

$$\mathbb{V}_e = \mathbb{V}_0 \otimes \mathbb{V}_s \tag{14}$$

where $\mathbb{V}_0$ is the infinite-dimensional spatial component and $\mathbb{V}_s$ is the 2-d spinor component. In terms of this space, we can create a unit operator as a sum over a complete set of states:

$$\mathbf{1} = \sum_{s_z} \int |xyzs_z\rangle \langle xyzs_z| \, dx \, dy \, dz \tag{15}$$

The normalization condition for a wave function thus becomes

$$1 = \langle \psi | \psi \rangle = \sum_{s_z} \int \langle \psi | xyzs_z \rangle \langle xyzs_z | \psi \rangle \, dx \, dy \, dz \tag{16}$$

$$= \int \left(|\psi_+|^2 + |\psi_-|^2 \right) dx \, dy \, dz \tag{17}$$

where we get the last line by substituting 13. The term

$$\int |\psi_+|^2 \, dx \, dy \, dz \tag{18}$$

represents the probability that the electron will be found in the spin state $+\frac{\hbar}{2}$ anywhere in space.

The important point to remember from this derivation is that spin is an essentially new phenomenon with no classical analogue. Thus the wave function for a particle that has spin is necessarily an expanded Hilbert space where the extra subspace $\mathbb{V}_s$ is introduced to allow the extra spin states. The two spaces $\mathbb{V}_0$ and $\mathbb{V}_s$ are completely separate from each other, with each possessing its own operators, eigenstates and eigenvalues. Of course, it's possible to construct operators that are composed of other operators from both spaces, but we'll leave that until later.

One final point is worth making. The above derivation of the Hilbert space for an electron relied on the experimental result that the electron has exactly two spin states, thus leading to the 2×2 spin matrices. This is the best we can do in non-relativistic quantum theory. Shankar promises us that when we study the Dirac equation, which arose out of the need to introduce special relativity, the two spin states of the electron can actually be derived.

EVERY SPIN-1/2 SPINOR IS AN EIGENKET OF SOME SPIN OPERATOR

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 14, Exercise 14.3.1.

Post date: 5 Aug 2017

[If some equations are too small to read easily, use your browser's magnifying option (Ctrl + on Chrome, probably something similar on other browsers).]

The eigenvectors of the spin $\frac{1}{2}$ matrix in an arbitrary direction are given by

$$|\hat{n}+\rangle = \begin{bmatrix} \cos\frac{\theta}{2}e^{-i\phi/2} \\ \sin\frac{\theta}{2}e^{i\phi/2} \end{bmatrix} \tag{1}$$

$$|\hat{n}-\rangle = \begin{bmatrix} -\sin\frac{\theta}{2}e^{-i\phi/2} \\ \cos\frac{\theta}{2}e^{i\phi/2} \end{bmatrix} \tag{2}$$

where the direction vector is given by

$$\hat{\mathbf{n}} = \sin\theta\cos\phi\hat{\mathbf{x}} + \sin\theta\sin\phi\hat{\mathbf{y}} + \cos\theta\hat{\mathbf{z}} \tag{3}$$

The corresponding spin operator is given by the matrix

$$\hat{\mathbf{n}}\cdot\mathbf{S} = \frac{\hbar}{2}\begin{bmatrix} \cos\theta & \sin\theta e^{-i\phi} \\ \sin\theta e^{i\phi} & -\cos\theta \end{bmatrix} \tag{4}$$

Any 2-component normalized spinor is an eigenvector of such a matrix. To see this, suppose we have an arbitrary spinor written as

$$|\chi\rangle = \rho_1 e^{i\phi_1}\begin{bmatrix} 1 \\ 0 \end{bmatrix} + \rho_2 e^{i\phi_2}\begin{bmatrix} 0 \\ 1 \end{bmatrix} \tag{5}$$

$$= \begin{bmatrix} \rho_1 e^{i\phi_1} \\ \rho_2 e^{i\phi_2} \end{bmatrix} \tag{6}$$

where $\rho_{1,2}$ and $\phi_{1,2}$ are arbitrary real numbers (so that the coefficients on the RHS are arbitrary complex numbers). From normalization we have

$$\langle\chi|\chi\rangle = 1 = \begin{bmatrix} \rho_1 e^{-i\phi_1} & \rho_2 e^{-i\phi_2} \end{bmatrix} \begin{bmatrix} \rho_1 e^{i\phi_1} \\ \rho_2 e^{i\phi_2} \end{bmatrix} = \rho_1^2 + \rho_2^2 \tag{7}$$

Thus we can write ρ_1 and ρ_2 as the sine and cosine of some angle, which we'll call $\frac{\theta}{2}$, giving

$$|\chi\rangle = \begin{bmatrix} \cos\frac{\theta}{2} e^{i\phi_1} \\ \sin\frac{\theta}{2} e^{i\phi_2} \end{bmatrix} \tag{8}$$

We can put this in the form 1 as follows. Since an overall phase doesn't affect the physics of the spinor, we can write

$$|\chi\rangle = e^{i\alpha} \begin{bmatrix} \cos\frac{\theta}{2} e^{-i\phi/2} \\ \sin\frac{\theta}{2} e^{i\phi/2} \end{bmatrix} = \begin{bmatrix} \cos\frac{\theta}{2} e^{i\phi_1} \\ \sin\frac{\theta}{2} e^{i\phi_2} \end{bmatrix} \tag{9}$$

We have the conditions

$$\phi_1 = \alpha - \frac{\phi}{2} \tag{10}$$

$$\phi_2 = \alpha + \frac{\phi}{2} \tag{11}$$

Solving, we get

$$\alpha = \frac{\phi_1 + \phi_2}{2} \tag{12}$$

$$\phi = \phi_2 - \phi_1 \tag{13}$$

giving

$$|\chi\rangle = e^{i(\phi_1+\phi_2)/2} \begin{bmatrix} \cos\frac{\theta}{2} e^{-i(\phi_2-\phi_1)/2} \\ \sin\frac{\theta}{2} e^{i(\phi_2-\phi_1)/2} \end{bmatrix} \tag{14}$$

Thus $|\chi\rangle$ as given by 6 is an eigenvector of the operator 4, where

$$\hat{\mathbf{n}} = \sin\theta\cos(\phi_2 - \phi_1)\,\hat{\mathbf{x}} + \sin\theta\sin(\phi_2 - \phi_1)\,\hat{\mathbf{y}} + \cos\theta\hat{\mathbf{z}} \tag{15}$$

PAULI MATRICES: PROPERTIES

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To leave a comment or report an error, please use the auxiliary blog.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 14, Exercise 14.3.3.

Post date: 6 Aug 2017

[If some equations are too small to read easily, use your browser's magnifying option (Ctrl + on Chrome, probably something similar on other browsers).]

The three components of the spin operator **S** for spin $\frac{1}{2}$ can be expressed in terms of the Pauli matrices

$$\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}; \quad \sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}; \quad \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \tag{1}$$

as

$$S_i = \frac{\hbar}{2}\sigma_i \tag{2}$$

As the trace of a matrix is the sum of its diagonal elements, it's obvious from their definitions that the σ_i are traceless, but for some reason Shankar wants us to show this by a roundabout method.

We can show by direct calculation that the Pauli matrices anticommute with each other. For example

$$\sigma_x\sigma_y = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \tag{3}$$

$$= \begin{bmatrix} i & 0 \\ 0 & -i \end{bmatrix} \tag{4}$$

$$= -\begin{bmatrix} -i & 0 \\ 0 & i \end{bmatrix} \tag{5}$$

$$= -\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \tag{6}$$

$$= -\sigma_y\sigma_x \tag{7}$$

In general, we have, for $i \neq j$:

$$[\sigma_i, \sigma_j]_+ = 0 \tag{8}$$
$$\sigma_i \sigma_j = -\sigma_j \sigma_i \tag{9}$$

Also, by direct calculation (or by using the commutation relations for S_i) we can show that

$$[\sigma_x, \sigma_y] = \sigma_x \sigma_y - \sigma_y \sigma_x \tag{10}$$
$$= 2\sigma_x \sigma_y \tag{11}$$
$$= 2 \begin{bmatrix} i & 0 \\ 0 & -i \end{bmatrix} \tag{12}$$
$$= 2i\sigma_z \tag{13}$$

This gives the relation

$$\sigma_x \sigma_y = i\sigma_z \tag{14}$$

and also for cyclic permutations of x, y and z. Also by direct calculation we can see that

$$\sigma_i^2 = I \tag{15}$$

We can write this more generally as

$$\sigma_i \sigma_j = \delta_{ij} I + i \sum_k \varepsilon_{ijk} \sigma_k \tag{16}$$

where ε_{ijk} is the Levi-Civita antisymmetric tensor.
Returning to the trace, we can use the theorem for the trace of a product:

$$\mathrm{Tr}\,(AB) = \mathrm{Tr}\,(BA) \tag{17}$$

Applying this to 9 we have

$$\mathrm{Tr}\,(\sigma_x \sigma_y) = \mathrm{Tr}\,(\sigma_y \sigma_x) = -\mathrm{Tr}\,(\sigma_y \sigma_x) \tag{18}$$

Any quantity equal to its negative must be zero, so

$$\mathrm{Tr}\,(\sigma_x \sigma_y) = 0 \tag{19}$$

Thus from 14 we get

$$\mathrm{Tr}\sigma_z = 0 \tag{20}$$

We can use the same argument for σ_x and σ_y by cyclic permutation.

PINGBACKS

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PAULI MATRICES: A USEFUL IDENTITY

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Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 14, Exercise 14.3.4.

Post date: 6 Aug 2017

[If some equations are too small to read easily, use your browser's magnifying option (Ctrl + on Chrome, probably something similar on other browsers).]

The three components of the spin operator **S** for spin $\frac{1}{2}$ can be expressed in terms of the Pauli matrices

$$\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}; \quad \sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}; \quad \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \tag{1}$$

We can derive an identity involving the Pauli matrices:

$$(\mathbf{A}\cdot\boldsymbol{\sigma})(\mathbf{B}\cdot\boldsymbol{\sigma}) = (\mathbf{A}\cdot\mathbf{B})\,I + i\,(\mathbf{A}\times\mathbf{B})\cdot\boldsymbol{\sigma} \tag{2}$$

One way of proving this is to use the commutation relations for the Pauli matrices. We have

$$\begin{aligned} [\sigma_i,\sigma_j]_+ &= 2\delta_{ij}I & (3)\\ [\sigma_i,\sigma_j] &= 2i\sum_k \varepsilon_{ijk}\sigma_k & (4) \end{aligned}$$

where ε_{ijk} is the Levi-Civita antisymmetric tensor.

We therefore have

$$\begin{aligned} \sigma_i\sigma_j &= \frac{1}{2}\left([\sigma_i,\sigma_j]_+ + [\sigma_i,\sigma_j]\right) & (5)\\ &= \delta_{ij}I + i\sum_k \varepsilon_{ijk}\sigma_k & (6) \end{aligned}$$

Using the summation convention where repeated indices are summed from 1 to 3 (that is, over x, y and z):

$$
\begin{aligned}
(\mathbf{A}\cdot\boldsymbol{\sigma})(\mathbf{B}\cdot\boldsymbol{\sigma}) &= A_i\sigma_i B_j\sigma_j && (7)\\
&= A_i B_j \sigma_i\sigma_j && (8)\\
&= A_i B_j \left(\delta_{ij} I + i\varepsilon_{ijk}\sigma_k\right) && (9)\\
&= A_i B_i I + i\varepsilon_{ijk} A_i B_j \sigma_k && (10)\\
&= (\mathbf{A}\cdot\mathbf{B})\, I + i\,(\mathbf{A}\times\mathbf{B})\cdot\boldsymbol{\sigma} && (11)
\end{aligned}
$$

where the last term on the RHS follows from writing the vector cross product in terms of ε_{ijk}. [Note that in the second line, we've assumed that $\mathbf{B}$ commutes with $\boldsymbol{\sigma}$.]

Another way of deriving this result is as follows. First, we add the 2×2 identity matrix I to the set of Pauli matrices, calling it $\sigma_0 \equiv I$. Then, because we have four independent matrices (Shankar shows they are linearly independent in his equations 14.3.40-41) each with 4 entries, we can write any 2×2 complex matrix as a linear combination of the σ_α (where a Greek subscript ranges from 0 to 3). That is, for a general 2×2 matrix M

$$M = \sum_\alpha m_\alpha \sigma_\alpha \tag{12}$$

From the trace identities

$$\mathrm{Tr}\left(\sigma_\alpha\sigma_\beta\right) = 2\delta_{\alpha\beta} \tag{13}$$

we can find m_α by right-multiplying by σ_β and taking the trace:

$$
\begin{aligned}
\mathrm{Tr}\left(M\sigma_\beta\right) &= \sum_\alpha m_\alpha \mathrm{Tr}\left(\sigma_\alpha\sigma_\beta\right) && (14)\\
&= 2\sum_\alpha m_\alpha \delta_{\alpha\beta} && (15)\\
&= 2m_\beta && (16)
\end{aligned}
$$

Thus

$$m_\alpha = \frac{1}{2}\mathrm{Tr}\left(M\sigma_\alpha\right) \tag{17}$$

Returning to 2, we can identify (again using the summation convention):

$$
\begin{aligned}
M &= (\mathbf{A}\cdot\boldsymbol{\sigma})(\mathbf{B}\cdot\boldsymbol{\sigma}) && (18)\\
&= A_i\sigma_i B_j\sigma_j && (19)\\
&= m_\alpha\sigma_\alpha && (20)
\end{aligned}
$$

For $\alpha = 0$ we have

$$\begin{aligned} m_0 &= \frac{1}{2}\mathrm{Tr}\left(M\sigma_0\right) && (21)\\ &= \frac{1}{2}\mathrm{Tr}\left(M\right) && (22)\\ &= \frac{1}{2}A_iB_j\mathrm{Tr}\left(\sigma_i\sigma_j\right) && (23)\\ &= \frac{1}{2}A_iB_j\left(2\delta_{ij}\right) && (24)\\ &= A_iB_i && (25)\\ &= \mathbf{A}\cdot\mathbf{B} && (26) \end{aligned}$$

where we used 13 to get the fourth line. This gives us the first term on the RHS of 2.

For the other three σ_i coefficients, we can use a similar argument. Consider σ_x.

$$\begin{aligned} m_x &= \frac{1}{2}\mathrm{Tr}\left(M\sigma_x\right) && (27)\\ &= \frac{1}{2}A_iB_j\mathrm{Tr}\left(\sigma_i\sigma_j\sigma_x\right) && (28) \end{aligned}$$

From 6 we see that $\sigma_i\sigma_j$ can always be written as a single Pauli matrix σ_α. Thus the product of 3 Pauli matrices $\sigma_i\sigma_j\sigma_x$ can be reduced to a product of 2: $\pm\sigma_\alpha\sigma_x$ (the plus or minus sign is determined by the order in which we multiply the two matrices σ_i and σ_j). However, from 13, we see that the trace of $\sigma_\alpha\sigma_x$ is non-zero only if $\alpha = x$. The only way this can happen is if either $i = y$ and $j = z$ or $i = z$ and $j = y$. Therefore we have

$$m_x = \frac{1}{2}A_yB_z\mathrm{Tr}\left(\sigma_y\sigma_z\sigma_x\right) + \frac{1}{2}A_zB_y\mathrm{Tr}\left(\sigma_z\sigma_y\sigma_x\right) \quad (29)$$

(Repeated indices are *not* summed here!) From 3 we have

$$\sigma_y\sigma_z = -\sigma_z\sigma_y = i\sigma_x \quad (30)$$

Thus

$$\mathrm{Tr}\left(\sigma_y\sigma_z\sigma_x\right) = i\mathrm{Tr}\left(\sigma_x^2\right) = 2i$$

Therefore

$$m_x = i\left(A_yB_z - A_zB_y\right) \quad (31)$$

and m_x is the x component of $i\left(\mathbf{A}\times\mathbf{B}\right)$. A similar argument gives m_y and m_z, so putting everything together we again arrive at 2.

COMMENTS

Remark 1. Danyel Cavazos
Nov 12, 2017 9:24 PM

Hi!

I'd like to ask something in this page.

How do we go from eq. 22 to eq. 23? I.e., how do we know that when we evaluate Tr(A_i s_i B_j s_j) we can take A_i and B_j out of the trace operation?

Thank you so much!

==========

A and **B** are ordinary vectors whose components are just numbers, not matrices, so they can be taken outside the trace operation.

==========

Danyel Cavazos
Nov 13, 2017 5:15 PM

That's what I imagined, but then that means that we should beware of using this identity when A or B is replaced by vector operators like L or S, right?

==========

You might be able to prove it for the case where **A** and **B** are matrices, since any 2×2 matrix can be written as a linear combination of the Pauli matrices and the unit matrix, but it looks like it would get quite messy. I guess we can just use the first proof above which seems to work in general.

PINGBACKS

Pingback: General 2x2 matrix in terms of pauli matrices
Pingback: Projection operators for spin-1/2 + spin-1/2

GENERAL 2X2 MATRIX IN TERMS OF PAULI MATRICES

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 14, Exercise 14.3.5.

Post date: 7 Aug 2017

[If some equations are too small to read easily, use your browser's magnifying option (Ctrl + on Chrome, probably something similar on other browsers).]

Any 2×2 matrix can be written as a linear combination of the three Pauli matrices and the unit matrix. That is, for an arbitrary matrix M we have

$$M = \sum_{\alpha} m_{\alpha} \sigma_{\alpha} \tag{1}$$

where the coefficients are found from

$$m_{\alpha} = \frac{1}{2} \mathrm{Tr}\left(M \sigma_{\alpha}\right) \tag{2}$$

We can write this out explicitly as follows

$$M = \begin{bmatrix} \alpha & \beta \\ \gamma & \delta \end{bmatrix} \tag{3}$$

We then get

$$m_0 = \frac{1}{2}\mathrm{Tr}\left(M\sigma_0\right) \tag{4}$$
$$= \frac{1}{2}\mathrm{Tr}\left(MI\right) \tag{5}$$
$$= \frac{1}{2}\mathrm{Tr}\left(M\right) \tag{6}$$
$$= \frac{\alpha+\delta}{2} \tag{7}$$
$$m_1 = \frac{1}{2}\mathrm{Tr}\left(M\sigma_1\right) \tag{8}$$
$$= \frac{1}{2}\mathrm{Tr}\left(\left[\begin{array}{cc}\alpha & \beta\\ \gamma & \delta\end{array}\right]\left[\begin{array}{cc}0 & 1\\ 1 & 0\end{array}\right]\right) \tag{9}$$
$$= \frac{1}{2}\mathrm{Tr}\left(\left[\begin{array}{cc}\beta & \alpha\\ \delta & \gamma\end{array}\right]\right) \tag{10}$$
$$= \frac{\beta+\gamma}{2} \tag{11}$$
$$m_2 = \frac{1}{2}\mathrm{Tr}\left(M\sigma_2\right) \tag{12}$$
$$= \frac{1}{2}\mathrm{Tr}\left(\left[\begin{array}{cc}\alpha & \beta\\ \gamma & \delta\end{array}\right]\left[\begin{array}{cc}0 & -i\\ i & 0\end{array}\right]\right) \tag{13}$$
$$= \frac{1}{2}\mathrm{Tr}\left(\left[\begin{array}{cc}i\beta & -i\alpha\\ i\delta & -i\gamma\end{array}\right]\right) \tag{14}$$
$$= i\frac{\beta-\gamma}{2} \tag{15}$$
$$m_3 = \frac{1}{2}\mathrm{Tr}\left(M\sigma_3\right) \tag{16}$$
$$= \frac{1}{2}\mathrm{Tr}\left(\left[\begin{array}{cc}\alpha & \beta\\ \gamma & \delta\end{array}\right]\left[\begin{array}{cc}1 & 0\\ 0 & -1\end{array}\right]\right) \tag{17}$$
$$= \frac{1}{2}\mathrm{Tr}\left(\left[\begin{array}{cc}\alpha & -\beta\\ \gamma & -\delta\end{array}\right]\right) \tag{18}$$
$$= \frac{\alpha-\delta}{2} \tag{19}$$

Thus, in more conventional notation

$$M = \frac{1}{2}\left[\left(\alpha+\delta\right)I + \left(\beta+\gamma\right)\sigma_x + i\left(\beta-\gamma\right)\sigma_y + \left(\alpha-\delta\right)\sigma_z\right] \tag{20}$$

PINGBACKS

Pingback: Pauli matrices: examples of linear combinations
Pingback: Ensemble of electrons in magnetic field
Pingback: Dirac equation: derivation

ROTATION OF SPINOR ABOUT ARBITRARY DIRECTION

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 14, Exercise 14.3.6.

Post date: 7 Aug 2017

[If some equations are too small to read easily, use your browser's magnifying option (Ctrl + on Chrome, probably something similar on other browsers).]

Just as orbital angular momentum operator $\mathbf{L}$ is the generator of rotations, the spin operator $\mathbf{S}$ can also be used as the generator of rotations in spin space by means of the unitary operator

$$U\left[R\left(\boldsymbol{\theta}\right)\right]=e^{-i\boldsymbol{\theta}\cdot\mathbf{S}/\hbar}=e^{-i\boldsymbol{\theta}\cdot\boldsymbol{\sigma}/2} \tag{1}$$

where we've written the operator in terms of the Pauli matrices $\boldsymbol{\sigma}$, the components of which are

$$\sigma_x=\begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix};\quad \sigma_y=\begin{bmatrix}0 & -i\\ i & 0\end{bmatrix};\quad \sigma_z=\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix} \tag{2}$$

For a spin pointing the direction $\hat{n}$, where $\hat{n}$ is defined in terms of the spherical angles as

$$\hat{n}=\sin\theta\cos\phi\hat{\mathbf{x}}+\sin\theta\sin\phi\hat{\mathbf{y}}+\cos\theta\hat{\mathbf{z}} \tag{3}$$

the corresponding eigenvectors of the operator $\hat{n}\cdot\mathbf{S}$ are

$$|\hat{n}+\rangle=\begin{bmatrix}\cos\frac{\theta}{2}e^{-i\phi/2}\\ \sin\frac{\theta}{2}e^{i\phi/2}\end{bmatrix} \tag{4}$$

$$|\hat{n}-\rangle=\begin{bmatrix}-\sin\frac{\theta}{2}e^{-i\phi/2}\\ \cos\frac{\theta}{2}e^{i\phi/2}\end{bmatrix} \tag{5}$$

If we start with spin pointing in the $+z$ direction, then it is in the state

$$\left|s_z=\frac{\hbar}{2}\right\rangle=\frac{\hbar}{2}\begin{bmatrix}1\\ 0\end{bmatrix} \tag{6}$$

then it should be possible to rotate this state into the general state 4 by applying the correct rotation operators in sequence.

Suppose we first rotate the state by an angle θ about the y axis. This rotates the axis of spin so that it lies in the xz plane in the first quadrant (that is, positive x and positive z), making an angle θ with the z axis. We can now rotate again by an angle ϕ about the (original) z axis. The axis of spin now points in the direction given by $\hat{n}$ in 3. That is, it should be true that

$$|\hat{n}+\rangle = U\left[R(\phi\hat{\mathbf{z}})\right]U\left[R(\theta\hat{\mathbf{y}})\right]\begin{bmatrix}1\\0\end{bmatrix} \tag{7}$$

In order to verify this by direct calculation, we need an explicit form for U. This is derived by Shankar in his equation 14.3.44 so we won't repeat the derivation here. Basically, it uses the fact that $(\hat{n}\cdot\boldsymbol{\sigma})^2 = I$ and expands the exponential 1 as a power series, with the result

$$U\left[R(\boldsymbol{\theta})\right] = \cos\frac{\theta}{2}I - i\sin\frac{\theta}{2}\left(\hat{\theta}\cdot\boldsymbol{\sigma}\right) \tag{8}$$

We can use this formula to do the calculation.

$$U\left[R(\theta\hat{\mathbf{y}})\right]\begin{bmatrix}1\\0\end{bmatrix} = \left[\cos\frac{\theta}{2}I - i\sin\frac{\theta}{2}\sigma_y\right]\begin{bmatrix}1\\0\end{bmatrix} \tag{9}$$

$$= \begin{bmatrix}\cos\frac{\theta}{2}\\0\end{bmatrix} - i\sin\frac{\theta}{2}\begin{bmatrix}0&-i\\i&0\end{bmatrix}\begin{bmatrix}1\\0\end{bmatrix} \tag{10}$$

$$= \begin{bmatrix}\cos\frac{\theta}{2}\\\sin\frac{\theta}{2}\end{bmatrix} \tag{11}$$

Applying the second rotation we get

$$U\left[R(\phi\hat{\mathbf{z}})\right]\begin{bmatrix}\cos\frac{\theta}{2}\\\sin\frac{\theta}{2}\end{bmatrix} = \left[\cos\frac{\phi}{2}I - i\sin\frac{\phi}{2}\sigma_z\right]\begin{bmatrix}\cos\frac{\theta}{2}\\\sin\frac{\theta}{2}\end{bmatrix} \tag{12}$$

$$= \begin{bmatrix}\cos\frac{\theta}{2}\cos\frac{\phi}{2}\\\sin\frac{\theta}{2}\cos\frac{\phi}{2}\end{bmatrix} - i\sin\frac{\phi}{2}\begin{bmatrix}1&0\\0&-1\end{bmatrix}\begin{bmatrix}\cos\frac{\theta}{2}\\\sin\frac{\theta}{2}\end{bmatrix} \tag{13}$$

$$= \begin{bmatrix}\cos\frac{\theta}{2}\left(\cos\frac{\phi}{2} - i\sin\frac{\phi}{2}\right)\\\sin\frac{\theta}{2}\left(\cos\frac{\phi}{2} + i\sin\frac{\phi}{2}\right)\end{bmatrix} \tag{14}$$

$$= \begin{bmatrix}\cos\frac{\theta}{2}e^{-i\phi/2}\\\sin\frac{\theta}{2}e^{i\phi/2}\end{bmatrix} \tag{15}$$

which agrees with 4.

PINGBACKS

Pingback: Spinor in oscillating magnetic field - part 1
Pingback: Spin flip of electron in magnetic field
Pingback: Rotation operator for spinors

PAULI MATRICES: EXAMPLES OF LINEAR COMBINATIONS

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 14, Exercise 14.3.7.

Post date: 8 Aug 2017

[If some equations are too small to read easily, use your browser's magnifying option (Ctrl + on Chrome, probably something similar on other browsers).]

Here are a few examples of calculations using the Pauli matrices $\boldsymbol{\sigma}$, the components of which are

$$\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}; \quad \sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}; \quad \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \tag{1}$$

From Shankar's equation 14.3.44, we know that the unitary rotation operator can be written as

$$U\left[R\left(\boldsymbol{\theta}\right)\right] = e^{-i\boldsymbol{\theta}\cdot\boldsymbol{\sigma}/2} \tag{2}$$

$$= \cos\frac{\theta}{2} I - i \sin\frac{\theta}{2}\left(\hat{\theta}\cdot\boldsymbol{\sigma}\right) \tag{3}$$

Example 1. Find $\left(I + i\sigma_x\right)^{1/2}$. As usual, the square root of a matrix M is the matrix $M^{1/2}$ such that $M^{1/2}M^{1/2} = M$. To solve this, we would like to express $I + i\sigma_x$ in the form 2, from which we can find the square root by simply dividing the exponent by 2. We first express it in the form 3, from which we see that we need an angle θ such that

$$\cos\frac{\theta}{2} = -\sin\frac{\theta}{2} \tag{4}$$

This is valid if

$$\theta = \frac{3\pi}{2} \tag{5}$$

$$\cos\frac{\theta}{2} = -\frac{\sqrt{2}}{2} = -\sin\frac{\theta}{2} \tag{6}$$

This gives

$$U = -\frac{\sqrt{2}}{2}(I + i\sigma_x) \tag{7}$$

$$I + i\sigma_x = -\sqrt{2}e^{i\sigma_x 3\pi/4} \tag{8}$$

$$= \sqrt{2}e^{i\pi}e^{i\sigma_x 3\pi/4} \tag{9}$$

Therefore

$$(I + i\sigma_x)^{1/2} = 2^{1/4}e^{i\pi/2}e^{i\sigma_x 3\pi/8} \tag{10}$$

$$= 2^{1/4}i\left(\cos\frac{3\pi}{8}I - i\sin\frac{3\pi}{8}\sigma_x\right) \tag{11}$$

We can check this by evaluating the cos and sin using the half-angle formulas

$$\sin\frac{\theta}{2} = \sqrt{\frac{1-\cos\theta}{2}} \tag{12}$$

$$\cos\frac{\theta}{2} = \sqrt{\frac{1+\cos\theta}{2}} \tag{13}$$

We therefore have

$$\sin\frac{3\pi}{8} = \frac{1}{2}\sqrt{2+\sqrt{2}} \tag{14}$$

$$\cos\frac{3\pi}{8} = \frac{1}{2}\sqrt{2-\sqrt{2}} \tag{15}$$

Plugging these into 11 we have

$$(I + i\sigma_x)^{1/2} = \frac{1}{2^{3/4}}\begin{bmatrix} i\sqrt{2-\sqrt{2}} & \sqrt{2+\sqrt{2}} \\ \sqrt{2+\sqrt{2}} & i\sqrt{2-\sqrt{2}} \end{bmatrix} \tag{16}$$

Squaring this gives

$$I + i\sigma_x = \frac{1}{2^{3/2}}\begin{bmatrix} -\left(2-\sqrt{2}\right)+2+\sqrt{2} & 2i\sqrt{2-\sqrt{2}}\sqrt{2+\sqrt{2}} \\ 2i\sqrt{2-\sqrt{2}}\sqrt{2+\sqrt{2}} & 2+\sqrt{2}-\left(2-\sqrt{2}\right) \end{bmatrix} \tag{17}$$

$$= \frac{1}{2\sqrt{2}}\begin{bmatrix} 2\sqrt{2} & 2\sqrt{2}i \\ 2\sqrt{2}i & 2\sqrt{2} \end{bmatrix} \tag{18}$$

$$= \begin{bmatrix} 1 & i \\ i & 1 \end{bmatrix} \tag{19}$$

which is correct.

[Incidentally, 11 is different from Shankar's answer in the back of the book, but both are correct as can be verified by squaring Shankar's answer. Unlike ordinary complex numbers, a 2×2 matrix can have more than 2 square roots.]

Example 2. Find $(2I + \sigma_x)^{-1}$. In principle, we could solve this the same way as in Example 1, but this time we would need to find θ such that $\cos\frac{\theta}{2} = -2\sin\frac{\theta}{2}$. This doesn't give a 'nice' value of θ (that is, a value that is some nice multiple of π). It seems easier to just calculate the matrix and then take its inverse using the standard formula for the inverse of a 2×2 matrix. We can then convert this back to a linear combination of Pauli matrices using the formula for a matrix M:

$$M = \begin{bmatrix} \alpha & \beta \\ \gamma & \delta \end{bmatrix} \tag{20}$$

$$= \frac{1}{2}\left[(\alpha+\delta)\, I + (\beta+\gamma)\,\sigma_x + i\,(\beta-\gamma)\,\sigma_y + (\alpha-\delta)\,\sigma_z\right] \tag{21}$$

We get

$$2I + \sigma_x = \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix} \tag{22}$$

The inverse of a matrix is given by

$$\begin{bmatrix} a & b \\ c & d \end{bmatrix}^{-1} = \frac{1}{ad-bc}\begin{bmatrix} d & -b \\ -c & a \end{bmatrix} \tag{23}$$

so

$$(2I + \sigma_x)^{-1} = \begin{bmatrix} \frac{2}{3} & -\frac{1}{3} \\ -\frac{1}{3} & \frac{2}{3} \end{bmatrix} \tag{24}$$

Using 21 we find

$$(2I + \sigma_x)^{-1} = \frac{1}{6}\,(4I - 2\sigma_x) = \frac{1}{3}\,(2I - \sigma_x) \tag{25}$$

We can check this by multiplication

$$\frac{1}{3}\,(2I - \sigma_x)\,(2I + \sigma_x) = \frac{1}{3}\left(4I - \sigma_x^2\right) \tag{26}$$

$$= \frac{1}{3}\,(4I - I) \tag{27}$$

$$= I \tag{28}$$

where we used $\sigma_x^2 = I$ to get the second line.

Example 3. Find σ_x^{-1}. Since $\sigma_x^2 = I$, $\sigma_x^{-1} = \sigma_x$.

PAULI MATRICES: COMMUTATION AND ANTICOMMUTATION PROPERTIES

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 14, Exercise 14.3.8.

Post date: 10 Aug 2017

[If some equations are too small to read easily, use your browser's magnifying option (Ctrl + on Chrome, probably something similar on other browsers).]

Here are a couple of theorems concerning the Pauli matrices$\boldsymbol{\sigma}$, the components of which are

$$\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}; \quad \sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}; \quad \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \tag{1}$$

Both theorems arise from the fact that an arbitrary 2×2 matrix can be written as a linear combination of the Pauli matrices and the unit matrix:

$$\begin{aligned} M &= \begin{bmatrix} \alpha & \beta \\ \gamma & \delta \end{bmatrix} && (2) \\ &= \frac{1}{2}\left[(\alpha+\delta)\, I + (\beta+\gamma)\,\sigma_x + i\,(\beta-\gamma)\,\sigma_y + (\alpha-\delta)\,\sigma_z\right] && (3) \end{aligned}$$

We'll also need the commutation and anticommutationsrelations

$$\begin{aligned} [\sigma_i, \sigma_j]_+ &= 2\delta_{ij} I && (4) \\ [\sigma_i, \sigma_j] &= 2i \sum_k \varepsilon_{ijk} \sigma_k && (5) \end{aligned}$$

Theorem 1. *Any matrix that commutes with $\boldsymbol{\sigma}$ (that is, it commutes with all 3 components of $\boldsymbol{\sigma}$) is a multiple of the unit matrix.*

Proof. First, since I commutes with every matrix, it commutes with $\boldsymbol{\sigma}$. Now, from 5, any one of the Pauli matrices does *not* commute with the other two Pauli matrices, so M cannot have any component that is one of the Pauli matrices. From 3, this means that

$$\beta+\gamma = 0 \quad (6)$$
$$\beta-\gamma = 0 \quad (7)$$
$$\alpha-\delta = 0 \quad (8)$$

The first two conditions say that $\beta = \gamma = -\gamma$ which implies $\beta = \gamma = 0$ and the last condition gives us $\alpha = \delta$, so M must be a multiple of the unit matrix. □

Theorem 2. *There is no matrix (apart from the zero matrix) that anticommutes with all 3 Pauli matrices.*

Proof. Since I doesn't anticommute with any matrix, M cannot contain a component with I. From 4, the anticommutator of two Pauli matrices is zero only if the two matrices are different. Therefore, if M contains a non-zero component for any one, say σ_x, of the Pauli matrices then M will not anticommute with σ_x. The same argument applies to the other two Pauli matrices, so there is no M that anticommutes with all 3 Pauli matrices. □

PINGBACKS

Pingback: Dirac equation: derivation

AVERAGE RATE OF CHANGE OF ANGULAR MOMENTUM IN MAGNETIC FIELD

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 14, Exercise 14.4.1.

Post date: 12 Aug 2017

[If some equations are too small to read easily, use your browser's magnifying option (Ctrl + on Chrome, probably something similar on other browsers).]

In classical electrodynamics, the torque on a magnetic moment $\boldsymbol{\mu}$ in a constant magnetic field $\mathbf{B}$ is given by (using Shankar's notation):

$$\mathbf{T} = \boldsymbol{\mu} \times \mathbf{B} \tag{1}$$

We can relate the magnetic moment to the angular momentum of a (classically) spinning charged object by introducing the gyromagnetic ratio

$$\gamma \equiv \frac{\mu}{l} \tag{2}$$

If we apply this to a single particle of charge q and mass m travelling at constant speed v around a circular orbit, then its angular momentum is

$$l = mvr \tag{3}$$

The magnetic moment can be calculated by taking the charge q to be smeared out over the circumference of the circle, giving a linear charge density of

$$\lambda = \frac{q}{2\pi r} \tag{4}$$

Since the loop is spinning with speed v, the current (rate at which charge passed a fixed point on the circle) is

$$I = \lambda v = \frac{q}{2\pi r} r\omega = \frac{q}{2\pi}\omega \tag{5}$$

where

$$\omega = \frac{2\pi}{P} = \frac{2\pi v}{2\pi r} = \frac{v}{r} \tag{6}$$

is the angular frequency (P is the period, or time it takes for one complete orbit).

The magnetic moment is defined as

$$\boldsymbol{\mu} \equiv \frac{I}{c}\mathbf{a} \tag{7}$$

where **a** is the area of the loop, whose direction is determined by using the right-hand rule on the direction of the current around the loop. Thus if the current is travelling counterclockwise when viewed from above, **a** points upwards. (The speed of light c enters because Shankar is using CGS units.) The magnetic moment here is then

$$\begin{aligned} \boldsymbol{\mu} &= \frac{qv}{2\pi r}\frac{\pi r^2}{c}\hat{\mathbf{a}} && (8)\\ &= \left(\frac{q}{2mc}\right)(mvr\hat{\mathbf{a}}) && (9)\\ &= \left(\frac{q}{2mc}\right)\mathbf{l} && (10) \end{aligned}$$

where **l** is the angular momentum vector. In this case, the gyromagnetic ratio is

$$\gamma = \frac{q}{2mc} \tag{11}$$

In this case, the torque 1 is given by

$$\mathbf{T} = \gamma\mathbf{l} \times \mathbf{B} \tag{12}$$

The interaction energy (between the angular momentum and magnetic field) is given by

$$H_{int} = \int T(\theta)\, d\theta \tag{13}$$

where the torque is given as a function of the angle between $\boldsymbol{\mu}$ and **B** in 1, so that

$$T = \mu B \sin\theta \tag{14}$$

Doing the integral (neglecting the constant of integration) we have

$$H_{int} = -\mu B\cos\theta = -\boldsymbol{\mu}\cdot\mathbf{B} \tag{15}$$

H_{int} is minimized when $\boldsymbol{\mu}$ and **B** are parallel, so the torque's effect is to try to bring these two vectors into alignment. This assumes that the magnetic moment doesn't actually involve any angular momentum, which obviously isn't the case with our rotating loop example above. In that case,

the torque causes a precession about the direction of **B**, which we can see as follows.

The angular version of Newton's law, relating torque and angular momentum, is

$$\mathbf{T} = \frac{d\mathbf{l}}{dt} = \gamma \mathbf{l} \times \mathbf{B} \tag{16}$$

Since the cross product is perpendicular to both its constituent vectors, the change in **l** is always perpendicular to **l** itself. The effect can be seen by looking at Shankar's Figure 14.2 (too much effort to reproduce that here), in which we can see that

$$\begin{aligned} \Delta\mathbf{l} &= \gamma\,(\mathbf{l} \times \mathbf{B})\,\Delta t & (17)\\ \Delta l &= \gamma l B \sin\theta \Delta t & (18) \end{aligned}$$

where θ is the angle between **l** and **B**, and $\Delta\mathbf{l}$ is tangent to the circle of radius $l\sin\theta$ that lies in the plane perpendicular to **B**. The net effect is that **l** precesses about the direction of **B**, so that the magnitude of angular momentum remains constant, but its direction changes at a constant rate. The change in azimuthal angle $\Delta\phi$ in time Δt is

$$\Delta\phi = \frac{-\Delta l}{l\sin\theta} = -\gamma B \Delta t \tag{19}$$

where the minus sign is because the angular momentum precesses clockwise (as seen from above) around **B**. The angular frequency of precession is therefore

$$\omega_0 = \frac{\Delta\phi}{\Delta t} = -\gamma B \tag{20}$$

If we include the direction of the axis of precession, which is parallel to **B**, then

$$\boldsymbol{\omega}_0 = -\gamma \mathbf{B} \tag{21}$$

We can see that these results transfer over to quantum mechanics if we use Ehrenfest's theorem. For an interaction hamiltonian 15, we can write it as

$$H = -\gamma \mathbf{L} \cdot \mathbf{B} \tag{22}$$

We want to find the average of the angular momentum over time, so we use Ehrenfest's theorem to write

$$\frac{d\,\langle \mathbf{L} \rangle}{dt} = -\frac{i}{\hbar}\,\langle [\mathbf{L}, H] \rangle \tag{23}$$

We can work out the RHS using the commutators of angular momentum:

$$[L_i, L_j] = i\hbar \sum_k \varepsilon_{ijk} L_k \tag{24}$$

As we're dealing with a vector operator, we can work out each component separately. For L_x we get, assuming that $\mathbf{B}$ is independent of position (and thus commutes with $\mathbf{L}$):

$$\begin{aligned}
-\frac{i}{\hbar}\left[L_x, H\right] &= \frac{i\gamma}{\hbar}\left[L_x, L_x B_x + L_y B_y + L_z B_z\right] && (25)\\
&= \frac{i\gamma}{\hbar}\left(\left[L_x, L_x\right] B_x + \left[L_x, L_y\right] B_y + \left[L_x, L_z\right] B_z\right) && (26)\\
&= -\gamma\left(0 + L_z B_y - L_y B_z\right) && (27)\\
&= \gamma\left(\mathbf{L} \times \mathbf{B}\right)_x && (28)\\
&= \left(\boldsymbol{\mu} \times \mathbf{B}\right)_x && (29)
\end{aligned}$$

The other two components work out similarly, so we have

$$-\frac{i}{\hbar}\left\langle[\mathbf{L}, H]\right\rangle = \boldsymbol{\mu} \times \mathbf{B} \tag{30}$$

As $\mathbf{B}$ doesn't depend on position, when we take the average over space we get

$$\frac{d\left\langle\mathbf{L}\right\rangle}{dt} = \left\langle\boldsymbol{\mu}\right\rangle \times \mathbf{B} \tag{31}$$

Thus the mean of the quantum angular momentum also precessed about $\mathbf{B}$. Since the only assumption we made was that $\mathbf{B}$ was independent of position, and all that was used in the derivation was the commutation relations of angular momentum, the result is also valid for spin angular momentum, and time-varying magnetic fields, provided they are constant over all space.

PINGBACKS

Pingback: Magnetic moment in oscillating magnetic field

Pingback: Spinor in oscillating magnetic field - part 1

Pingback: Spin flip of electron in magnetic field

Pingback: Effective magnetic field in rotating frame - axis of rotation not parallel

Pingback: Ensemble of electrons in magnetic field

Pingback: Coupling of proton's magnetic moment to external field

Pingback: Wigner-Eckart Theorem - adding orbital and spin angular momenta

MAGNETIC MOMENT IN OSCILLATING MAGNETIC FIELD

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 14, Exercise 14.4.2.

Post date: 15 Aug 2017

[If some equations are too small to read easily, use your browser's magnifying option (Ctrl + on Chrome, probably something similar on other browsers).]

In classical electromagnetism, a magnetic moment precessesif placed in a constant magnetic field whose direction is not parallel to that of the magnetic moment. For a magnetic moment $\boldsymbol{\mu}$ in a constant field $\mathbf{B}_0$, the precession has a frequency of

$$\boldsymbol{\omega}_0 = -\gamma \mathbf{B}_0 \tag{1}$$

where γ is the gyromagnetic ratio.

Now suppose we view this precession in a frame of reference that is rotating about the same axis as $\boldsymbol{\omega}_0$, but with a frequency $\boldsymbol{\omega}$ that may not be the same as $\boldsymbol{\omega}_0$. The precession frequency will now appear to be

$$\boldsymbol{\omega}_r = \boldsymbol{\omega}_0 - \boldsymbol{\omega} \tag{2}$$

[Although this is a vector equation, all vectors in it have the same direction.] Comparing this with 1, we see that, in the rotating frame, the effective magnetic field is

$$\mathbf{B}_r = -\frac{1}{\gamma}\boldsymbol{\omega}_r = \mathbf{B}_0 + \frac{\omega}{\gamma} \tag{3}$$

Now suppose the magnetic field is taken to be constant in the z direction with component $B_0\hat{\mathbf{z}}$, but with a small oscillating component in the xy plane, so that the total field is

$$\mathbf{B} = B\cos\omega t\hat{\mathbf{x}} - B\sin\omega t\hat{\mathbf{y}} + B_0\hat{\mathbf{z}} \tag{4}$$

where $B \ll B_0$.

This is a magnetic field that precesses about the z axis, so it's similar to the case we treated earlier, although in the earlier post we were concerned only with the behaviour of an electron in such a field, so we were interested in the quantum mechanics. The present treatment is purely classical.

If we place a magnetic moment in this field so that at $t = 0$ it's pointing in the $+z$ direction, we want to find how the magnetic moment varies with time. To analyze the problem, it's easiest to transform to a rotating frame with frequency $\boldsymbol{\omega} = -\omega\hat{\mathbf{z}}$ (minus, because it's precessing in a clockwise direction). Since the frame is rotating at the same rate as the magnetic field, the field appears frozen in this rotating frame. For simplicity, we'll assume that the field's horizontal component lies along the $+x$ direction, so the field lies in the xz plane. The z component of the field is thus effectively reduced to

$$B_z = B_0 - \frac{\omega}{\gamma} \tag{5}$$

In this frame, we therefore have a constant magnetic field given by

$$\mathbf{B}_r = B\hat{\mathbf{x}} + \left(B_0 - \frac{\omega}{\gamma}\right)\hat{\mathbf{z}} \tag{6}$$

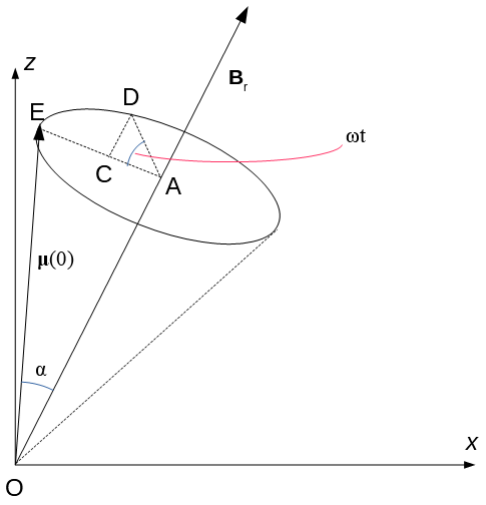
The magnetic moment should then precess about $\mathbf{B}_r$. To get the frequency $\boldsymbol{\omega}_r$ of this precession, we get the magnitude of the magnetic field:

$$B_r = \sqrt{B^2 + \left(B_0 - \frac{\omega}{\gamma}\right)^2} \tag{7}$$

The precession frequency is then

$$\boldsymbol{\omega}_r = -\gamma\mathbf{B}_r \tag{8}$$

Refer to the following figure (similar to Shankar's Fig. 14.3, but with a few added points) for what follows.



In the figure $\boldsymbol{\mu}(0)$ is given by the vector OE, so it starts off pointing in the $+z$ direction. [Just as in Shankar's figure, we've drawn this vector so it's not quite parallel to the z axis, although in the problem $\boldsymbol{\mu}(0)$ does actually point directly along the z axis. Drawing it this way makes the figure a bit easier to follow.] To get the z component of $\boldsymbol{\mu}$ as it precesses about $\mathbf{B}_r$, suppose we look at $\boldsymbol{\mu}$ at time t, when it has precessed through an angle ωt, so $\boldsymbol{\mu}$ now lies along the vector OD (I haven't drawn the vector in the diagram since it would get too cluttered, but you can imagine the vector.) To get the z component of this vector, we look at its components parallel and perpendicular to the plane followed by the tip of $\boldsymbol{\mu}$ as it precesses. This is the plane occupied by the circle in the diagram (well, ok, in the diagram it's an ellipse because we're looking at the circle from an angle). If the angle between $\boldsymbol{\mu}$ and $\mathbf{B}_r$ is α, then the components of $\boldsymbol{\mu}(\omega t)$ are

$$AD = \mu \sin\alpha \tag{9}$$

$$OA = \mu \cos\alpha \tag{10}$$

Note that the magnitude of $\boldsymbol{\mu}$ is constant; only its direction changes by precession. The angle α between $\boldsymbol{\mu}$ and $\mathbf{B}_r$ is also constant.

To get the projections of these two segments onto the z axis, we look first at the projection of OA since OA always lies in the xz plane. From the diagram

$$OA_z = (\mu \cos\alpha)\cos\alpha = \mu \cos^2\alpha \tag{11}$$

To get the z projection of AD, we first project it onto the xz plane by projecting it onto AE, giving the segment AC:

$$AC = AD\cos\omega t \tag{12}$$

$$= \mu \sin\alpha \cos\omega t \tag{13}$$

We then project AC onto the z axis. The line AC makes an angle α with the x axis, so the projection introduces another factor of $\sin\alpha$:

$$AC_z = AC\sin\alpha = \mu \sin^2\alpha \cos\omega t \tag{14}$$

The z component of $\boldsymbol{\mu}$ is therefore the sum of 11 and 14:

$$\mu_z = \mu\cos^2\alpha + \mu\sin^2\alpha\cos\omega t \tag{15}$$

To get the final form, we need to eliminate α which we can do from 6, since α is the angle between $\mathbf{B}_r$ and the z axis. Therefore

$$\sin\alpha = \frac{B}{B_r} \tag{16}$$

$$= \frac{B}{\sqrt{B^2+\left(B_0-\frac{\omega}{\gamma}\right)^2}} \tag{17}$$

$$= \frac{\gamma B}{\sqrt{\gamma^2B^2+\left(\gamma B_0-\omega\right)^2}} \tag{18}$$

$$\cos\alpha = \frac{B_0-\frac{\omega}{\gamma}}{\sqrt{B^2+\left(B_0-\frac{\omega}{\gamma}\right)^2}} \tag{19}$$

$$= \frac{\gamma B_0-\omega}{\sqrt{\gamma^2B^2+\left(\gamma B_0-\omega\right)^2}} \tag{20}$$

We can write this in terms of the frequency ω_0 by which the magnetic moment would precess if the field were constant, which is

$$\omega_0 = |\boldsymbol{\omega}_0| = \gamma B_0 \tag{21}$$

So we get

$$\sin\alpha = \frac{\gamma B}{\sqrt{\gamma^2B^2+\left(\omega_0-\omega\right)^2}} \tag{22}$$

$$\cos\alpha = \frac{\omega_0-\omega}{\sqrt{\gamma^2B^2+\left(\omega_0-\omega\right)^2}} \tag{23}$$

Plugging this into 15 we get

$$\mu_z(t) = \mu_z(0)\left[\frac{\left(\omega_0-\omega\right)^2}{\gamma^2B^2+\left(\omega_0-\omega\right)^2}+\frac{\gamma^2B^2\cos\omega t}{\gamma^2B^2+\left(\omega_0-\omega\right)^2}\right] \tag{24}$$

PINGBACKS

Pingback: Spinor in oscillating magnetic field - part 1

Pingback: Spinor in oscillating magnetic field - part 2

Pingback: Effective magnetic field in rotating frame - axis of rotation not parallel

SPINOR IN OSCILLATING MAGNETIC FIELD - PART 1

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 14, Exercise 14.4.3, Part 1.

Post date: 17 Aug 2017

[If some equations are too small to read easily, use your browser's magnifying option (Ctrl + on Chrome, probably something similar on other browsers).]

Classically, if a magnetic moment $\boldsymbol{\mu}$ is placed in a magnetic field that precesses about the z axis, the magnetic moment itself precesses. If the field is given as

$$\mathbf{B} = B\cos\omega t\hat{\mathbf{x}} - B\sin\omega t\hat{\mathbf{y}} + B_0\hat{\mathbf{z}} \tag{1}$$

then in a frame that rotates with the same frequency as the field, the magnetic field appears to be constant with value

$$\mathbf{B}_r = B\hat{\mathbf{x}}_r + \left(B_0 - \frac{\omega}{\gamma}\right)\hat{\mathbf{z}} \tag{2}$$

where

$$\hat{\mathbf{x}}_r = \cos\omega t\hat{\mathbf{x}} - \sin\omega t\hat{\mathbf{y}} \tag{3}$$

is a unit vector along the x axis in the rotating frame. We now want to see how this result transfers into quantum mechanics.

We begin with the Schrödinger equation for the state $|\psi(t)\rangle$ in the lab (non-rotating) frame, which is, as usual

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = H|\psi(t)\rangle \tag{4}$$

We'll study the case where $|\psi(t)\rangle$ is a spin $\frac{1}{2}$ state, for which the Hamiltonian is

$$H = -\gamma\mathbf{S}\cdot\mathbf{B} \tag{5}$$

We can analyze the situation in the rotating frame by applying a unitary rotation operator to the lab state. That is

$$|\psi_r(t)\rangle = e^{-i\omega t S_z/\hbar}|\psi(t)\rangle = e^{-i\omega t\sigma_z/2}|\psi(t)\rangle \tag{6}$$

$$= \left[\cos\frac{\omega t}{2}I - i\sin\frac{\omega t}{2}\sigma_z\right]|\psi(t)\rangle \tag{7}$$

[It seems to me that this unitary operator is for a rotation by an angle ωt, and since the rotation of the field in 1 is given by a frequency $-\omega\hat{\mathbf{z}}$, we should really be using the rotation operator $e^{i\omega t\sigma_z/2}$. However if we do this (I tried) we get the wrong answer, so presumably the transformation 6 is correct.]

Our first goal is to find the Schrödinger equation for $|\psi_r(t)\rangle$, which involves finding the corresponding Hamiltonian. The Schrödinger equation is

$$i\hbar\frac{\partial}{\partial t}|\psi_r(t)\rangle = H_r|\psi_r(t)\rangle \tag{8}$$

Inserting 6 into the LHS and differentiating, we get

$$i\hbar\frac{\partial}{\partial t}|\psi_r(t)\rangle = \frac{\hbar\omega\sigma_z}{2}e^{-i\omega t\sigma_z/2}|\psi(t)\rangle + i\hbar e^{-i\omega t\sigma_z/2}\frac{\partial}{\partial t}|\psi(t)\rangle \tag{9}$$

$$= \frac{\hbar\omega\sigma_z}{2}|\psi_r(t)\rangle + e^{-i\omega t\sigma_z/2}H|\psi(t)\rangle \tag{10}$$

$$= \frac{\hbar\omega\sigma_z}{2}|\psi_r(t)\rangle - e^{-i\omega t\sigma_z/2}\gamma\mathbf{S}\cdot\mathbf{B}|\psi(t)\rangle \tag{11}$$

We would like the RHS to be in the form of the RHS of 8, but in the second term, the problem is that $e^{-i\omega t\sigma_z/2}$ does not commute with $\mathbf{S}$ so we can't just swap the $e^{-i\omega t\sigma_z/2}$ and $\mathbf{S}\cdot\mathbf{B}$ factors. We need to multiply out the terms and see what simplifications we can do.

In what follows, it's easier to work with the Pauli matrices defined by

$$\mathbf{S} = \frac{\hbar}{2}\boldsymbol{\sigma} \tag{12}$$

We'll also need a few theorems involving σ_i

$$\sigma_i\sigma_j = -\sigma_j\sigma_i \tag{13}$$

$$\sigma_i\sigma_j = \delta_{ij}I + i\sum_k \varepsilon_{ijk}\sigma_k \tag{14}$$

We'll also define some shorthand for the trig functions:

$$c \equiv \cos\frac{\omega t}{2} \tag{15}$$
$$s \equiv \sin\frac{\omega t}{2} \tag{16}$$
$$c_1 \equiv \cos\omega t \tag{17}$$
$$s_1 \equiv \sin\omega t \tag{18}$$

The standard double-angle formulas are

$$c_1 = c^2 - s^2 \tag{19}$$
$$s_1 = 2sc \tag{20}$$

Using 1 and 7 we have

$$-e^{-i\omega t\sigma_z/2}\gamma\mathbf{S}\cdot\mathbf{B} = -\frac{\gamma\hbar}{2}\left[B\left(c-is\sigma_z\right)\left(\sigma_x c_1-\sigma_y s_1\right)+B_0\left(c-is\sigma_z\right)\sigma_z\right] \tag{21}$$

The last term on the RHS is in the correct form since there are no commutation problems here. So we need to work on the first term, which we'll isolate here:

$$\left(c-is\sigma_z\right)\left(\sigma_x c_1-\sigma_y s_1\right) = c_1 c\sigma_x + ic_1 s\sigma_x\sigma_z - s_1 c\sigma_y - is_1 s\sigma_y\sigma_z \tag{22}$$

We can now use the identities 13 and 14 and the trig identities above to get

$$\left(c-is\sigma_z\right)\left(\sigma_x c_1-\sigma_y s_1\right) = \left(c^2-s^2\right)c\sigma_x + i\left(c^2-s^2\right)s\sigma_x\sigma_z - 2sc^2\sigma_y - 2is^2 c\sigma_y\sigma_z \tag{23}$$
$$= \left(c^2-s^2\right)c\sigma_x + i\left(c^2-s^2\right)s\sigma_x\sigma_z - 2isc^2\sigma_x\sigma_z + 2s^2 c\sigma_x \tag{24}$$
$$= \left(c^3 - s^2 c + 2s^2 c\right)\sigma_x + i\left(-s^3 + c^2 s - 2sc^2\right)\sigma_x\sigma_z \tag{25}$$
$$= \left(c^2+s^2\right)c\sigma_x - i\left(c^2+s^2\right)s\sigma_x\sigma_z \tag{26}$$
$$= \sigma_x\left(c-is\sigma_z\right) \tag{27}$$
$$= \sigma_x e^{-i\omega t\sigma_z/2} \tag{28}$$

Plugging this into 21 and then back into 11 we get

$$i\hbar\frac{\partial}{\partial t}\left|\psi_r\left(t\right)\right\rangle = \frac{\hbar\omega\sigma_z}{2}\left|\psi_r\left(t\right)\right\rangle - \frac{\gamma\hbar}{2}\left[B\sigma_x + B_0\sigma_z\right]e^{-i\omega t\sigma_z/2}\left|\psi\left(t\right)\right\rangle \quad (29)$$

$$= \left[\left(\omega - \gamma B_0\right)S_z - \gamma B S_x\right]\left|\psi_r\left(t\right)\right\rangle \quad (30)$$

Comparing this with 2, we see that we can write the result as

$$i\hbar\frac{\partial}{\partial t}\left|\psi_r\left(t\right)\right\rangle = -\gamma\mathbf{S}\cdot\mathbf{B}_r\left|\psi_r\left(t\right)\right\rangle \quad (31)$$

Thus in the rotating frame, the Schrödinger equation has the same form as the classical relation, with a time-independent magnetic field $\mathbf{B}_r$.

COMMENTS

From: Petra Axolotl, 3 Jul 2018, 00:37.

The transformation 6 is indeed correct, for the following reason. - At time t, the rotating frame has rotated by $-\omega t$ relative to the rest frame. - Therefore everything in the rest frame, including the wave function $\psi\left(t\right)$, should be rotated by $+\omega t$ to get $\psi_r(t)$. - The unitary operator for a rotation by $+\omega t$ is $\exp(-i\omega t S_z/h)$.

Conclusion: $\psi_r(t) = \exp(-i\omega t S_z/h)\psi(t)$.

This is in fact the same as in certain derivations regarding translational invariance, where moving the frame by $-\Delta$ means moving the wave function by $+\Delta$ and $\psi(x)$ becomes $\psi(x-\Delta)$, or $\psi_r(x) = \exp(-i\Delta P/h)\psi(x)$.

PINGBACKS

Pingback: Spinor in oscillating magnetic field - part 2

SPINOR IN OSCILLATING MAGNETIC FIELD - PART 2

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Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 14, Exercise 14.4.3, Part 2.

Post date: 18 Aug 2017

[If some equations are too small to read easily, use your browser's magnifying option (Ctrl + on Chrome, probably something similar on other browsers).]

In the first part of this article, we saw that a particle with spin placed in a precessing magnetic field can be analyzed by moving to a frame rotating with the same frequency as the field. In this rotating frame, the magnetic field is independent of time and looks like this:

$$\mathbf{B}_r = B\hat{\mathbf{x}}_r + \left(B_0 - \frac{\omega}{\gamma}\right)\hat{\mathbf{z}} \tag{1}$$

where $\hat{\mathbf{x}}_r$ is a unit vector along the rotating x axis. In this frame, the Schrödinger equation has the form

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}\left|\psi_r(t)\right\rangle &= -\gamma\mathbf{S}\cdot\mathbf{B}_r\left|\psi_r(t)\right\rangle & (2)\\ &= \left[\left(\omega-\gamma B_0\right)S_z - \gamma B S_x\right]\left|\psi_r(t)\right\rangle & (3)\end{aligned}$$

where $\left|\psi_r(t)\right\rangle$ is the state vector in the rotating frame, in the S_z basis. The Hamiltonian in the rotating frame is thus

$$\begin{aligned} H &= \left(\omega-\gamma B_0\right)S_z - \gamma B S_x & (4)\\ &= \frac{\hbar}{2}\left(\omega-\gamma B_0\right)\sigma_z - \frac{\hbar}{2}\gamma B\sigma_x & (5)\end{aligned}$$

Given the initial state $\left|\psi_r(0)\right\rangle$ we can find the state at other times if we can find the propagator in the rotating frame

$$U_r(t) = e^{-iHt/\hbar} \tag{6}$$

The propagator is complicated by the fact that the Hamiltonian 5 contains two operators (σ_x and σ_z) that don't commute, so we can't split the exponential into the product of two simpler exponentials. However, if we

expand the exponential in a power series, we see that it does actually have a fairly simple form. We have

$$\begin{aligned} e^{-iHt/\hbar} &= e^{-i[(\omega-\gamma B_0)\sigma_z-\gamma B\sigma_x]t/2} && (7)\\ &= e^{i[(\gamma B_0-\omega)\sigma_z+\gamma B\sigma_x]t/2} && (8)\end{aligned}$$

We can expand this in a power series, but first it's useful to introduce some shorthand. We have

$$\begin{aligned} \omega_0 &\equiv \gamma B_0 && (9)\\ \omega_r &\equiv \sqrt{(\gamma B_0-\omega)^2+\gamma^2B^2} && (10)\\ &= \sqrt{(\omega_0-\omega)^2+\gamma^2B^2} && (11)\end{aligned}$$

We get

$$\begin{aligned} e^{-iHt/\hbar} = I + \frac{it}{2}\left[(\omega_0-\omega)\,\sigma_z+\gamma B\sigma_x\right]+ && (12)\\ -\frac{1}{2!}\frac{t^2}{2^2}\left(\left[(\omega_0-\omega)\,\sigma_z+\gamma B\sigma_x\right]\right)^2+ && (13)\\ -\frac{1}{3!}\frac{it^3}{2^3}\left(\left[(\omega_0-\omega)\,\sigma_z+\gamma B\sigma_x\right]\right)^3+\ldots && (14)\end{aligned}$$

Consider the square term in the second line. Multiplying it out, we get

$$\begin{aligned} \left((\omega_0-\omega)\,\sigma_z+\gamma B\sigma_x\right)^2 = (\omega_0-\omega)^2\,\sigma_z^2+\gamma^2B^2\sigma_x^2+ && (15)\\ (\omega_0-\omega)\,\gamma B\left(\sigma_z\sigma_x+\sigma_x\sigma_z\right) && (16)\end{aligned}$$

Using a couple of identities for Pauli matrices:

$$\begin{aligned} \sigma_i^2 &= I && (17)\\ \left[\sigma_z,\sigma_x\right]_+ &= 0 && (18)\end{aligned}$$

we see that the last term vanishes and the first two terms can be combined, so we get

$$\begin{aligned} \left((\omega_0-\omega)\,\sigma_z+\gamma B\sigma_x\right)^2 &= \left[(\omega_0-\omega)^2+\gamma^2B^2\right]I && (19)\\ &= \omega_r^2 I && (20)\end{aligned}$$

This simple form means that all higher terms in the power series 12 are easy to calculate. If we call the nth term in the series a_n, the terms with an even exponent are

$$a_{2n} = (-1)^n \frac{t^{2n}}{(2n)!2^{2n}} \omega_r^{2n} I \tag{21}$$

The $(-1)^n$ comes in because of the i in the exponent which gets raised to successively higher powers in the series. The series of even terms is therefore a cosine:

$$\sum_{n=0}^{\infty} a_{2n} = \cos\frac{\omega_r t}{2} I \tag{22}$$

For odd terms, we have

$$a_{2n+1} = (-1)^n i\omega_r^{2n} \frac{t^{2n+1}}{(2n+1)!2^{2n+1}} \left[(\omega_0 - \omega)\sigma_z + \gamma B \sigma_x\right] \tag{23}$$

The series of odd terms comes out to

$$\sum_{n=0}^{\infty} a_{2n+1} = \frac{i}{\omega_r}\left[(\omega_0 - \omega)\sigma_z + \gamma B\sigma_x\right] \sum_{n=0}^{\infty} \frac{(-1)^n t^{2n+1} \omega_r^{2n+1}}{(2n+1)!2^{2n+1}} \tag{24}$$

$$= \frac{i}{\omega_r}\left[(\omega_0 - \omega)\sigma_z + \gamma B\sigma_x\right] \sin\frac{\omega_r t}{2} \tag{25}$$

We can therefore write out U as a matrix by using the Pauli matrices:

$$\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}; \quad \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \tag{26}$$

$$U_r(t) = \begin{bmatrix} \cos\frac{\omega_r t}{2} + \frac{\omega_0 - \omega}{\omega_r} i \sin\frac{\omega_r t}{2} & \frac{i\gamma B}{\omega_r}\sin\frac{\omega_r t}{2} \\ \frac{i\gamma B}{\omega_r}\sin\frac{\omega_r t}{2} & \cos\frac{\omega_r t}{2} - \frac{\omega_0 - \omega}{\omega_r} i \sin\frac{\omega_r t}{2} \end{bmatrix} \tag{27}$$

To rotate this back to the lab frame, we apply the inverse rotation operator

$$e^{+i\omega t S_z/\hbar} = e^{i\omega t \sigma_z/2} \tag{28}$$

$$= \begin{bmatrix} e^{i\omega t/2} & 0 \\ 0 & e^{-i\omega t/2} \end{bmatrix} \tag{29}$$

For a particle that starts in the spin up state

$$|\psi(0)\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \tag{30}$$

Since the spin z direction is also the axis of rotation for the rotating frame, we have (except for a phase factor that isn't observable physically):

$$|\psi_r(0)\rangle = e^{-i\omega t/2}\begin{bmatrix} 1 \\ 0 \end{bmatrix} \tag{31}$$

The general state at time t is

$$|\psi(t)\rangle = e^{i\omega t\sigma_z/2}U_r(t)\,|\psi_r(0)\rangle \tag{32}$$

$$= e^{-i\omega t/2}\begin{bmatrix} \left[\cos\frac{\omega_r t}{2} + \frac{\omega_0-\omega}{\omega_r} i\sin\frac{\omega_r t}{2}\right] e^{i\omega t/2} \\ \frac{i\gamma B}{\omega_r}\sin\frac{\omega_r t}{2} e^{-i\omega t/2} \end{bmatrix} \tag{33}$$

In the case $\omega = \omega_0 = \gamma B_0$, we have $\omega_r = \gamma B$ from 11, so the state vector becomes

$$|\psi(t)\rangle = e^{-i\omega t/2}\begin{bmatrix} \cos\frac{\gamma B t}{2} e^{i\omega t/2} \\ i\sin\frac{\gamma B t}{2} e^{-i\omega t/2} \end{bmatrix} \tag{34}$$

If we compare this to the eigenvector $|\hat{n}+\rangle$ for spin up along a general direction given by the spherical angles θ and ϕ, which is

$$|\hat{n}+\rangle = \begin{bmatrix} \cos\frac{\theta}{2} e^{-i\phi/2} \\ \sin\frac{\theta}{2} e^{i\phi/2} \end{bmatrix} \tag{35}$$

we see that, apart from the extra i in the sine term, the state $|\psi(t)\rangle$ is the spin-up state for polar angles $\theta = \gamma B t$, $\phi = -\omega t$. The probability of finding an up or down state is

$$P_{up} = \left|\cos\frac{\gamma B t}{2} e^{i\omega t/2}\right|^2 = \cos^2\frac{\gamma B t}{2} \tag{36}$$

$$P_{down} = \left|i\sin\frac{\gamma B t}{2} e^{-i\omega t/2}\right|^2 = \sin^2\frac{\gamma B t}{2} \tag{37}$$

The spin oscillates between a pure up state when $\gamma B t/2$ is a multiple of π to a pure down state when $\gamma B t/2$ is an odd multiple of $\frac{\pi}{2}$.

Finally, we can check that $\langle\mu_z(t)\rangle$ agrees with the classical result

$$\mu_z(t) = \mu_z(0)\left[\frac{(\omega_0-\omega)^2}{\gamma^2 B^2 + (\omega_0-\omega)^2} + \frac{\gamma^2 B^2\cos\omega t}{\gamma^2 B^2 + (\omega_0-\omega)^2}\right] \tag{38}$$

To find $\langle\mu_z(t)\rangle$ we evaluate as follows.

$$\langle \mu_z(t) \rangle = \langle \psi(t) | \mu_z | \psi(t) \rangle \tag{39}$$
$$= \gamma \langle \psi(t) | S_z | \psi(t) \rangle \tag{40}$$
$$= \frac{\gamma\hbar}{2} \langle \psi(t) | \sigma_z | \psi(t) \rangle \tag{41}$$
$$= \frac{\gamma\hbar}{2} \left[\begin{array}{cc} \left(\cos\frac{\omega_r t}{2} - \frac{\omega_0-\omega}{\omega_r} i \sin\frac{\omega_r t}{2}\right) e^{-i\omega t/2} & -\frac{i\gamma B}{\omega_r} \sin\frac{\omega_r t}{2} e^{i\omega t/2} \end{array} \right] \times \tag{42}$$
$$\left[\begin{array}{cc} 1 & 0 \\ 0 & -1 \end{array} \right] \left[\begin{array}{c} \left(\cos\frac{\omega_r t}{2} + \frac{\omega_0-\omega}{\omega_r} i \sin\frac{\omega_r t}{2}\right) e^{i\omega t/2} \\ \frac{i\gamma B}{\omega_r} \sin\frac{\omega_r t}{2} e^{-i\omega t/2} \end{array} \right] \tag{43}$$

We introduce shorthand for the trig functions:

$$c \equiv \cos\frac{\omega_r t}{2} \tag{44}$$
$$s \equiv \sin\frac{\omega_r t}{2} \tag{45}$$

Then we have (note that complex exponentials cancel out):

$$\frac{2}{\gamma\hbar} \langle \mu_z(t) \rangle = \left[\begin{array}{cc} \left[c - \frac{\omega_0-\omega}{\omega_r} is\right] e^{-i\omega t/2} & -\frac{i\gamma B}{\omega_r} s e^{i\omega t/2} \end{array} \right] \left[\begin{array}{cc} 1 & 0 \\ 0 & -1 \end{array} \right] \left[\begin{array}{c} \left[c + \frac{\omega_0-\omega}{\omega_r} is\right] e^{i\omega t/2} \\ \frac{i\gamma B}{\omega_r} s e^{-i\omega t/2} \end{array} \right] \tag{46}$$
$$\left[\begin{array}{cc} c - \frac{\omega_0-\omega}{\omega_r} is & -\frac{i\gamma B}{\omega_r} s \end{array} \right] \left[\begin{array}{c} c + \frac{\omega_0-\omega}{\omega_r} is \\ -\frac{i\gamma B}{\omega_r} s \end{array} \right] \tag{47}$$
$$= c^2 + \left(\frac{\omega_0-\omega}{\omega_r}\right)^2 s^2 - \left(\frac{\gamma B}{\omega_r}\right)^2 s^2 \tag{48}$$
$$= \frac{1}{\omega_r^2} \left[\omega_r^2 c^2 + \left((\omega_0-\omega)^2 - \gamma^2 B^2 \right) s^2 \right] \tag{49}$$
$$= \frac{1}{\omega_r^2} \left[\left((\omega_0-\omega)^2 + \gamma^2 B^2 \right) c^2 + \left((\omega_0-\omega)^2 - \gamma^2 B^2 \right) s^2 \right] \tag{50}$$
$$= \frac{1}{\omega_r^2} \left((\omega_0-\omega)^2 + \gamma^2 B^2 \left(c^2 - s^2 \right) \right) \tag{51}$$

where we used 11 in the fourth line.
Using the trig identity

$$\cos 2\theta = \cos^2\theta - \sin^2\theta \tag{52}$$

we see that

$$c^2 - s^2 = \cos^2 \frac{\omega_r t}{2} - \sin^2 \frac{\omega_r t}{2} = \cos \omega_r t \tag{53}$$

So we have

$$\langle \mu_z (t) \rangle = \frac{\gamma \hbar}{2} \frac{(\omega_0 - \omega)^2 + \gamma^2 B^2 \cos \omega_r t}{\omega_r^2} \tag{54}$$

$$= \frac{\gamma \hbar}{2} \frac{(\omega_0 - \omega)^2 + \gamma^2 B^2 \cos \omega_r t}{(\omega_0 - \omega)^2 + \gamma^2 B^2} \tag{55}$$

This agrees with 38 provided $\mu_z (0) = \frac{\gamma \hbar}{2}$, which is true, since the magnitude of the magnetic moment is $\frac{\gamma \hbar}{2}$ and it starts in the spin up position so $\mu_z (0) = \frac{\gamma \hbar}{2}$.

SPIN FLIP OF ELECTRON IN MAGNETIC FIELD

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 14, Exercise 14.4.4.

Post date: 20 Aug 2017

[If some equations are too small to read easily, use your browser's magnifying option (Ctrl + on Chrome, probably something similar on other browsers).]

The fact that the rotation operator in 2-d spin space can be written in terms of the Pauli matrices as

$$U\left[R(\boldsymbol{\theta})\right] = e^{-i\boldsymbol{\theta}\cdot\boldsymbol{\sigma}/2} = \cos\frac{\theta}{2}I - i\sin\frac{\theta}{2}\left(\hat{\theta}\cdot\boldsymbol{\sigma}\right) \tag{1}$$

allows us to do some calculations involving an electron in a magnetic field. We've seen that placing a magnetic moment that is due to angular momentum in a constant magnetic field causes the magnetic moment to precess about the direction of the field. The Hamiltonian of an electron with spin **S** in a constant field **B** is

$$\begin{aligned} H &= -\gamma\mathbf{S}\cdot\mathbf{B} && (2)\\ &= -\frac{\gamma\hbar}{2}\boldsymbol{\sigma}\cdot\mathbf{B} && (3)\end{aligned}$$

where γ is the gyromagnetic ratio

$$\begin{aligned} \gamma &= \frac{-e}{m}\,(\text{SI}) = \frac{-e}{mc}\,(\text{CGS}) && (4)\\ &= 1.76\times10^{11}\ \text{s}^{-1}\text{T}^{-1} && (5)\\ &= 1.76\times10^{7}\ \text{s}^{-1}\text{G}^{-1} && (6)\end{aligned}$$

As an example, suppose we have an electron initially in the spin-up state, with $s_z = +\frac{\hbar}{2}$ and turn on a magnetic field of $\mathbf{B} = (100\ \text{G})\,\hat{\mathbf{x}}$ at $t = 0$. As the applied field is perpendicular to the initial spin, the precession will cause the spin vector to rotate in the yz plane about the x axis. To find how long it takes the spin to flip, we need the propagator, which is

$$\begin{aligned} U(t) &= e^{-iHt/\hbar} && (7)\\ &= e^{i\gamma\boldsymbol{\sigma}\cdot\mathbf{B}t/2} && (8)\\ &= e^{i\gamma Bt\sigma_x/2} && (9) \end{aligned}$$

Comparing with 1 we see that $U(t)$ is equivalent to a rotation operator with angle $\theta = -\gamma Bt$. Thus we have

$$\begin{aligned} U(t) &= \cos\frac{\gamma Bt}{2} I + i\sin\frac{\gamma Bt}{2}\sigma_x && (10)\\ &= \begin{bmatrix} \cos\frac{\gamma Bt}{2} & i\sin\frac{\gamma Bt}{2} \\ i\sin\frac{\gamma Bt}{2} & \cos\frac{\gamma Bt}{2} \end{bmatrix} && (11) \end{aligned}$$

The electron's state as a function of time is thus

$$\begin{aligned} |\psi(t)\rangle &= U(t)|\psi(0)\rangle && (12)\\ &= \begin{bmatrix} \cos\frac{\gamma Bt}{2} & i\sin\frac{\gamma Bt}{2} \\ i\sin\frac{\gamma Bt}{2} & \cos\frac{\gamma Bt}{2} \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} && (13)\\ &= \begin{bmatrix} \cos\frac{\gamma Bt}{2} \\ i\sin\frac{\gamma Bt}{2} \end{bmatrix} && (14) \end{aligned}$$

The state first has a 100% probability of being found with spin down when (using 6):

$$\begin{aligned} \sin\frac{\gamma Bt}{2} &= 1 && (15)\\ t &= \frac{\pi}{\gamma B} && (16)\\ &= \frac{\pi}{(1.76\times 10^7)(100)} && (17)\\ &= 1.78\times 10^{-9}\ \text{s} && (18) \end{aligned}$$

EFFECTIVE MAGNETIC FIELD IN ROTATING FRAME - AXIS OF ROTATION NOT PARALLEL TO FIELD

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 14, Exercise 14.4.5.

Post date: 21 Aug 2017

[If some equations are too small to read easily, use your browser's magnifying option (Ctrl + on Chrome, probably something similar on other browsers).]

Returning to classical physics for this post, we recall that if we have a magnetic moment $\boldsymbol{\mu}$ placed in a constant magnetic field $\mathbf{B}_0$, then if we move to a frame of reference that rotates with frequency $\boldsymbol{\omega}$ which is parallel to $\mathbf{B}_0$, the effective magnetic field as seen in the rotating frame is

$$\mathbf{B}_r = \mathbf{B}_0 + \frac{\boldsymbol{\omega}}{\gamma} \tag{1}$$

where γ is the gyromagnetic ratio. However, suppose the rotating frame has an axis of rotation that is not parallel to $\mathbf{B}_0$, that is $\boldsymbol{\omega}$ is not parallel to $\mathbf{B}_0$. In this case, we have the following situation.

Suppose we have some arbitrary vector $\mathbf{V}$ which changes by $\Delta\mathbf{V}$ in time interval Δt, as viewed in the non-rotating frame. As we've seen earlier, if a vector $\mathbf{r}$ that makes an angle α with the axis of rotation is rotated through an angle $\Delta\boldsymbol{\theta}$ where the direction of $\Delta\boldsymbol{\theta}$ is the axis of rotation, then the change in $\mathbf{r}$ is given by

$$\mathbf{r} \rightarrow \mathbf{r} + (\delta\boldsymbol{\theta}) \times \mathbf{r} \tag{2}$$

In the rotating frame, in the time interval Δt, the vector changes due to two separate effects: the change $\Delta\mathbf{V}$ that occurs in the lab frame *plus* the change due to the angle $\delta\boldsymbol{\theta} = -\boldsymbol{\omega}\Delta t$ that occurs due to the frame's rotation. (The minus sign arises because if the frame is rotating counterclockwise, objects in the lab frame appear to be rotating clockwise as seen in the rotating frame.) If we take the vector to be at the same position in both frames at time t, then our job is to find the relation between the changes to $\mathbf{V}$ that occur in the two frames after interval Δt.

In the inertial (lab) frame, we have

$$\mathbf{V}(t + \Delta t) = \mathbf{V}(t) + \Delta\mathbf{V} \tag{3}$$

In the rotating frame, we have

$$\begin{aligned} \mathbf{V}_r(t+\Delta t) &= \mathbf{V}_r(t) + \Delta\mathbf{V}_r && (4)\\ &= \mathbf{V}(t) + \Delta\mathbf{V}_r && (5)\end{aligned}$$

where the last line follows because the two vectors are identical at the initial time t.

Now by applying 2 to a rotation angle of $\delta\boldsymbol{\theta} = -\boldsymbol{\omega}\Delta t$ we have

$$\begin{aligned} \mathbf{V}_r(t+\Delta t) &= \mathbf{V}(t+\Delta t) - \boldsymbol{\omega}\times\mathbf{V}(t+\Delta t)\Delta t && (6)\\ &= \mathbf{V}(t) + \Delta\mathbf{V} - \boldsymbol{\omega}\times[\mathbf{V}(t) + \Delta\mathbf{V}]\Delta t && (7)\\ &= \mathbf{V}_r(t) + \Delta\mathbf{V} - \boldsymbol{\omega}\times\mathbf{V}(t)\Delta t + \mathcal{O}\left((\Delta t)^2\right) && (8)\\ \Delta\mathbf{V}_r &= \mathbf{V}_r(t+\Delta t) - \mathbf{V}_r(t) && (9)\\ &= \Delta\mathbf{V} - \boldsymbol{\omega}\times\mathbf{V}(t)\Delta t && (10)\end{aligned}$$

where the last line drops higher order terms. Dividing through by Δt and taking the limit we get

$$\frac{d\mathbf{V}_r}{dt} = \frac{d\mathbf{V}}{dt} - \boldsymbol{\omega}\times\mathbf{V} \tag{11}$$

If we now apply this to the precession of magnetic moments, we begin with the relation between torque $\mathbf{T}$ and angular momentum $\boldsymbol{\ell}$:

$$\mathbf{T} = \frac{d\boldsymbol{\ell}}{dt} = \gamma\boldsymbol{\ell}\times\mathbf{B}_0 \tag{12}$$

In the rotating frame, we have

$$\begin{aligned} \frac{d\boldsymbol{\ell}_r}{dt} &= \frac{d\boldsymbol{\ell}}{dt} - \boldsymbol{\omega}\times\boldsymbol{\ell} && (13)\\ &= \gamma\boldsymbol{\ell}\times\mathbf{B}_0 + \boldsymbol{\ell}\times\boldsymbol{\omega} && (14)\\ &= \gamma\boldsymbol{\ell}\times\left(\mathbf{B}_0 + \frac{\boldsymbol{\omega}}{\gamma}\right) && (15)\end{aligned}$$

Thus the effective field in the rotating frame is again

$$\mathbf{B}_r = \mathbf{B}_0 + \frac{\boldsymbol{\omega}}{\gamma} \tag{16}$$

and this applies even if $\mathbf{B}_0$ and $\boldsymbol{\omega}$ are not parallel.

ENSEMBLE OF ELECTRONS IN MAGNETIC FIELD

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Exercise 14.4.6.

Post date: 22 Aug 2017

[If some equations are too small to read easily, use your browser's magnifying option (Ctrl + on Chrome, probably something similar on other browsers).]

As an example of a density matrix, we can apply it to an ensemble of spin $\frac{1}{2}$ particles. The density matrix is defined as

$$\rho \equiv \sum_i p_i \left|i\right\rangle \left\langle i\right| \tag{1}$$

where p_i is the probability of a single system being state $|i\rangle$. For a spin $\frac{1}{2}$ particle, there are only 2 states, so the density matrix can be written as a 2×2 matrix, once we define a basis for the states (for example, the basis of S_z states where $S_z = \pm\frac{\hbar}{2}$). Since any 2×2 matrix can be written as a linear combination of the Pauli matrices and the identity matrix, the density matrix can be written as

$$\rho = a_0 I + \mathbf{A} \cdot \boldsymbol{\sigma} \tag{2}$$

Since the trace of each of the Pauli matrices is zero, and $\text{Tr}I = 2$, we have

$$\text{Tr}\rho = 2a_0 \tag{3}$$

However, we know that $\text{Tr}\rho = 1$, so we must have $a_0 = \frac{1}{2}$, so we can write

$$\rho = \frac{1}{2}\left(I + \mathbf{a} \cdot \boldsymbol{\sigma}\right) \tag{4}$$

for some vector **a** whose elements are complex numbers.

To find the average value $\left\langle \bar{\Omega} \right\rangle$ of an observable Ω in an ensemble, we can use the density matrix in the form

$$\left\langle \bar{\Omega} \right\rangle = \text{Tr}\left(\Omega\rho\right) \tag{5}$$

To find $\langle \bar{\boldsymbol{\sigma}} \rangle$, we can work out each component separately. For σ_x we have, using the properties of the σ_i:

$$\langle \bar{\sigma}_x \rangle = \mathrm{Tr}\,(\sigma_x \rho) \tag{6}$$
$$= \frac{1}{2}\mathrm{Tr}\left(\sigma_x I + a_x \sigma_x^2 + a_y \sigma_x \sigma_y + a_z \sigma_x \sigma_z\right) \tag{7}$$
$$= \frac{1}{2}\mathrm{Tr}\,(\sigma_x + a_x I + i a_y \sigma_z - i a_z \sigma_y) \tag{8}$$
$$= \frac{1}{2}\,(0 + 2a_x + 0 + 0) \tag{9}$$
$$= a_x \tag{10}$$

We can do similar calculations to get the other two components, with the result

$$\langle \bar{\boldsymbol{\sigma}} \rangle = \mathbf{a} \tag{11}$$

Finally, suppose we have an ensemble of electrons in a constant magnetic field $\mathbf{B} = B\hat{\mathbf{z}}$, and that this ensemble is in thermal equilibrium at temperature T. A central result of statistical mechanics (which we haven't covered yet) is that particles in thermal equilibrium obey the Boltzmann distribution, which states that the probability of finding a particle with energy E in the ensemble is

$$p_E \propto e^{-E/kT} \tag{12}$$

where k is the Boltzmann constant. In this case, the energy is that of a magnetic moment $\boldsymbol{\mu}$ in a constant magnetic field $\mathbf{B}$, which is

$$H = -\boldsymbol{\mu} \cdot \mathbf{B} = -\gamma \mathbf{S} \cdot \mathbf{B} = -\gamma S_z B \tag{13}$$

There are only two states ($S_z = \pm\frac{\hbar}{2}$), so the probabilities are

$$p_\uparrow = \frac{1}{P} e^{\gamma B\hbar/2kT} \tag{14}$$
$$p_\downarrow = \frac{1}{P} e^{-\gamma B\hbar/2kT} \tag{15}$$
$$P = e^{\gamma B\hbar/2kT} + e^{-\gamma B\hbar/2kT} \tag{16}$$

The density matrix is therefore

$$\rho = \frac{1}{P}\left(e^{\gamma B\hbar/2kT} \left|\uparrow\right\rangle \left\langle\uparrow\right| + e^{-\gamma B\hbar/2kT} \left|\downarrow\right\rangle \left\langle\downarrow\right|\right) \tag{17}$$

In the S_z basis, this is

$$\rho = \frac{1}{P}\begin{bmatrix} e^{\gamma B\hbar/2kT} & 0 \\ 0 & e^{-\gamma B\hbar/2kT} \end{bmatrix} \tag{18}$$

We can work out the average magnetic moment for the ensemble as

$$\langle \bar{\boldsymbol{\mu}} \rangle = \mathrm{Tr}\,(\boldsymbol{\mu}\rho) \tag{19}$$

$$= \frac{\hat{\mathbf{z}}}{P}\left[\frac{\gamma\hbar}{2}e^{\gamma B\hbar/2kT} - \frac{\gamma\hbar}{2}e^{-\gamma B\hbar/2kT}\right] \tag{20}$$

$$= \frac{e^{\gamma B\hbar/2kT} - e^{-\gamma B\hbar/2kT}}{e^{\gamma B\hbar/2kT} + e^{-\gamma B\hbar/2kT}}\frac{\gamma\hbar}{2}\hat{\mathbf{z}} \tag{21}$$

$$= \frac{\gamma\hbar}{2}\tanh\frac{\gamma B\hbar}{2kT}\hat{\mathbf{z}} \tag{22}$$

$$= -\frac{e\hbar}{2mc}\tanh\left(-\frac{eB\hbar}{2mckT}\right)\hat{\mathbf{z}} \tag{23}$$

$$= \frac{e\hbar}{2mc}\tanh\frac{eB\hbar}{2mckT}\hat{\mathbf{z}} \tag{24}$$

COUPLING OF PROTON'S MAGNETIC MOMENT TO EXTERNAL FIELD

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Exercise 14.5.1.

Post date: 27 Aug 2017

[If some equations are too small to read easily, use your browser's magnifying option (Ctrl + on Chrome, probably something similar on other browsers).]

We've dealt with the Zeeman effect in a lot of detail before, but Shankar deals with it using the approximation of negelecting the coupling of the proton's magnetic moment to the external magnetic field **B**. Using classical arguments, we can see why this is a reasonable approximation.

The proton, like the electron, has both orbital and spin angular momentum. The proton's spin is $\frac{\hbar}{2}$, the same as the electron, so its spin magnetic moment is given by

$$\mu_{ps} = \frac{q}{2Mc}\frac{\hbar}{2} \tag{1}$$

where M is the proton's mass. Since (apart from the sign) the proton and electron have the same charge q and spin, the equivalent formula for the electron is

$$\mu_{es} = \frac{q}{2mc}\frac{\hbar}{2} \tag{2}$$

where m is the electron mass. Thus

$$\mu_{ps} = \frac{m}{M}\mu_{es} \tag{3}$$

so that the proton's spin magnetic moment is about $\frac{1}{1836}$ times that of the electron.

For the orbital magnetic moment, we can consider a classical system in which the electron and proton are orbiting about their centre of mass. The period T of the orbit is the same for both particles, and the radius of each orbit is

$$r_p = \frac{m}{m+M} r \approx \frac{m}{M} r \tag{4}$$

$$r_e = \frac{M}{m+M} r \approx r \tag{5}$$

where r is the distance between the two particles. The orbital magnetic moment can be written as

$$\mu_i = \frac{q v_i r_i}{2c} \tag{6}$$

where the subscript i is either e or p. Since the proton moves in a smaller orbit but at the same frequency as the electron, its velocity is smaller. We have

$$v_p = \frac{2\pi r_p}{T} = \frac{2\pi r}{T} \frac{m}{m+M} \approx \frac{2\pi r}{T} \frac{m}{M} \tag{7}$$

$$v_e = \frac{2\pi r_e}{T} = \frac{2\pi r}{T} \frac{M}{m+M} \approx \frac{2\pi r}{T} \tag{8}$$

Therefore

$$\mu_p \approx \frac{\pi q r^2}{cT} \left(\frac{m}{M}\right)^2 \tag{9}$$

$$\mu_e \approx \frac{\pi q r^2}{cT} \tag{10}$$

Thus the orbital magnetic moment of the proton is about $\left(\frac{m}{M}\right)^2$ times that of the electron.

PINGBACKS

Pingback: Stern-gerlach experiment
Pingback: Hyperfine interaction in hydrogen - a rough calculation

SECOND-ORDER CORRECTION TO ZEEMAN EFFECT IN HYDROGEN

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Exercise 14.5.2.

Post date: 1 Sep 2017

[If some equations are too small to read easily, use your browser's magnifying option (Ctrl + on Chrome, probably something similar on other browsers).]

Shankar derives the interaction Hamiltonian between a magnetic moment and a magnetic field in quantum theory in his equations 14.4.11 to 14.4.15, so we won't repeat the derivation here. Rather we can summarize the main points.

The starting point is the classical Hamiltonian for the electromagnetic force

$$H = \frac{|\mathbf{p} - q\mathbf{A}/c|^2}{2m} + q\phi \tag{1}$$

In the current example, there is no electrostatic field, so $\phi = 0$, and we make the transition to quantum theory by interpreting $\mathbf{p}$ as the momentum operator $\mathbf{P}$. This gives

$$H = \frac{|\mathbf{P}|^2}{2m} - \frac{q}{2mc}(\mathbf{P}\cdot\mathbf{A} + \mathbf{A}\cdot\mathbf{P}) + \frac{q^2|\mathbf{A}|^2}{2mc^2} \tag{2}$$

We then assume that we have a constant magnetic field that points along the z axis, which can be produced by taking the vector potential $\mathbf{A}$ to be

$$\mathbf{A} = \frac{B}{2}(-y\hat{\mathbf{x}} + x\hat{\mathbf{y}}) \tag{3}$$

Using the standard relation between the vector potential and field, we have

$$\mathbf{B} = \nabla \times \mathbf{A} = B\hat{\mathbf{z}} \tag{4}$$

Shankar then assumes that the field is fairly weak, so we can ignore the last term in 2. He then shows that the middle term in 2 comes out to

$$H = -\boldsymbol{\mu}\cdot\mathbf{B} \tag{5}$$

where the magnetic moment is defined as

$$\boldsymbol{\mu} \equiv \frac{q}{2mc}\mathbf{L} \tag{6}$$

where $\mathbf{L}$ is the orbital angular momentum.

For the hydrogen atom, this analysis leads to the prediction of energy levels for the state $|nlmm_x\rangle$ of

$$E = -\frac{\text{Ry}}{n^2} + \frac{eB\hbar}{2m_e c}\left(m + 2m_s\right) \tag{7}$$

Here, m_e is the mass of the electron, m is the z component of orbital angular momentum (Shankar confusingly uses the same symbol m for the electron mass and z component of orbital angular momentum) and m_s is the z component of spin (both in units of $\hbar$). The Rydberg (Ry) has a value of 13.6 eV and is the energy level of the ground state of hydrogen. Also, note that all these equations use the Gaussian system of units (rather than SI, which we used in both of Griffiths's books). For calculation, it's useful to use the Bohr magneton for the electron, which is (using Gaussian units):

$$\mu_B \equiv \frac{e\hbar}{2m_e c} \tag{8}$$

$$= \frac{\left(4.8 \times 10^{-10}\text{ esu}\right)\left(1.05 \times 10^{-27}\text{ erg s}\right)}{2\left(9.1 \times 10^{-28}\text{ g}\right)\left(3 \times 10^{10}\text{ cm s}^{-1}\right)} \tag{9}$$

$$= 9.23 \times 10^{-21}\text{ erg G}^{-1} \tag{10}$$

$$\simeq 0.6 \times 10^{-8}\text{ eV G}^{-1} \tag{11}$$

To see the effect of the level splitting on the ground state (this is the Zeeman effect for $l = 0$, which we treated earlier), we have $n = 1$ and $m = 0$ with $m_s = \frac{1}{2}$, so the size of the level splitting is

$$\Delta E = \mu_B B \tag{12}$$

For $B = 1000$ kG $= 10^6$ G we have $\Delta E \simeq 0.6 \times 10^{-2}$ eV so the relative size, compared to the ground state energy, is

$$\frac{\Delta E}{E} = \frac{0.6 \times 10^{-2}}{13.6} = 4.4 \times 10^{-4} \tag{13}$$

[In Shankar's answer at the back of the book, he says the relative size is about one in a million, which seems much too small.]

We can also calculate the effect that we neglected by ignoring the $|\mathbf{A}|^2$ term in 2. If we assume that the electron is in a classical orbit of radius a_0 (the Bohr radius), then from 3, we have

$$|\mathbf{A}|^2 = \frac{B^2 a_0^2}{4} \tag{14}$$

The neglected term is therefore (using $a_0 \simeq 5.3 \times 10^{-9}$ cm)

$$\frac{e^2 B^2 a_0^2}{8mc^2} = \frac{\left(4.8 \times 10^{-10} \text{ esu}\right)^2 B^2 \left(5.3 \times 10^{-9} \text{ cm}\right)^2}{8 \left(9.1 \times 10^{-28} \text{ g}\right) \left(3 \times 10^{10} \text{ cm s}^{-1}\right)^2} \tag{15}$$

$$\simeq 10^{-32} B^2 \text{ erg} \tag{16}$$

$$= 6 \times 10^{-19} B^2 \text{ eV} \tag{17}$$

Thus in order for this term to make much of a difference, it would need to be the same order of magnitude as ΔE in 12. That is, we're looking for B such that

$$\Delta E \simeq \frac{e^2 B^2 a_0^2}{8mc^2} \tag{18}$$

$$\mu_B B \simeq \frac{e^2 B^2 a_0^2}{8mc^2} = 6 \times 10^{-19} B^2 \text{ eV} \tag{19}$$

$$B \simeq \frac{\mu_B}{6 \times 10^{-19}} \tag{20}$$

$$= \frac{0.6 \times 10^{-8}}{6 \times 10^{-19}} \tag{21}$$

$$= 10^{10} \text{ G} \tag{22}$$

STERN-GERLACH EXPERIMENT

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Exercises 14.5.3 - 14.5.4.

Post date: 5 Sep 2017

[If some equations are too small to read easily, use your browser's magnifying option (Ctrl + on Chrome, probably something similar on other browsers).]

The Stern-Gerlach experiment is the classic experiment that revealed the existence of electron spin. Shankar describes the ideas behind the experiment at the end of Chapter 14, so we'll just summarize them here.

The idea is to pass a beam of particles possessing magnetic moments through a non-uniform magnetic field **B**. The **B** field has a gradient along the z axis and the beam of particles is fired into this field along the y axis. The force exerted by this non-uniform field on a particle with magnetic moment $\boldsymbol{\mu}$ is given by

$$\mathbf{F} = -\nabla H = \mu_z \frac{\partial B_z}{\partial z}\hat{\mathbf{z}} \tag{1}$$

(see Shankar for the details of this calculation). If the magnetic moments μ_z have a continuous spread (as would be expected classically), then the force ranges continuously and we'd expect to see the particles smeared out over a uniform strip on the detector. What is actually observed is that the particles are deflected in discrete intervals, so we get a series of dots on the detector rather than a continuous line. This is explained by the fact that the magnetic moment (arising either from spin or orbital angular momentum) is quantized.

Here are some examples of what the experiment would reveal.

If we start with a beam of spin-$\frac{1}{2}$ particles (such as electrons or neutral hydrogen atoms where we can neglect the magnetic moment of the proton) then, because the possible values of spin are $\pm\frac{\hbar}{2}$, we see the incident beam split into two beams. If we block the lower beam, and allow the upper beam through, then we have a beam containing particles all with spin up, or $+\frac{\hbar}{2}$. If we pass this beam into a second appartus with a **B** field along the x axis (so the field gradient is at an angle of $\frac{\pi}{2}$ relative to the first apparatus), this second apparatus will also split the beam into two sub-beams. Because the

spin operators S_z and S_x don't commute, we can't measure the spin components in both directions simultaneously so, as far as the second apparatus is concerned, the x component of spin is unknown and could be either $\pm\frac{\hbar}{2}$. If we block the lower beam from the second apparatus, what fraction of the particles will get through?

To answer this, recall that the eigenspinors for the x direction in the basis of z spinors are

$$\chi_+^{(x)} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \tag{2}$$

$$\chi_-^{(x)} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} \tag{3}$$

Thus a particle with x spin $+\frac{\hbar}{2}$ is equally likely to be measured with a z spin of $\pm\frac{\hbar}{2}$. We can apply this argument in reverse by swapping the definitions of the x and z axes, so that if we send a beam of particles with z spin $+\frac{\hbar}{2}$ into the second apparatus, then a particle is equally likely to have a spin of $\pm\frac{\hbar}{2}$ in the x direction. In other words, on average, half the particles being fed into the second apparatus will go into the latter's 'up' beam and half into its 'down' beam. Combining the two apparatuses, we'd expect on average $\frac{1}{4}$ of the incident particles to emerge in the upper beam of the second apparatus.

Another way of saying this is that if we arrange a sequence of apparatuses where each apparatus is rotated by $\frac{\pi}{2}$ relative to its predecessor and one of the exit beams in each case is blocked, then the number of particles getting through each apparatus is half the number that entered it.

Now suppose we return to the case where the first apparatus transmits only spin z of $+\frac{\hbar}{2}$ but the second (aligned along the x axis) transmits everything (no blocked beam) into a third apparatus, which is aligned again along the z axis, but now transmits only particles with spin z of $-\frac{\hbar}{2}$. In this case, the middle (x axis) apparatus has no effect since it doesn't filter the particles at all, with the result that we're feeding a stream of $+\frac{\hbar}{2}$ particles into an apparatus that detects only spin $-\frac{\hbar}{2}$. In this case, nothing will get through.

Now let's look at a somewhat more complex situation. We now have a stream of spin-1 particles moving along the y axis into an apparatus with a **B** field aligned on the the z axis. Because m has three possible values $(\pm\hbar, 0)$, the output will be split into 3 beams. Suppose we take only the $+\hbar$ beam and feed it into a second apparatus in which the **B** field is rotated by an angle θ relative to the first. What fraction of the particles will get through?

To solve this, we need the unitary rotation operator that relates the two apparatuses. We worked this out before for both spin-$\frac{1}{2}$ and spin-1, and the result we need is the matrix

$$U\left[R\left(\theta\right)\right]=D^{(1)}\left[R\left(\theta\right)\right]=I^{(1)}+\frac{\left(\hat{\boldsymbol{\theta}}\cdot\mathbf{J}^{(1)}\right)^{2}}{\hbar^{2}}\left(\cos\theta-1\right)-\frac{i\hat{\boldsymbol{\theta}}\cdot\mathbf{J}^{(1)}}{\hbar}\sin\theta \quad (4)$$

Here, $\hat{\boldsymbol{\theta}}$ is a unit vector along the axis of rotation and $\mathbf{J}^{(1)}$ is the angular momentum operator for spin-1. In our case, the rotation is around the y axis, so

$$\hat{\boldsymbol{\theta}}=\hat{\mathbf{y}}=(0,1,0) \quad (5)$$

The components of $\mathbf{J}^{(1)}$ are given in Shankar's equations 12.5.23 and 12.5.24. We need only $J_y^{(1)}$:

$$J_y^{(1)}=\frac{i\hbar}{\sqrt{2}}\begin{bmatrix}0&-1&0\\1&0&-1\\0&1&0\end{bmatrix} \quad (6)$$

We then have

$$\frac{\hat{\boldsymbol{\theta}}\cdot\mathbf{J}^{(1)}}{\hbar}=\frac{i}{\sqrt{2}}\begin{bmatrix}0&-1&0\\1&0&-1\\0&1&0\end{bmatrix} \quad (7)$$

$$\frac{\left(\hat{\boldsymbol{\theta}}\cdot\mathbf{J}^{(1)}\right)^{2}}{\hbar^{2}}=\frac{1}{2}\begin{bmatrix}1&0&-1\\0&2&0\\-1&0&1\end{bmatrix} \quad (8)$$

From 4 we have

$$U\left[R\left(\theta\right)\right]=\begin{bmatrix}1+\frac{\cos\theta-1}{2}&\frac{\sin\theta}{\sqrt{2}}&-\frac{\cos\theta-1}{2}\\-\frac{\sin\theta}{\sqrt{2}}&\cos\theta&\frac{\sin\theta}{\sqrt{2}}\\-\frac{\cos\theta-1}{2}&-\frac{\sin\theta}{\sqrt{2}}&1+\frac{\cos\theta-1}{2}\end{bmatrix} \quad (9)$$

$$=\begin{bmatrix}\frac{1+\cos\theta}{2}&\frac{\sin\theta}{\sqrt{2}}&\frac{1-\cos\theta}{2}\\-\frac{\sin\theta}{\sqrt{2}}&\cos\theta&\frac{\sin\theta}{\sqrt{2}}\\\frac{1-\cos\theta}{2}&-\frac{\sin\theta}{\sqrt{2}}&\frac{1+\cos\theta}{2}\end{bmatrix} \quad (10)$$

The first column is the rotated version of the state $\begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}$, so a particle in this rotated state has probability of $\left(\frac{1+\cos\theta}{2}\right)^2$ of being in the $+\hbar$ spin state, so this is the fraction of particles leaving the first apparatus that will pass the second. [As a check, note that the sums of the squares of the elements in each column of 10 are 1.]

COMMENTS

Remark 1. I have some confusion about your solution to problem 14.05.03, Principles of Quantum Mechanics, Shankar. (Link: http://physicspages.com/pdf/Shankar/Shankar%20%2014.05.04.pdf) "Now suppose we return to the case where the first apparatus transmits only spin z of +h/2 but the second (aligned along the x axis) transmits everything (no blocked beam) into a third apparatus, which is aligned again along the z axis, but now transmits only particles with spin z of -h/2. In this case, the middle (x axis) apparatus has no effect since it doesn't filter the particles at all, with the result that we're feeding a stream of +h/2 particles into an apparatus that detects only spin -h/2. In this case, nothing will get through." My opinion is: When the spin +z electrons pass through the second SG (along x axis) apparatus, the outcome is electrons in the +x and -x spin state. The state is no more +z spin. So when the +x and -x spin electrons pass through the 3rd SG apparatus (along z axis) 50% of them should get through.

==========

I originally thought the same thing, but I think the point is that we aren't allowed to look at the output of the middle detector, so we don't ever measure a particle's x-spin. In that case, all the particles remain in the $+z$ state, so they all get blocked in the third detector. I suspect you're right that if we did measure the x-spin in the middle detector that would place the particle in either the $+x$ or $-x$ state, with z-spin undetermined, so that 50% of them would indeed get through the third detector. Shankar gives zero as the answer at the back of the book, so my guess is that's what's happening.

SPIN 1/2 ALONG AN ARBITRARY DIRECTION

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

Reference: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Problem 4.30.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 14, Exercise 14.3.2.

Post date: 19 Jan 2013.

[If some equations are too small to read easily, use your browser's magnifying option (Ctrl + on Chrome, probably something similar on other browsers).]

We've seen what the spin 1/2 matrices look like along the 3 rectangular coordinate axes. From this, we can derive an expression for the spin component along an arbitrary direction $\hat{\mathbf{r}}$. The unit radius vector is

$$\hat{\mathbf{r}} = \sin\theta\cos\phi\hat{\mathbf{i}} + \sin\theta\sin\phi\hat{\mathbf{j}} + \cos\theta\hat{\mathbf{k}} \tag{1}$$

We can get S_r by combining S_x, S_y and S_z according to the formula for the radius vector:

$$\begin{aligned} \mathsf{S}_r &= \mathsf{S}\cdot\hat{\mathbf{r}} && (2)\\ &= \sin\theta\cos\phi S_x + \sin\theta\sin\phi S_y + \cos\theta S_z && (3) \end{aligned}$$

By using the forms for the matrices derived earlier, and $\cos\phi \pm i\sin\phi = e^{\pm i\phi}$ we get

$$\mathsf{S}_r = \frac{\hbar}{2}\begin{pmatrix} \cos\theta & \sin\theta e^{-i\phi} \\ \sin\theta e^{i\phi} & -\cos\theta \end{pmatrix} \tag{4}$$

The eigenvalues of this matrix are calculated in the usual way

$$\begin{vmatrix} \frac{\hbar}{2}\cos\theta - \lambda & \frac{\hbar}{2}\sin\theta e^{-i\phi} \\ \frac{\hbar}{2}\sin\theta e^{i\phi} & -\frac{\hbar}{2}\cos\theta - \lambda \end{vmatrix} = -\frac{\hbar^2}{4}\left[\cos^2\theta + \sin^2\theta\right] + \lambda^2 = 0 \tag{5}$$

We get $\lambda = \pm\hbar/2$ as before so all is well at this stage.

To get the eigenspinors, we must solve

$$\frac{\hbar}{2}\begin{pmatrix} \cos\theta \pm 1 & \sin\theta e^{-i\phi} \\ \sin\theta e^{i\phi} & -\cos\theta \pm 1 \end{pmatrix}\begin{pmatrix} \alpha \\ \beta \end{pmatrix} = 0 \tag{6}$$

We get the equations

$$(\cos\theta \pm 1)\alpha + \sin\theta e^{-i\phi}\beta = 0 \quad (7)$$

$$\sin\theta e^{i\phi}\alpha - (-\cos\theta \pm 1)\beta = 0 \quad (8)$$

The two solutions (one for each sign) are

$$\beta_+ = -e^{i\phi}\frac{\cos\theta - 1}{\sin\theta}\alpha_+ \quad (9)$$

$$\beta_- = -e^{i\phi}\frac{\cos\theta + 1}{\sin\theta}\alpha_- \quad (10)$$

We can use the double-angle trig identities to simplify these expressions:

$$\sin\theta = 2\sin(\theta/2)\cos(\theta/2) \quad (11)$$

$$\cos\theta = \cos^2(\theta/2) - \sin^2(\theta/2) \quad (12)$$

Substituting these together with $\cos^2(\theta/2) + \sin^2(\theta/2) = 1$ and simplifying leads to

$$\beta_+ = e^{i\phi}\frac{\sin(\theta/2)}{\cos(\theta/2)}\alpha_+ \quad (13)$$

$$\beta_- = -e^{i\phi}\frac{\cos(\theta/2)}{\sin(\theta/2)}\alpha_- \quad (14)$$

The eigenspinors should be normalized, so

$$|\beta_+|^2 + |\alpha_+|^2 = |\alpha_+|^2\left(\frac{\sin^2(\theta/2)}{\cos^2(\theta/2)} + 1\right) \quad (15)$$

$$= |\alpha_+|^2\left(\frac{\sin^2(\theta/2) + \cos^2(\theta/2)}{\cos^2(\theta/2)}\right) \quad (16)$$

$$= \frac{|\alpha_+|^2}{\cos^2(\theta/2)} \quad (17)$$

$$= 1 \quad (18)$$

Thus we can take

$$\alpha_+ = \cos\frac{\theta}{2} \quad (19)$$

Other answers are possible, since we can multiply α_+ by any complex exponential, as all that is important is that its magnitude is 1.

A similar calculation for the other solution leads to

$$\frac{|\alpha_-|^2}{\sin^2(\theta/2)} = 1 \tag{20}$$

We can take

$$\alpha_- = \sin\frac{\theta}{2} \tag{21}$$

These choices lead to

$$\chi_+^{(r)} = \begin{pmatrix} \cos(\theta/2) \\ e^{i\phi}\sin(\theta/2) \end{pmatrix} \tag{22}$$

$$\chi_-^{(r)} = \begin{pmatrix} \sin(\theta/2) \\ -e^{i\phi}\cos(\theta/2) \end{pmatrix} \tag{23}$$

If we want the answer in Griffiths, we would choose $\alpha_- = e^{-i\phi}\sin\frac{\theta}{2}$, which leads to the answer:

$$\chi_+^{(r)} = \begin{pmatrix} \cos(\theta/2) \\ e^{i\phi}\sin(\theta/2) \end{pmatrix} \tag{24}$$

$$\chi_-^{(r)} = \begin{pmatrix} e^{-i\phi}\sin(\theta/2) \\ -\cos(\theta/2) \end{pmatrix} \tag{25}$$

The phase difference between the two components is the same in each solution.

Shankar's equations 14.3.28 use a slightly different phase, giving

$$|\hat{n}+\rangle = \begin{bmatrix} \cos\frac{\theta}{2}e^{-i\phi/2} \\ \sin\frac{\theta}{2}e^{i\phi/2} \end{bmatrix} \tag{26}$$

$$|\hat{n}-\rangle = \begin{bmatrix} -\sin\frac{\theta}{2}e^{-i\phi/2} \\ \cos\frac{\theta}{2}e^{i\phi/2} \end{bmatrix} \tag{27}$$

We can calculate $\langle \mathbf{S} \rangle$ by using the spin matrices

$$S_x = \frac{\hbar}{2}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \tag{28}$$

$$S_y = \frac{\hbar}{2}\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \tag{29}$$

$$S_z = \frac{\hbar}{2}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \tag{30}$$

We have

$$\langle \hat{n}+|S_x|\hat{n}+\rangle = \frac{\hbar}{2}\begin{bmatrix} \cos\frac{\theta}{2}e^{i\phi/2} & \sin\frac{\theta}{2}e^{-i\phi/2} \end{bmatrix}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}\begin{bmatrix} \cos\frac{\theta}{2}e^{-i\phi/2} \\ \sin\frac{\theta}{2}e^{i\phi/2} \end{bmatrix} \tag{31}$$

$$= \frac{\hbar}{2}\begin{bmatrix} \cos\frac{\theta}{2}e^{i\phi/2} & \sin\frac{\theta}{2}e^{-i\phi/2} \end{bmatrix}\begin{bmatrix} \sin\frac{\theta}{2}e^{i\phi/2} \\ \cos\frac{\theta}{2}e^{-i\phi/2} \end{bmatrix} \tag{32}$$

$$= \frac{\hbar}{2}\sin\frac{\theta}{2}\cos\frac{\theta}{2}\left(e^{i\phi}+e^{-i\phi}\right) \tag{33}$$

$$= \frac{\hbar}{2}\sin\theta\cos\phi \tag{34}$$

$$\langle \hat{n}+|S_y|\hat{n}+\rangle = \frac{\hbar}{2}\begin{bmatrix} \cos\frac{\theta}{2}e^{i\phi/2} & \sin\frac{\theta}{2}e^{-i\phi/2} \end{bmatrix}\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}\begin{bmatrix} \cos\frac{\theta}{2}e^{-i\phi/2} \\ \sin\frac{\theta}{2}e^{i\phi/2} \end{bmatrix} \tag{35}$$

$$= \frac{i\hbar}{2}\begin{bmatrix} \cos\frac{\theta}{2}e^{i\phi/2} & \sin\frac{\theta}{2}e^{-i\phi/2} \end{bmatrix}\begin{bmatrix} -\sin\frac{\theta}{2}e^{i\phi/2} \\ \cos\frac{\theta}{2}e^{-i\phi/2} \end{bmatrix} \tag{36}$$

$$= -\frac{\hbar}{2i}\sin\frac{\theta}{2}\cos\frac{\theta}{2}\left(-e^{i\phi}+e^{-i\phi}\right) \tag{37}$$

$$= \frac{\hbar}{2}\sin\theta\sin\phi \tag{38}$$

$$\langle \hat{n}+|S_z|\hat{n}+\rangle = \frac{\hbar}{2}\begin{bmatrix} \cos\frac{\theta}{2}e^{i\phi/2} & \sin\frac{\theta}{2}e^{-i\phi/2} \end{bmatrix}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}\begin{bmatrix} \cos\frac{\theta}{2}e^{-i\phi/2} \\ \sin\frac{\theta}{2}e^{i\phi/2} \end{bmatrix} \tag{39}$$

$$= \frac{\hbar}{2}\begin{bmatrix} \cos\frac{\theta}{2}e^{i\phi/2} & \sin\frac{\theta}{2}e^{-i\phi/2} \end{bmatrix}\begin{bmatrix} \cos\frac{\theta}{2}e^{-i\phi/2} \\ -\sin\frac{\theta}{2}e^{i\phi/2} \end{bmatrix} \tag{40}$$

$$= \frac{\hbar}{2}\left(\cos^2\frac{\theta}{2}-\sin^2\frac{\theta}{2}\right) \tag{41}$$

$$= \frac{\hbar}{2}\cos\theta \tag{42}$$

PINGBACKS

Pingback: Angular momentum: adding spins in arbitrary directions
Pingback: Electron in a precessing magnetic field
Pingback: Every spin-1/2 spinor is an eigenket of some spin operator
Pingback: Spinor in oscillating magnetic field - part 2

ADDING TWO SPIN-1/2 SYSTEMS - PRODUCT AND TOTAL-S BASES

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 15.1.

Post date: 9 Sep 2017

[If some equations are too small to read easily, use your browser's magnifying option (Ctrl + on Chrome, probably something similar on other browsers).]

When adding two spins we can work in the product basis, which is the vector space formed by the direct product of the two vector spaces which correspond to the two spins, taken separately. For spin-$\frac{1}{2}$, the single-spin basis consists of two spinors

$$\chi_{\uparrow} = \frac{\hbar}{2}\begin{bmatrix} 1 \\ 0 \end{bmatrix} \tag{1}$$

$$\chi_{\downarrow} = \frac{\hbar}{2}\begin{bmatrix} 0 \\ 1 \end{bmatrix} \tag{2}$$

In this basis, the spin operator $\mathbf{S}$ is formed from the 3 Pauli matrices as

$$\mathbf{S}_i = \frac{\hbar}{2}\boldsymbol{\sigma} \tag{3}$$

$$\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \tag{4}$$

$$\sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \tag{5}$$

$$\sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \tag{6}$$

where the subscript i labels which particle we're considering.

When we add two independent spins, we get a total spin operator $\mathbf{S} = \mathbf{S}_1 + \mathbf{S}_2$. However, if we use the product basis, the vector space in which $\mathbf{S}$ resides is the direct product of the two vector spaces for the individual spins:

$$\mathbb{V}_{tot} = \mathbb{V}^{(1)} \otimes \mathbb{V}^{(2)} \tag{7}$$

where $\mathbb{V}^{(i)}$ is the 2-d vector space corresponding to spin i. We've seen in an earlier post how to construct the components of **S** in this vector space, so we'll quote the results:

$$S_x = S_{1x} + S_{2x} = \frac{\hbar}{2} \begin{bmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{bmatrix} \tag{8}$$

$$S_y = S_{1y} + S_{2y} = \frac{\hbar}{2} \begin{bmatrix} 0 & -i & -i & 0 \\ i & 0 & 0 & -i \\ i & 0 & 0 & -i \\ 0 & i & i & 0 \end{bmatrix} \tag{9}$$

$$S_z = S_{1z} + S_{2z} = \hbar \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix} \tag{10}$$

We also have, again working directly from the earlier results in the product basis

$$S_1^2 = S_2^2 = \frac{3\hbar^2}{4} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} = \frac{3\hbar^2}{4} I \tag{11}$$

The square of the total spin operator in the product basis comes out to

$$S^2 = \hbar^2 \begin{bmatrix} 2 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 2 \end{bmatrix} \tag{12}$$

From these results, we see that (since S_1^2 and S_2^2 are multiplies of the identity matrix) both S_z and S^2 commute with S_1^2 and S_2^2. We can also see by direct calculation that $\left[S^2, S_z\right] = 0$, so S^2, S_z, S_1^2 and S_2^2 form a set of 4 mutually commuting matrices. Since the matrices are all hermitian (they represent observable quantities), it must be possible to find a basis in which all 4 are diagonal. The problem in this case is fairly simple, since in the product basis, only S^2 is not diagonal, so if we can find the unitary transformation that diagonalizes S^2, we should have our new basis. The desired

unitary transformation matrix is the matrix whose columns are the normalized eigenvectors of S^2. In the previous post we found these eigenvectors to be

$$v_0 = \frac{1}{\sqrt{2}} \begin{bmatrix} 0 \\ 1 \\ -1 \\ 0 \end{bmatrix} \tag{13}$$

$$v_{2a} = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} \tag{14}$$

$$v_{2b} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix} \tag{15}$$

$$v_{2c} = \frac{1}{\sqrt{2}} \begin{bmatrix} 0 \\ 1 \\ 1 \\ 0 \end{bmatrix} \tag{16}$$

The first eigenvector v_0 corresponds to eigenvalue 0, and the other 3 to eigenvalue 2. The unitary transformation matrix is then

$$U = \begin{bmatrix} 0 & 1 & 0 & 0 \\ \frac{1}{\sqrt{2}} & 0 & 0 & \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} & 0 & 0 & \frac{1}{\sqrt{2}} \\ 0 & 0 & 1 & 0 \end{bmatrix} \tag{17}$$

By direct multiplication, we find that S^2 in what Shankar calls the total-s basis is

$$U^T S^2 U = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 2 \end{bmatrix} \tag{18}$$

The normalized eigenvectors are

$$u_i = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix} \tag{19}$$

The first eigenvector corresponds to the singlet state and the last 3 to the triplet state. We can verify by direct calculation that S_z, S_1^2 and S_2^2 are unchanged by this transformation, remaining as given in 10 and 11.

The basis is related to the product basis by (using the notation $|ss_z s_1 s_2\rangle$ for the vectors in the total-s basis):

$$\left|00\frac{1}{2}\frac{1}{2}\right\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right) \tag{20}$$

$$\left|11\frac{1}{2}\frac{1}{2}\right\rangle = |\uparrow\uparrow\rangle \tag{21}$$

$$\left|10\frac{1}{2}\frac{1}{2}\right\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\right) \tag{22}$$

$$\left|1-1\frac{1}{2}\frac{1}{2}\right\rangle = |\downarrow\downarrow\rangle \tag{23}$$

We can use either basis in practical calculations. The choice depends on the form of the Hamiltonian: if it can be expressed entirely in terms of S^2,S_z, S_1^2 and S_2^2 then it makes sense to use the total-s basis.

PINGBACKS

Pingback: Clebsch-Gordan coefficients for addition of spin-1/2 and general L

Pingback: Symmetry of states formed from two equal spins

TOTAL-S MATRIX AND EIGENSTATES IN PRODUCT BASIS

Link to: physicspages home page.

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Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Exercise 15.1.1.

Post date: 7 Sep 2017

[If some equations are too small to read easily, use your browser's magnifying option (Ctrl + on Chrome, probably something similar on other browsers).]

Although we've looked at the addition of two spins while working through Griffiths's book, this problem from Shankar is a nice exercise in dealing with a direct product of two vector spaces, so we'll analyze it that way.

The problem is to find the spin operator **S** obtained by adding two spin-$\frac{1}{2}$ systems. Each spin comprises a vector space of dimension 2, and the components can be written using the spin matrices

$$S_x = \frac{\hbar}{2}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}; \quad S_y = \frac{\hbar}{2}\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}; \quad S_z = \frac{\hbar}{2}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \tag{1}$$

Each spin resides in its own 2-dim vector space, so the vector space for the combined system is formed by taking the direct product of the two spin spaces. We can write the matrices for the combined space by following the formulas we gave earlier. The notation we'll use is to add a subscript 1 or 2 to indicate which particle we're considering. In the product space, for particle 1 we have

$$S_{1x} = S_x^{(1)} \otimes I^{(2)} \tag{2}$$

$$= \frac{\hbar}{2} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \otimes \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \tag{3}$$

$$= \frac{\hbar}{2} \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix} \tag{4}$$

$$S_{1y} = S_y^{(1)} \otimes I^{(2)} \tag{5}$$

$$= \frac{\hbar}{2} \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \otimes \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \tag{6}$$

$$= \frac{\hbar}{2} \begin{bmatrix} 0 & 0 & -i & 0 \\ 0 & 0 & 0 & -i \\ i & 0 & 0 & 0 \\ 0 & i & 0 & 0 \end{bmatrix} \tag{7}$$

$$S_{1z} = S_z^{(1)} \otimes I^{(2)} \tag{8}$$

$$= \frac{\hbar}{2} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \otimes \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \tag{9}$$

$$= \frac{\hbar}{2} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix} \tag{10}$$

For particle 2, we have

$$S_{2x} = I^{(1)} \otimes S_x^{(2)} \tag{11}$$

$$= \frac{\hbar}{2} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \otimes \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \tag{12}$$

$$= \frac{\hbar}{2} \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \tag{13}$$

$$S_{2y} = I^{(1)} \otimes S_y^{(2)} \tag{14}$$

$$= \frac{\hbar}{2} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \otimes \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \tag{15}$$

$$= \frac{\hbar}{2} \begin{bmatrix} 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \\ 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \end{bmatrix} \tag{16}$$

$$S_{2z} = I^{(1)} \otimes S_z^{(2)} \tag{17}$$

$$= \frac{\hbar}{2} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \otimes \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \tag{18}$$

$$= \frac{\hbar}{2} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix} \tag{19}$$

Given these matrices, it's just a matter of matrix multiplication and addition to obtain the overall operators. For the overall z component we have

$$S_z = S_{1z} + S_{2z} = \hbar \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix} \tag{20}$$

We can get S^2 from the above components

$$S^2 = (\mathbf{S}_1 + \mathbf{S}_2) \cdot (\mathbf{S}_1 + \mathbf{S}_2) \tag{21}$$

$$= S_1^2 + S_2^2 + 2\mathbf{S}_1 \cdot \mathbf{S}_2 \tag{22}$$

We could just use brute force and calculate these by multiplying out the matrices above. For example

$$S_1^2 = S_{1x}^2 + S_{1y}^2 + S_{1z}^2 \tag{23}$$

and so on. However, if we use Shankar's suggestion and remember that $S_1^2 = S_2^2 = \frac{3}{4}\hbar^2 I$ (where I refers to the identity matrix within the appropriate vector space), then we need to work out the last term in 22. Using the raising and lowering operators for spin

$$S_\pm = S_x \pm iS_y \tag{24}$$

we have

$$S_{1+}S_{2-} + S_{1-}S_{2+} = S_{1x}S_{2x} + S_{1y}S_{2y} + i\left(-S_{1x}S_{2y} + S_{1y}S_{2x}\right) + \tag{25}$$

$$S_{1x}S_{2x} + S_{1y}S_{2y} - i\left(-S_{1x}S_{2y} + S_{1y}S_{2x}\right) \tag{26}$$

$$= 2\left(S_{1x}S_{2x} + S_{1y}S_{2y}\right) \tag{27}$$

We therefore get

$$2\mathbf{S}_1 \cdot \mathbf{S}_2 = S_{1+}S_{2-} + S_{1-}S_{2+} + 2S_{1z}S_{2z} \tag{28}$$

We can work out the matrix forms of the raising and lowering operators from the above matrices, and we have

$$S_{1+} = S_{1x} + iS_{1y} \tag{29}$$

$$= \hbar \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \tag{30}$$

$$S_{1-} = S_{1x} - iS_{1y} \tag{31}$$

$$= \hbar \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix} \tag{32}$$

$$S_{2+} = S_{2x} + iS_{2y} \tag{33}$$

$$= \hbar \begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{bmatrix} \tag{34}$$

$$S_{2-} = S_{2x} - iS_{2y} \tag{35}$$

$$= \hbar \begin{bmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix} \tag{36}$$

For the products, we have

$$S_{1+}S_{2-} = \hbar^2 \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \tag{37}$$

$$S_{1-}S_{2+} = \hbar^2 \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \tag{38}$$

$$2S_{1z}S_{2z} = \frac{\hbar^2}{2} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \tag{39}$$

For the total, we have

$$S^2 = 2 \times \frac{3\hbar^2}{4} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} + \hbar^2 \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} + \tag{40}$$

$$\hbar^2 \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} + \frac{\hbar^2}{2} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \tag{41}$$

$$= \hbar^2 \begin{bmatrix} 2 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 2 \end{bmatrix} \equiv \hbar^2 \Lambda \tag{42}$$

The eigenvalues and eigenvectors of the matrix in 42 are found in the usual way, by calculating the characteristic determinant:

$$|\Lambda - \lambda I| = \begin{vmatrix} 2-\lambda & 0 & 0 & 0 \\ 0 & 1-\lambda & 1 & 0 \\ 0 & 1 & 1-\lambda & 0 \\ 0 & 0 & 0 & 2-\lambda \end{vmatrix} = 0 \tag{43}$$

This gives the polynomial

$$(2-\lambda)^2 \left[(1-\lambda)^2 - 1 \right] = 0 \tag{44}$$

The roots (eigenvalues) are 0 (once) and 2 (3 times). The corresponding normalized eigenvectors can be found from solving the equations:

For the eigenvalue $\lambda = 0$, we have for the eigenvector $v_0 = \begin{bmatrix} a & b & c & d \end{bmatrix}^T$

$$\Lambda v_0 = 0 \tag{45}$$

$$a = d = 0 \tag{46}$$

$$b = -c \tag{47}$$

Thus the normalized eigenvector is

$$v_0 = \frac{1}{\sqrt{2}} \begin{bmatrix} 0 \\ 1 \\ -1 \\ 0 \end{bmatrix} \tag{48}$$

This is the singlet state with $s = 0$, $m = 0$.

For the triply degenerate eigenvalue $\lambda = 2$, we have

$$\Lambda v_2 = 2v_2 \tag{49}$$

$$\begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & -1 & 1 & 0 \\ 0 & 1 & -1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} a \\ b \\ c \\ d \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} \tag{50}$$

The normalized eigenvectors are then

$$v_{2a} = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} \tag{51}$$

$$v_{2b} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix} \tag{52}$$

$$v_{2c} = \frac{1}{\sqrt{2}} \begin{bmatrix} 0 \\ 1 \\ 1 \\ 0 \end{bmatrix} \tag{53}$$

This gives us the triplet state, with $s = 1$ and $m = 1, 0, -1$.

PINGBACKS

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HYPERFINE INTERACTION IN HYDROGEN - A ROUGH CALCULATION

Link to: physicspages home page.

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Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Exercise 15.1.2.

Post date: 9 Sep 2017

[If some equations are too small to read easily, use your browser's magnifying option (Ctrl + on Chrome, probably something similar on other browsers).]

We've looked at the hyperfine splitting and the resulting 21 cm line of hydrogen in some detail before, but it's worth doing Shankar's approximate treatment in this problem to get some experience with calculations using the total-s basis for the addition of two spins.

The interaction between the spins of the proton and electron is due to the interaction between their magnetic moments, and has the form

$$H_{hf} = A\mathbf{S}_1 \cdot \mathbf{S}_2 \tag{1}$$

where A is some constant. The total Hamiltonian is thus the sum of the dominant Coulomb interaction and H_{hf}. The Coulomb interaction gives rise to the Bohr energy levels

$$E_n = -\frac{me^4}{2n^2\hbar^2} \tag{2}$$

The complete energy is

$$E = E_n + H_{hf} \tag{3}$$

The perturbation H_{hf} can be written as

$$H_{hf} = \frac{1}{2}A\left(S^2 - S_1^2 - S_2^2\right) \tag{4}$$

Because H_{hf} involves S^2, S_1^2 and S_2^2 we can use the total-s basis, and its four basis vectors, one of which is the singlet state $\left|00\tfrac{1}{2}\tfrac{1}{2}\right\rangle$ and the other three of which are the triplet states $\left|11\tfrac{1}{2}\tfrac{1}{2}\right\rangle, \left|10\tfrac{1}{2}\tfrac{1}{2}\right\rangle, \left|1-1\tfrac{1}{2}\tfrac{1}{2}\right\rangle$. All four vectors are eigenvectors of both S_1^2 and S_2^2 with eigenvalue $\frac{3\hbar^2}{4}$. As $s = 0$ in the singlet state, $S^2\left|00\tfrac{1}{2}\tfrac{1}{2}\right\rangle = 0$, while for the triplet states $s = 1$, so

$S^2\left|11\tfrac{1}{2}\tfrac{1}{2}\right\rangle = s(s+1)\hbar^2\left|11\tfrac{1}{2}\tfrac{1}{2}\right\rangle = 2\hbar^2\left|11\tfrac{1}{2}\tfrac{1}{2}\right\rangle$ and similarly for the other two triplet states.

Thus in the singlet state (we'll take hydrogen to be in its ground state, so $n = 1$):

$$E_- = -\frac{me^4}{2\hbar^2} + \frac{A}{2}\left(0 - \frac{3\hbar^2}{4} - \frac{3\hbar^2}{4}\right) \tag{5}$$

$$= -\frac{me^4}{2\hbar^2} - \frac{3\hbar^2 A}{4} \tag{6}$$

and in the triplet states

$$E_+ = -\frac{me^4}{2\hbar^2} + \frac{A}{2}\left(2\hbar^2 - \frac{3\hbar^2}{4} - \frac{3\hbar^2}{4}\right) \tag{7}$$

$$= -\frac{me^4}{2\hbar^2} + \frac{\hbar^2 A}{4} \tag{8}$$

To get a rough idea of the frequency of the photon that is emitted when the atom jumps from E_+ to E_-, we can approximate the atom as two interacting dipoles separated by the Bohr radius a_0. The interaction energy between two magnetic dipoles is roughly the product of their magnetic moments divided by the cube of the distance between them, so we have

$$H_{hf} \simeq \frac{\mu_e \mu_p}{a_0^3} \tag{9}$$

The magnetic moments are

$$\mu_e = \frac{g_e e}{2mc}\frac{\hbar}{2} = \frac{2e}{2mc}\frac{\hbar}{2} \tag{10}$$

$$\mu_p = \frac{g_p e}{2Mc}\frac{\hbar}{2} = \frac{5.6e}{2Mc}\frac{\hbar}{2} \tag{11}$$

where m is the electron mass and M is the proton mass, and g_e and g_p are the g factors for the electron and proton. The Bohr radius is (in Gaussian units):

$$a_0 = \frac{\hbar^2}{me^2} \tag{12}$$

so we get

$$H_{hf} \simeq \frac{2e}{2mc}\frac{5.6e}{2Mc}\frac{\hbar^2}{4} = \frac{2.8e^2}{mMc^2a_0^3}\frac{\hbar^2}{4} \tag{13}$$

Comparing with 8, we see that

$$A \simeq \frac{2.8e^2}{mMc^2a_0^3} \tag{14}$$

The energy difference between the two hyperfine states 8 and 6 is

$$\begin{aligned} \Delta E &= E_+ - E_- && (15)\\ &= A\hbar^2 && (16)\\ &= \frac{2.8e^2\hbar^2}{mMc^2a_0^3} && (17)\\ &= \frac{2.8e^8m^2}{\hbar^4Mc^2} && (18) \end{aligned}$$

In terms of the fine structure constant $\alpha = e^2/\hbar c = \frac{1}{137}$, this energy is, as a fraction of the Coulomb energy:

$$\frac{\Delta E}{E_n} = \frac{5.6e^4m}{\hbar^2Mc^2} = 5.6\frac{m}{M}\alpha^2 \tag{19}$$

Given that the ground state energy is $E_1 = -13.6$ eV, and the electron-proton mass ratio is $\frac{1}{1836}$, the energy of the hyperfine photon is

$$\begin{aligned} \Delta E &= 5.6\frac{m}{M}\alpha^2\,(13.6\text{ eV}) && (20)\\ &= \frac{5.6}{1836}\frac{1}{137^2}\,(13.6\text{ eV}) && (21)\\ &= 2.2\times10^{-6}\text{ eV} && (22)\\ &= 3.5\times10^{-25}\text{ J} && (23) \end{aligned}$$

From Planck's formula relating energy to frequency, the frequency of the photon is

$$\nu = \frac{\Delta E}{h} = \frac{3.5\times10^{-25}}{6.6\times10^{-34}} = 5.3\times10^8\text{ s}^{-1} \tag{24}$$

This corresponds to a wavelength of

$$\lambda = \frac{c}{\nu} = 0.56\text{ m} \tag{25}$$

The measured wavelength is 21.4 cm, so this estimate isn't terribly accurate, but it's in the right order of magnitude.

Since the hyperfine energy is very small, it's interesting to find the relative number of atoms that are in the two states at room temperature. Using the Boltzmann factor, the number of atoms in an energy state E is proportional to $e^{-E/kT}$, so the ratio of atoms in the two states is

$$\frac{N_+}{N_-} = \frac{e^{-E_+/kT}}{e^{-E_-/kT}} \tag{26}$$

$$= e^{-\Delta E/kT} \tag{27}$$

At room temperature $T = 293$ K and Boltzmann's constant is

$$k = 1.38 \times 10^{-23} \text{ SI units} \tag{28}$$

so we have

$$\frac{N_+}{N_-} = e^{-3.5\times10^{-25}/(293)\left(1.38\times10^{-23}\right)} \tag{29}$$

$$= 0.99991 \tag{30}$$

That is, the ratio of number of atoms in the singlet state to *one* of the triplet states is about 1:1. However, there are 3 states with the higher energy, so the ratio of total number of atoms in the upper state to the number in the lower state is 3 times this, which is essentially just 3.

TOTAL J FOR SUM OF TWO ANGULAR MOMENTA

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Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 15.2; Exercise 15.2.1.

Post date: 10 Sep 2017

[If some equations are too small to read easily, use your browser's magnifying option (Ctrl + on Chrome, probably something similar on other browsers).]

When we add two spins (or angular momenta) in quantum mechanics, we can express the states in one of two ways. The first is in the vector space which is the direct product of the two spaces for the two spins. This is called the *product space* and formally is

$$\mathbb{V}_p = \mathbb{V}_1 \otimes \mathbb{V}_2 \tag{1}$$

where $\mathbb{V}_i$ is the vector space of the single spin i. If we're interested in the total spin $\mathbf{J} = \mathbf{J}_1 + \mathbf{J}_2$, we could also use the total-j vector space, which is the direct sum of the two spin spaces:

$$\mathbb{V}_t = \mathbb{V}_1 \oplus \mathbb{V}_2 \tag{2}$$

As each space is complete, we can express any state in terms of a basis from either space. We've seen an example of this when adding two spin-$\frac{1}{2}$ systems.

In general, if we have two angular momenta $\mathbf{J}_1$ and $\mathbf{J}_2$, we would like to be able to write a state in one space as a linear combination of states from the other space. The Clebsch-Gordan coefficients allow us to this. Calculating the C-G coefficients in general is quite complicated, but for systems with small spins or angular momenta, Shankar gives a method that is simpler than the more tedious brute-force method. We ground through one of these brute-force calculations earlier for the addition of spin-$\frac{1}{2}$ and another, arbitrary, spin.

In this post, we'll work through Shankar's method for the explicit case of adding spin-$\frac{1}{2}$ and spin-1 so you can see how the calculations are done.

We have two sets of kets. In the product space, each ket is labelled by the two spins and their z components, as in

$$\mathbb{V}_p = \{|j_1 m_1; j_2 m_2\rangle\} \tag{3}$$

The curly brackets here represent the set of all kets of form $|j_1 m_1; j_2 m_2\rangle$ where j_i is the value (in units of $\hbar$) of spin $\mathbf{J}_i$ and m_i is its z component.

In the total-j space $\mathbb{V}_t$, the labels are the total spin j, its z component m and the two component spins j_1 and j_2:

$$\mathbb{V}_t = \{|j m j_1 j_2\rangle\} \tag{4}$$

To work out the linear combinations, we start with the state where both j and m are maximum, which occurs when $m_1 = j_1$ and $m_2 = j_2$, which gives $j = j_1 + j_2$ and $m = j_1 + j_2$. There is only one member of the set 3 satisfying this condition, so we begin by stating that

$$|(j_1 + j_2)\,(j_1 + j_2)\,j_1 j_2\rangle = |j_1 j_1; j_2 j_2\rangle \tag{5}$$

To get states with lower values of m but the same value of j, we can apply the lowering operator J_- to the LHS of 5 and its equivalent in the product space, which is $J_{1-} + J_{2-}$, to the RHS. We use the formula

$$J_\pm |j m j_1 j_2\rangle = \hbar\sqrt{(j \mp m)\,(j \pm m + 1)}\,|j\,(m-1)\,j_1 j_2\rangle \tag{6}$$

Shankar gives the details of this calculation in the general case; here we'll apply it to $j_1 = 1$ and $j_2 = \frac{1}{2}$. We begin with the top state, where $j = 1 + \frac{1}{2} = \frac{3}{2}$ and $m = \frac{3}{2}$:

$$\left|\frac{3}{2}\frac{3}{2}1\frac{1}{2}\right\rangle_t = \left|11;\frac{1}{2}\frac{1}{2}\right\rangle_p \tag{7}$$

In what follows, to simplify the notation, we'll omit $j_1 j_2$ from the total-j kets (since they are always $1\frac{1}{2}$) and also omit j_1 and j_2 from the product kets (again, because they are always 1 and $\frac{1}{2}$). We'll use a subscript t for a total-j ket and p for a product space ket. In this notation 7 is

$$\left|\frac{3}{2}\frac{3}{2}\right\rangle_t = \left|1\frac{1}{2}\right\rangle_p \tag{8}$$

Now we apply the lowering operator to both sides. On the LHS, we have

$$J_- \left|\frac{3}{2}\frac{3}{2}\right\rangle_t = \hbar\sqrt{\left(\frac{3}{2}+\frac{3}{2}\right)\left(\frac{3}{2}-\frac{3}{2}+1\right)}\left|\frac{3}{2}\frac{1}{2}\right\rangle_t \tag{9}$$

$$= \sqrt{3}\hbar\left|\frac{3}{2}\frac{1}{2}\right\rangle_t \tag{10}$$

On the RHS, we have (remember that J_{1-} operates only on spin 1 and J_{2-} only on spin 2):

$$(J_{1-}+J_{2-})\left|1\frac{1}{2}\right\rangle_p = \hbar\sqrt{(1+1)(1-1+1)}\left|0\frac{1}{2}\right\rangle_p + \tag{11}$$

$$\hbar\sqrt{\left(\frac{1}{2}+\frac{1}{2}\right)\left(\frac{1}{2}-\frac{1}{2}+1\right)}\left|1,-\frac{1}{2}\right\rangle_p \tag{12}$$

$$= \sqrt{2}\hbar\left|0\frac{1}{2}\right\rangle_p + \hbar\left|1,-\frac{1}{2}\right\rangle_p \tag{13}$$

Combining 10 and 13, we find

$$\left|\frac{3}{2}\frac{1}{2}\right\rangle_t = \sqrt{\frac{2}{3}}\left|0\frac{1}{2}\right\rangle_p + \frac{1}{\sqrt{3}}\left|1,-\frac{1}{2}\right\rangle_p \tag{14}$$

To get the next lower value of m, we apply lowering operators again:

$$J_-\left|\frac{3}{2}\frac{1}{2}\right\rangle_t = 2\hbar\left|\frac{3}{2},-\frac{1}{2}\right\rangle_t \tag{15}$$

$$(J_{1-}+J_{2-})\left(\sqrt{\frac{2}{3}}\left|0\frac{1}{2}\right\rangle_p + \frac{1}{\sqrt{3}}\left|1,-\frac{1}{2}\right\rangle_p\right) = \sqrt{\frac{2}{3}}\sqrt{2}\hbar\left|-1,\frac{1}{2}\right\rangle_p + \tag{16}$$

$$\sqrt{\frac{2}{3}}\hbar\left|0,-\frac{1}{2}\right\rangle_p + \frac{1}{\sqrt{3}}\sqrt{2}\hbar\left|0,-\frac{1}{2}\right\rangle_p \tag{17}$$

$$= \frac{2}{\sqrt{3}}\hbar\left|-1,\frac{1}{2}\right\rangle_p + 2\sqrt{\frac{2}{3}}\hbar\left|0,-\frac{1}{2}\right\rangle_p \tag{18}$$

$$\left|\frac{3}{2},-\frac{1}{2}\right\rangle_t = \frac{1}{\sqrt{3}}\hbar\left|-1,\frac{1}{2}\right\rangle_p + \sqrt{\frac{2}{3}}\hbar\left|0,-\frac{1}{2}\right\rangle_p \tag{19}$$

To get the bottom ket, we could apply the lowering operator again, but it's easier to notice that there is only one way of getting the state $\left|\frac{3}{2},-\frac{3}{2}\right\rangle_t$ so we have

$$\left|\frac{3}{2},-\frac{3}{2}\right\rangle_t = \left|-1,-\frac{1}{2}\right\rangle_p \tag{20}$$

This completes the states with $j=\frac{3}{2}$. There are two total-j states with $j=\frac{1}{2}$: one with $m=+\frac{1}{2}$ and the other with $m=-\frac{1}{2}$. To get the state $\left|\frac{1}{2}\frac{1}{2}\right\rangle_t$,

we observe that it must be a combination of the product kets $\left|1,-\frac{1}{2}\right\rangle_p$ and $\left|0,\frac{1}{2}\right\rangle_p$. These are the same two kets that were combined to get $\left|\frac{3}{2},\frac{1}{2}\right\rangle_t$ in 14. As usual, we're looking for a mutually orthonormal sets of states, so $\left|\frac{1}{2}\frac{1}{2}\right\rangle_t$ must be orthogonal to $\left|\frac{3}{2}\frac{1}{2}\right\rangle_t$ and also be normalized. By inspection, we see that the state must be

$$\left|\frac{1}{2}\frac{1}{2}\right\rangle_t = \sqrt{\frac{2}{3}}\left|1,-\frac{1}{2}\right\rangle_p - \frac{1}{\sqrt{3}}\left|0\frac{1}{2}\right\rangle_p \tag{21}$$

[Actually, we could multiply this by any phase factor $e^{i\alpha}$ for real α, but by convention, the coefficients are taken to be real. A further convention makes the coefficient of the product ket with $m_1 = j_1$ positive.]

To get the state $\left|\frac{1}{2},-\frac{1}{2}\right\rangle_t$ we again use lowering operators:

$$J_-\left|\frac{1}{2}\frac{1}{2}\right\rangle_t = \hbar\left|\frac{1}{2},-\frac{1}{2}\right\rangle_t \tag{22}$$

$$(J_{1-}+J_{2-})\left(\sqrt{\frac{2}{3}}\left|1,-\frac{1}{2}\right\rangle_p - \frac{1}{\sqrt{3}}\left|0\frac{1}{2}\right\rangle_p\right) = \sqrt{\frac{2}{3}}\sqrt{2}\hbar\left|0,-\frac{1}{2}\right\rangle_p - \tag{23}$$

$$\frac{\sqrt{2}}{\sqrt{3}}\hbar\left|-1,\frac{1}{2}\right\rangle_p - \frac{1}{\sqrt{3}}\hbar\left|0,-\frac{1}{2}\right\rangle_p \tag{24}$$

$$= \frac{\hbar}{\sqrt{3}}\left|0,-\frac{1}{2}\right\rangle_p - \sqrt{\frac{2}{3}}\hbar\left|-1,\frac{1}{2}\right\rangle_p \tag{25}$$

$$\left|\frac{1}{2},-\frac{1}{2}\right\rangle_t = \frac{1}{\sqrt{3}}\left|0,-\frac{1}{2}\right\rangle_p - \sqrt{\frac{2}{3}}\left|-1,\frac{1}{2}\right\rangle_p \tag{26}$$

This completes the transformations.

From here, it's actually not too hard to construct the matrix J^2 in the product basis. We first note that J^2 in the total-j basis is diagonal, with the diagonal entries being the eigenvalues, which are the values of $j\,(j+1)$ for the 6 states. If we list the states in the order

$$\left|\frac{3}{2}\frac{3}{2}\right\rangle_t, \left|\frac{3}{2}\frac{1}{2}\right\rangle_t, \left|\frac{1}{2}\frac{1}{2}\right\rangle_t, \left|\frac{1}{2}-\frac{1}{2}\right\rangle_t, \left|\frac{3}{2},-\frac{1}{2}\right\rangle_t, \left|\frac{3}{2},-\frac{3}{2}\right\rangle_t \tag{27}$$

then the eigenvalues are $\frac{15}{4}\hbar^2, \frac{15}{4}\hbar^2, \frac{3}{4}\hbar^2, \frac{3}{4}\hbar^2, \frac{15}{4}\hbar^2, \frac{15}{4}\hbar^2$ so we have

$$J_t^2 = \frac{3\hbar^2}{4}\begin{bmatrix} 5 & 0 & 0 & 0 & 0 & 0 \\ 0 & 5 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 5 & 0 \\ 0 & 0 & 0 & 0 & 0 & 5 \end{bmatrix} \tag{28}$$

To construct J_p^2, we observe that the kets 27 are the eigenvectors of J^2 (in both bases) and we know that the unitary matrix U whose columns are the normalized eigenvectors of J_p^2 will diagonalize J_p^2. In this case, we already have the diagonalized form, which is just J_t^2, so we know that

$$U^T J_p^2 U = J_t^2 \tag{29}$$

Since U is unitary, $U^T = U^{-1}$, so we get

$$J_p^2 = U J_t^2 U^T \tag{30}$$

Using the eigenvector order given in 27 to order the columns of U, we have

$$U = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{3}} & \sqrt{\frac{2}{3}} & 0 & 0 & 0 \\ 0 & \sqrt{\frac{2}{3}} & -\frac{1}{\sqrt{3}} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{\sqrt{3}} & -\sqrt{\frac{2}{3}} & 0 \\ 0 & 0 & 0 & \sqrt{\frac{2}{3}} & \frac{1}{\sqrt{3}} & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} \tag{31}$$

We can now just do the matrix multiplications (I used Maple, since multiplying 6×6 matrices is quite tedious), and we find

$$J_p^2 = \hbar^2 \begin{bmatrix} \frac{15}{4} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{7}{4} & \sqrt{2} & 0 & 0 & 0 \\ 0 & \sqrt{2} & \frac{11}{4} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{11}{4} & \sqrt{2} & 0 \\ 0 & 0 & 0 & \sqrt{2} & \frac{7}{4} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{15}{4} \end{bmatrix} \tag{32}$$

To finish, we return to the general results given by Shankar. First, for the general state $|j_1 j_1; j_2 j_2\rangle_p$ we can find the total angular momentum by operating with

$$J^2 = J_1^2 + J_2^2 + 2J_{1z}J_{2z} + J_{1+}J_{2-} + J_{1-}J_{2+} \tag{33}$$

[This formula was derived earlier.] Since the state $|j_1 j_1; j_2 j_2\rangle_p$ has maximum values for m_1 and m_2, operating with J_{1+} or J_{2+} will give zero. Therefore

$$\begin{aligned} J^2 |j_1 j_1; j_2 j_2\rangle_p &= \left(J_1^2 + J_2^2 + 2J_{1z}J_{2z}\right) |j_1 j_1; j_2 j_2\rangle_p && (34)\\ &= \left[j_1 (j_1+1) + j_2 (j_2+1) + 2m_1 m_2\right] \hbar^2 |j_1 j_1; j_2 j_2\rangle_p && (35)\\ &= \left[j_1 (j_1+1) + j_2 (j_2+1) + 2j_1 j_2\right] \hbar^2 |j_1 j_1; j_2 j_2\rangle_p && (36)\\ &= \left[(j_1+j_2)(j_1+j_2+1)\right] \hbar^2 |j_1 j_1; j_2 j_2\rangle_p && (37) \end{aligned}$$

Thus the total j value is $j = j_1 + j_2$.

The second exercise is a bit messier, since we're dealing with the top ket whose j value is one unit less than the maximum, which is given by Shankar's equation 15.2.8.

$$|j_1 + j_2 - 1, j_1 + j_2 - 1\rangle_t = \frac{1}{\sqrt{j_1 + j_2}} \left[\sqrt{j_1}\, |j_1, j_2 - 1\rangle_p - \sqrt{j_2}\, |j_1 - 1, j_2\rangle_p\right] \tag{38}$$

This time, operating with 33 must include the two terms with raising operators, so we need to use 6. We'll deal with these terms first. We note that operating with J_{1+} on the first term in 38 gives zero, since $m_1 = j_1$, and similarly for J_{2+}on the second term. We're left with

$$\begin{aligned} J_{1+}J_{2-} |j_1 - 1, j_2\rangle_p &= \sqrt{2j_2}\hbar J_{1+} |j_1 - 1, j_2 - 1\rangle_p && (39)\\ &= \sqrt{2j_2}\hbar^2 \sqrt{2j_1}\, |j_1, j_2 - 1\rangle_p && (40)\\ &= 2\sqrt{j_1 j_2}\hbar^2 |j_1, j_2 - 1\rangle_p && (41)\\ J_{1-}J_{2+} |j_1, j_2 - 1\rangle_p &= 2\sqrt{j_1 j_2}\hbar^2 |j_1 - 1, j_2\rangle_p && (42) \end{aligned}$$

Combining these two results in 38 we have, for these terms

$$\begin{aligned} \left(J_{1+}J_{2-} + J_{1-}J_{2+}\right) \left[\sqrt{j_1}\, |j_1, j_2 - 1\rangle_p - \sqrt{j_2}\, |j_1 - 1, j_2\rangle_p\right] = && (43)\\ 2j_1\sqrt{j_2}\hbar^2 |j_1 - 1, j_2\rangle_p - 2j_2\sqrt{j_1}\hbar^2 |j_1, j_2 - 1\rangle_p && (44) \end{aligned}$$

Now for the first 3 terms in 33. First, we apply them to the first term in 38:

$$\left(J_1^2 + J_2^2 + 2J_{1z}J_{2z}\right) \sqrt{j_1}\, |j_1, j_2 - 1\rangle_p = \sqrt{j_1}\hbar^2 \left[j_1 (j_1+1) + j_2 (j_2+1) + 2j_1 (j_2 - 1)\right] |j_1, j_2 - 1\rangle_p \tag{45}$$

Combining this with 44 we get the coefficient of $|j_1, j_2 - 1\rangle_p$ to be

$$\sqrt{j_1}\hbar^2 \left[j_1 (j_1+1) + j_2 (j_2+1) + 2j_1 (j_2-1) - 2j_2\right] = \tag{46}$$

$$\sqrt{j_1}\hbar^2 \left[(j_1 + j_2 - 1)(j_1 + j_2)\right] \tag{47}$$

Now we apply $\left(J_1^2 + J_2^2 + 2J_{1z}J_{2z}\right)$ to the second term in 38:

$$-\left(J_1^2 + J_2^2 + 2J_{1z}J_{2z}\right)\sqrt{j_2}\,|j_1 - 1, j_2\rangle_p = -\sqrt{j_2}\hbar^2 \left[j_1 (j_1+1) + j_2 (j_2+1) + 2(j_1-1) j_2\right] |j_1 - 1, j_2\rangle \tag{48}$$

Again, combining this with 44 we get the coefficient of $|j_1 - 1, j_2\rangle_p$ to be

$$-\sqrt{j_2}\hbar^2 \left[j_1 (j_1+1) + j_2 (j_2+1) + 2(j_1-1) j_2 - 2j_1\right] = \tag{49}$$

$$-\sqrt{j_2}\hbar^2 \left[(j_1 + j_2 - 1)(j_1 + j_2)\right] \tag{50}$$

Thus the net result of operating on 38 with J^2 is to multiply by $(j_1 + j_2 - 1)(j_1 + j_2)$, this state has angular momentum $j_1 + j_2 - 1$.

PINGBACKS

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Pingback: Clebsch-Gordan coefficients for addition of spin-1/2 and general L

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CLEBSCH-GORDAN COEFFICIENTS - EXAMPLES

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Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 15.2; Exercises 15.2.2 - 15.2.3.

Post date: 12 Sep 2017

[If some equations are too small to read easily, use your browser's magnifying option (Ctrl + on Chrome, probably something similar on other browsers).]

We've seen a detailed example of calculating Clebsch-Gordan coefficients by using the angular momentum lowering operator, where we calculated the coefficients for the case of spin-1 combined with spin-$\frac{1}{2}$. Here we'll give a slightly more involved example by combining two spin-1 systems.

Shankar gives the conditions satisfied by the CG coefficients, so we'll apply these here. We start with the combined system with the maximum values of j (the total angular momentum number) and m (the z component of the total angular momentum), which here means we have $j = m = 2$. As there is only one member of the product space ($m_1 = m_2 = 1$) satisfying this condition, we have

$$|22\rangle_t = |11\rangle_p \tag{1}$$

As in the previous post, we give the ket in the total-j space as $|jm\rangle_t$ (subscript t for 'total-j') and in the product space as $|m_1 m_2\rangle_p$ (subscript p for 'product'). The two individual spins j_1 and j_2 are always the same in all cases, so we omit them from the notation.

We now apply the lowering operator to both sides to generate the next state. This operator is, in the total-j space:

$$J_- |jm\rangle_t = \hbar\sqrt{(j+m)(j-m+1)}\,|j\,(m-1)\rangle_t \tag{2}$$

In the product space, we have

$$(J_{1-} + J_{2-})\,|m_1 m_2\rangle_p = \hbar\sqrt{(j_1+m_1)(j_1-m_1+1)}\,|(m_1-1)\,m_2\rangle_p + \tag{3}$$

$$\hbar\sqrt{(j_2+m_2)(j_2-m_2+1)}\,|m_1\,(m_2-1)\rangle_p \tag{4}$$

In what follows, we'll omit the $\hbar$ since it always occurs in every term on both sides of the equation, so it always cancels out in the final result.

Starting from 1 we have

$$J_- |22\rangle_t = 2 |21\rangle_t \tag{5}$$

$$(J_{1-} + J_{2-}) |11\rangle_p = \sqrt{2} |01\rangle_p + \sqrt{2} |10\rangle_p \tag{6}$$

$$|21\rangle_t = \frac{1}{\sqrt{2}} |01\rangle_p + \frac{1}{\sqrt{2}} |10\rangle_p \tag{7}$$

For the next state, we have

$$J_- |21\rangle_t = \sqrt{6} |20\rangle_t \tag{8}$$

$$\frac{1}{\sqrt{2}} (J_{1-} + J_{2-}) \left(|01\rangle_p + |10\rangle_p \right) = \frac{1}{\sqrt{2}} \left(\sqrt{2} |-11\rangle_p + \sqrt{2} |00\rangle_p \right) + \tag{9}$$

$$\frac{1}{\sqrt{2}} \left(\sqrt{2} |00\rangle_p + \sqrt{2} |1,-1\rangle_p \right) \tag{10}$$

$$= |-11\rangle_p + 2 |00\rangle_p + |1,-1\rangle_p \tag{11}$$

$$|20\rangle_t = \frac{1}{\sqrt{6}} |-11\rangle_p + \sqrt{\frac{2}{3}} |00\rangle_p + \frac{1}{\sqrt{6}} |1,-1\rangle_p \tag{12}$$

[The last line equates the first line with the fourth line.]

To get the states with negative m, we can use equation 15.2.11 in Shankar:

$$\langle m_1 m_2 | jm \rangle = (-1)^{j_1 + j_2 - j} \langle -m_1, -m_2 | j, -m \rangle \tag{13}$$

Here, the bracket $\langle m_1 m_2 | jm \rangle$ is the CG coefficient that multiplies $|m_1 m_2\rangle$ in the expansion of $|jm\rangle$. For example, in 12

$$\langle -11 | 20 \rangle = \frac{1}{\sqrt{6}} \tag{14}$$

$$\langle 00 | 20 \rangle = \sqrt{\frac{2}{3}} \tag{15}$$

$$\langle 1,-1 | 20 \rangle = \frac{1}{\sqrt{6}} \tag{16}$$

Using 13 and 7, we have $j_1 + j_2 - j = 1 + 1 - 2 = 0$, so

$$|2,-1\rangle_t = \frac{1}{\sqrt{2}} |0,-1\rangle_p + \frac{1}{\sqrt{2}} |-10\rangle_p \tag{17}$$

The final ket in the column with $j = 2$ is

$$|2,-2\rangle_t = |-1,-1\rangle_p \tag{18}$$

For the next column, we have $j=1$ and the top entry therefore has $m=1$. This total-j state $|11\rangle_t$ must be a combination of the product states $|10\rangle_p$ and $|01\rangle_p$, must be orthogonal to 7 and the coefficient of the term with $m_1 = j_1$ is by convention positive. By inspection, we have

$$|11\rangle_t = -\frac{1}{\sqrt{2}}|01\rangle_p + \frac{1}{\sqrt{2}}|10\rangle_p \tag{19}$$

Note that $m_1 = j_1 = 1$ in the second term, so it's the positive one.

To get the next ket, we apply the lowering operator again:

$$J_-|11\rangle_t = \sqrt{2}|10\rangle_t \tag{20}$$

$$\frac{1}{\sqrt{2}}(J_{1-}+J_{2-})\left(|01\rangle_p - |10\rangle_p\right) = -\frac{1}{\sqrt{2}}\left(\sqrt{2}|-11\rangle_p + \sqrt{2}|00\rangle_p\right) + \tag{21}$$

$$\frac{1}{\sqrt{2}}\left(\sqrt{2}|00\rangle_p + \sqrt{2}|1,-1\rangle_p\right) \tag{22}$$

$$= -|-11\rangle_p + |1,-1\rangle_p \tag{23}$$

$$|10\rangle_t = -\frac{1}{\sqrt{2}}|-11\rangle_p + \frac{1}{\sqrt{2}}|1,-1\rangle_p \tag{24}$$

We apply 13 to get the final entry in this column. This time $j_1+j_2-j=1$ so

$$|1,-1\rangle_t = \frac{1}{\sqrt{2}}|0,-1\rangle_p - \frac{1}{\sqrt{2}}|-10\rangle_p \tag{25}$$

Finally, there is one total-j ket in the third column, where $j=m=0$. This time, the ket $|00\rangle_t$ must be a combination of $|-11\rangle_p$, $|00\rangle_p$ and $|1,-1\rangle_p$, and must be orthogonal to both 12 and 24. Suppose

$$|00\rangle_t = a|-11\rangle_p + b|00\rangle_p + c|1,-1\rangle_p \tag{26}$$

Then the orthogonality conditions tell us that

$$\frac{a}{\sqrt{6}} + \sqrt{\frac{2}{3}}b + \frac{c}{\sqrt{6}} = 0 \tag{27}$$

$$-\frac{a}{\sqrt{2}} + \frac{c}{\sqrt{2}} = 0 \tag{28}$$

We can solve these to find

$$c = a \tag{29}$$
$$2a+2b = 0 \tag{30}$$
$$b = -a \tag{31}$$

We can find a from the normalization condition

$$a^2+b^2+c^2 = 1 \tag{32}$$
$$3a^2 = 1 \tag{33}$$

Thus we have

$$a = c = \frac{1}{\sqrt{3}} \tag{34}$$
$$b = -\frac{1}{\sqrt{3}} \tag{35}$$
$$|00\rangle_t = \frac{1}{\sqrt{3}}|-11\rangle_p - \frac{1}{\sqrt{3}}|00\rangle_p + \frac{1}{\sqrt{3}}|1,-1\rangle_p \tag{36}$$

These CG coefficients agree with those given in Griffiths's Table 4.8, for example.

A final comment on the dimensionality of the various spaces. If we combine two single spins j_1 and j_2, then the dimensionality of the product space $j_1 \otimes j_2$ is $(2j_1+1)(2j_2+1)$, since there are $2j_i+1$ possible m_i values for spin j_i. In the above example, both j_1 and j_2 are 1, so the dimensionality of $1 \otimes 1$ is $3 \times 3 = 9$. The dimensionality of the corresponding total-j space is the sum of the dimensions for each possible value of j within this space. For $1 \otimes 1$, there are 5 states with $j = 2$, 3 states with $j = 1$ and 1 state with $j = 0$, for a total of $5+3+1 = 9$.

If we combine more than 2 spins, we can apply the same argument, provided we count the number of total-j states properly. For $\frac{1}{2} \otimes \frac{1}{2} \otimes \frac{1}{2}$, the product space contains $2 \times 2 \times 2 = 8$ dimensions, so the total-j space must also contain 8 dimensions. In the total-j space, j can be $\frac{3}{2}$ or $\frac{1}{2}$. We have 4 states with $j = \frac{3}{2}$. For $j = \frac{1}{2}$, we can have $m = \pm\frac{1}{2}$. Consider the ket $\left|\frac{1}{2}\frac{1}{2}\right\rangle_t$. It must be a combination of product states where two spins are up and one is down (that is, two of the m_i are $+\frac{1}{2}$ and one is $-\frac{1}{2}$), so we have

$$\left|\frac{1}{2}\frac{1}{2}\right\rangle_t = a|\uparrow\uparrow\downarrow\rangle + b|\uparrow\downarrow\uparrow\rangle + c|\downarrow\uparrow\uparrow\rangle \tag{37}$$

The only constraints we have on a, b and c are (1) the state $\left|\frac{1}{2}\frac{1}{2}\right\rangle_t$ must be orthogonal to $\left|\frac{3}{2}\frac{1}{2}\right\rangle_t$ and (2) the state must be normalized. As we have

only 2 constraints on 3 unknowns, the subspace occupied by $\left|\frac{1}{2}\frac{1}{2}\right\rangle_t$ is two-dimensional. The same argument applies to $\left|\frac{1}{2},-\frac{1}{2}\right\rangle_t$ so it, too, is two-dimensional. Thus the total dimensionality of the total-j space is $4+2+2=8$, or in other words, $\frac{1}{2}\otimes\frac{1}{2}\otimes\frac{1}{2}=\frac{3}{2}\oplus\frac{1}{2}\oplus\frac{1}{2}$.

CLEBSCH-GORDAN COEFFICIENTS FOR ADDITION OF SPIN-1/2 AND GENERAL L

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Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 15.2; Exercise 15.2.4.

Post date: 18 Sep 2017

[If some equations are too small to read easily, use your browser's magnifying option (Ctrl + on Chrome, probably something similar on other browsers).]

We've looked at the problem of adding spin-$\frac{1}{2}$ to another arbitrary spin s_2 before, but Shankar provides a different method to get this result. In Shankar's book, the problem is to add a general angular momentum $\mathbf{L}$ to a spin-$\frac{1}{2}$ system. In the product space, there are four states in such a system. In all of these states ℓ and $s = \frac{1}{2}$ are always the same. We wish to construct the total-j state for a given total angular momentum $\mathbf{J} = \mathbf{L} + \mathbf{S}$ and a specified z component of total angular momentum m from these four states. In a given product state, the z component of spin is either $m_s = \pm\frac{1}{2}$ and since we must have $m = m_\ell + m_s$, the orbital z component must be $m_\ell = m - m_s$. Therefore, for a given m, the two possible total-j states are

$$\left|\ell + \frac{1}{2}, m\right\rangle_t = \alpha \left|m - \frac{1}{2}, \frac{1}{2}\right\rangle_p + \beta \left|m + \frac{1}{2}, -\frac{1}{2}\right\rangle_p \tag{1}$$

$$\left|\ell - \frac{1}{2}, m\right\rangle_t = \alpha' \left|m - \frac{1}{2}, \frac{1}{2}\right\rangle_p + \beta' \left|m + \frac{1}{2}, -\frac{1}{2}\right\rangle_p \tag{2}$$

As usual, a subscript t on a ket indicates a total-j state and a subscript p indicates a product state. We've omitted ℓ and s in the product states since they are always the same.

The coefficients α, β, α' and β' can be determined by applying several constraints. The two states must be orthonormal which gives us three constraints

$$\alpha^2 + \beta^2 = 1 \tag{3}$$

$$\alpha'^2 + \beta'^2 = 1 \tag{4}$$

$$\alpha\alpha' + \beta\beta' = 0 \tag{5}$$

[As usual for Clebsch-Gordan coefficients, we're taking them to be real, so we don't need to indicate norms in these equations.] To get a fourth constraint, we can apply the total angular momentum operator J^2 in the form

$$\begin{aligned} J^2 &= (\mathbf{L}+\mathbf{S})^2 && (6)\\ &= L^2+S^2+2\mathbf{L}\cdot\mathbf{S} && (7)\\ &= L^2+S^2+2L_zS_z+L_-S_++L_+S_- && (8)\end{aligned}$$

Applying this operator to the LHS of 1 and 2, we have

$$J^2\left|\ell+\frac{1}{2},m\right\rangle_t=\hbar^2\left(\ell+\frac{1}{2}\right)\left(\ell+\frac{3}{2}\right)\left|\ell+\frac{1}{2},m\right\rangle_t \quad (9)$$

$$J^2\left|\ell-\frac{1}{2},m\right\rangle_t=\hbar^2\left(\ell-\frac{1}{2}\right)\left(\ell+\frac{1}{2}\right)\left|\ell-\frac{1}{2},m\right\rangle_t \quad (10)$$

On the RHS, we need the formulas for the raising and lowering operators (which also apply if we replace J by L or S):

$$J_\pm\left|jm\right\rangle_p=\hbar\sqrt{(j\mp m)(j\pm m+1)}\left|j(m-1)\right\rangle_p \quad (11)$$

To apply this formula to 1, for example, we see that $L_-S_+\left|m-\frac{1}{2},\frac{1}{2}\right\rangle_p=0$ since m_s is at its maximum value so applying the raising operator to that state gives zero. To calculate $L_-S_+\left|m+\frac{1}{2},-\frac{1}{2}\right\rangle_p$ we need to consider the two operators in turn.

We have

$$S_+ \left| m+\frac{1}{2},-\frac{1}{2} \right\rangle_p = \hbar\sqrt{(s-m_s)(s+m_s+1)} \left| m+\frac{1}{2},\frac{1}{2} \right\rangle_p \tag{12}$$

$$= \hbar\sqrt{\left(\frac{1}{2}+\frac{1}{2}\right)\left(\frac{1}{2}-\frac{1}{2}+1\right)} \left| m+\frac{1}{2},\frac{1}{2} \right\rangle_p \tag{13}$$

$$= \hbar \left| m+\frac{1}{2},\frac{1}{2} \right\rangle_p \tag{14}$$

$$L_-\hbar \left| m+\frac{1}{2},\frac{1}{2} \right\rangle_p = \hbar^2\sqrt{(\ell+m_\ell)(\ell-m_\ell+1)} \left| m-\frac{1}{2},\frac{1}{2} \right\rangle_p \tag{15}$$

$$= \hbar^2\sqrt{\left(\ell+m+\frac{1}{2}\right)\left(\ell-m-\frac{1}{2}+1\right)} \left| m-\frac{1}{2},\frac{1}{2} \right\rangle_p \tag{16}$$

$$= \hbar^2\sqrt{\left(\ell+\frac{1}{2}\right)^2-m^2} \left| m-\frac{1}{2},\frac{1}{2} \right\rangle_p \tag{17}$$

Similarly we have $L_+S_- \left|m+\frac{1}{2},-\frac{1}{2}\right\rangle_p = 0$ and

$$S_- \left| m-\frac{1}{2},\frac{1}{2} \right\rangle_p = \hbar\sqrt{(s+m_s)(s-m_s+1)} \left| m-\frac{1}{2},-\frac{1}{2} \right\rangle_p \tag{18}$$

$$= \hbar\sqrt{\left(\frac{1}{2}+\frac{1}{2}\right)\left(\frac{1}{2}-\frac{1}{2}+1\right)} \left| m-\frac{1}{2},-\frac{1}{2} \right\rangle_p \tag{19}$$

$$= \hbar \left| m-\frac{1}{2},-\frac{1}{2} \right\rangle_p \tag{20}$$

$$L_+\hbar \left| m-\frac{1}{2},-\frac{1}{2} \right\rangle_p = \hbar^2\sqrt{(\ell-m_\ell)(\ell+m_\ell+1)} \left| m+\frac{1}{2},-\frac{1}{2} \right\rangle_p \tag{21}$$

$$= \hbar^2\sqrt{\left(\ell-m+\frac{1}{2}\right)\left(\ell+m-\frac{1}{2}+1\right)} \left| m+\frac{1}{2},-\frac{1}{2} \right\rangle_p \tag{22}$$

$$= \hbar^2\sqrt{\left(\ell+\frac{1}{2}\right)^2-m^2} \left| m+\frac{1}{2},-\frac{1}{2} \right\rangle_p \tag{23}$$

Therefore (I'll drop the factor of $\hbar^2$ from now on, since it cancels out in the end):

$$\left[L^2+S^2+2L_zS_z+L_-S_++L_+S_-\right]\left[\alpha\left|m-\frac{1}{2},\frac{1}{2}\right\rangle_p+\beta\left|m+\frac{1}{2},-\frac{1}{2}\right\rangle_p\right]= \tag{24}$$

$$\left[\ell(\ell+1)+\frac{3}{4}\right]\left[\alpha\left|m-\frac{1}{2},\frac{1}{2}\right\rangle_p+\beta\left|m+\frac{1}{2},-\frac{1}{2}\right\rangle_p\right]+ \tag{25}$$

$$\left[\alpha\left(m-\frac{1}{2}\right)\left|m-\frac{1}{2},\frac{1}{2}\right\rangle_p-\beta\left(m+\frac{1}{2}\right)\left|m+\frac{1}{2},-\frac{1}{2}\right\rangle_p\right]+ \tag{26}$$

$$\sqrt{\left(\ell+\frac{1}{2}\right)^2-m^2}\left[\beta\left|m-\frac{1}{2},\frac{1}{2}\right\rangle_p+\alpha\left|m+\frac{1}{2},-\frac{1}{2}\right\rangle_p\right]= \tag{27}$$

$$\alpha\left[\left(\ell(\ell+1)+\frac{3}{4}+\left(m-\frac{1}{2}\right)\right)\left|m-\frac{1}{2},\frac{1}{2}\right\rangle+\sqrt{\left(\ell+\frac{1}{2}\right)^2-m^2}\left|m+\frac{1}{2},-\frac{1}{2}\right\rangle_p\right]+ \tag{28}$$

$$\beta\left[\left(\ell(\ell+1)+\frac{3}{4}-\left(m+\frac{1}{2}\right)\right)\left|m+\frac{1}{2},-\frac{1}{2}\right\rangle_p+\sqrt{\left(\ell+\frac{1}{2}\right)^2-m^2}\left|m-\frac{1}{2},\frac{1}{2}\right\rangle_p\right]= \tag{29}$$

$$\left(\ell+\frac{1}{2}\right)\left(\ell+\frac{3}{2}\right)\left[\alpha\left|m-\frac{1}{2},\frac{1}{2}\right\rangle_p+\beta\left|m+\frac{1}{2},-\frac{1}{2}\right\rangle_p\right] \tag{30}$$

where the last equality comes from equating the result with 9.
Equating coefficients in the last equation gives us

Thanks to Petra Axolotl for corrections to my original post.

$$\left(\ell(\ell+1)+\frac{3}{4}+\left(m-\frac{1}{2}\right)\right)\alpha+\sqrt{\left(\ell+\frac{1}{2}\right)^2-m^2}\beta=\left(\ell+\frac{1}{2}\right)\left(\ell+\frac{3}{2}\right)\alpha \tag{31}$$

$$\sqrt{\left(\ell+\frac{1}{2}\right)^2-m^2}\alpha+\left(\ell(\ell+1)+\frac{3}{4}-\left(m+\frac{1}{2}\right)\right)\beta=\left(\ell+\frac{1}{2}\right)\left(\ell+\frac{3}{2}\right)\beta \tag{32}$$

Dividing the first equation by α we get

$$\frac{\beta}{\alpha} = \frac{\left(\ell+\frac{1}{2}\right)\left(\ell+\frac{3}{2}\right) - \left(\ell(\ell+1)+\frac{3}{4}+\left(m-\frac{1}{2}\right)\right)}{\sqrt{\left(\ell+\frac{1}{2}\right)^2 - m^2}} \tag{33}$$

We can simplify this by noting that

$$\ell(\ell+1)+\frac{3}{4}+\left(m-\frac{1}{2}\right) = \left(\ell+\frac{1}{2}\right)^2 + m \tag{34}$$

$$\left(\ell+\frac{1}{2}\right)\left(\ell+\frac{3}{2}\right) = \left(\ell+\frac{1}{2}\right)^2 + \left(\ell+\frac{1}{2}\right) \tag{35}$$

so that

$$\frac{\beta}{\alpha} = \frac{\left(\ell+\frac{1}{2}\right)-m}{\sqrt{\left(\ell+\frac{1}{2}\right)^2 - m^2}} \tag{36}$$

$$= \frac{\ell+\frac{1}{2}-m}{\sqrt{\ell+\frac{1}{2}+m}\sqrt{\ell+\frac{1}{2}-m}} \tag{37}$$

$$= \sqrt{\frac{\ell+\frac{1}{2}-m}{\ell+\frac{1}{2}+m}} \tag{38}$$

From here, we can use 3 to get

The other equation 32 gives the same result for $\frac{\beta}{\alpha}$.

$$\alpha^2+\beta^2 = \alpha^2\left(1+\frac{\beta^2}{\alpha^2}\right) \tag{39}$$

$$= \alpha^2\left(1+\frac{\ell+\frac{1}{2}-m}{\ell+\frac{1}{2}+m}\right) \tag{40}$$

$$= \alpha^2\frac{2\ell+1}{\ell+\frac{1}{2}+m} = 1 \tag{41}$$

$$\alpha = \sqrt{\frac{\ell+\frac{1}{2}+m}{2\ell+1}} \tag{42}$$

$$\beta = \alpha\sqrt{\frac{\ell+\frac{1}{2}-m}{\ell+\frac{1}{2}+m}} \tag{43}$$

$$= \sqrt{\frac{\ell+\frac{1}{2}-m}{2\ell+1}} \tag{44}$$

We can get α' and β' from 4 and 5:

$$\frac{\beta'}{\alpha'} = -\frac{\alpha}{\beta} = -\sqrt{\frac{\ell+\frac{1}{2}+m}{\ell+\frac{1}{2}-m}} \tag{45}$$

A bit of algebra gives

$$\alpha' = -\sqrt{\frac{\ell+\frac{1}{2}-m}{2\ell+1}} \tag{46}$$

$$\beta' = \sqrt{\frac{\ell+\frac{1}{2}+m}{2\ell+1}} \tag{47}$$

The sign of α' is determined from the convention that the coefficient of the product ket with the highest m is positive. Combining these results gives Shankar's equation 15.2.20:

$$\left|\ell\pm\frac{1}{2},m\right\rangle_t = \pm\sqrt{\frac{\ell+\frac{1}{2}\pm m}{2\ell+1}}\left|m-\frac{1}{2},\frac{1}{2}\right\rangle_p + \sqrt{\frac{\ell+\frac{1}{2}\mp m}{2\ell+1}}\left|m+\frac{1}{2},-\frac{1}{2}\right\rangle_p \tag{48}$$

PINGBACKS

Pingback: Symmetry of states formed from two equal spins

PROJECTION OPERATORS FOR SPIN-1/2 + SPIN-1/2

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Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 15.2; Exercise 15.2.5.

Post date: 15 Sep 2017

[If some equations are too small to read easily, use your browser's magnifying option (Ctrl + on Chrome, probably something similar on other browsers).]

We've seen projection operators in a formal mathematical sense, but in this post, we'll see a practical example of projection operators in spin space. We look at a system of two spin-$\frac{1}{2}$ particles, with spin operators $\mathbf{S}_1$ and $\mathbf{S}_2$ for each of the two particles. Now consider the operators

$$\mathbb{P}_1 = \frac{3}{4}I + \frac{1}{\hbar^2}\mathbf{S}_1 \cdot \mathbf{S}_2 \tag{1}$$

$$\mathbb{P}_2 = \frac{1}{4}I - \frac{1}{\hbar^2}\mathbf{S}_1 \cdot \mathbf{S}_2 \tag{2}$$

A projection operator projects an arbitrary vector onto a subscape of the vector space in which that vector resides. The two projection operators here project onto orthogonal subspaces, which means if we project some vector V first with $\mathbb{P}_1$ and then with $\mathbb{P}_2$ (or vice versa), we'll end up with the zero vector. Also, if we project V twice (or more) with the same projection operator, all projections after the first have no further effect. That is

$$\mathbb{P}_i\mathbb{P}_j = \delta_{ij}\mathbb{P}_j \tag{3}$$

To show that this is true for the two projection operators above, we can make use of an identity derived earlier:

$$(\mathbf{A}\cdot\boldsymbol{\sigma})(\mathbf{B}\cdot\boldsymbol{\sigma}) = (\mathbf{A}\cdot\mathbf{B})I + i(\mathbf{A}\times\mathbf{B})\cdot\boldsymbol{\sigma} \tag{4}$$

which is valid if $\mathbf{A}$ and $\mathbf{B}$ commute with $\boldsymbol{\sigma}$.

Here $\mathbf{A}$ and $\mathbf{B}$ are vector operators that commute with the Pauli matrices $\boldsymbol{\sigma}$.

First, we'll look at $\mathbb{P}_1\mathbb{P}_2$:

$$\mathbb{P}_1\mathbb{P}_2 = \left[\frac{3}{4}I + \frac{1}{\hbar^2}\mathbf{S}_1\cdot\mathbf{S}_2\right]\left[\frac{1}{4}I - \frac{1}{\hbar^2}\mathbf{S}_1\cdot\mathbf{S}_2\right] \tag{5}$$

$$= \left[\frac{3}{4}I + \frac{1}{4}\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2\right]\left[\frac{1}{4}I - \frac{1}{4}\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2\right] \tag{6}$$

$$= \frac{3}{16}I - \frac{2}{16}\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2 - \frac{1}{16}\left(\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2\right)^2 \tag{7}$$

We can write the last term as

$$\left(\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2\right)^2 = \left(\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2\right)\left(\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2\right) \tag{8}$$

We see that this has the same form as 4 with $\mathbf{A} = \mathbf{B} = \boldsymbol{\sigma}_1$ and $\boldsymbol{\sigma} = \boldsymbol{\sigma}_2$. Since $\boldsymbol{\sigma}_1$ and $\boldsymbol{\sigma}_2$ refer to different spins, they commute, so the identity is valid. We get

$$\left(\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2\right)^2 = \boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_1 I + i\left(\boldsymbol{\sigma}_1\times\boldsymbol{\sigma}_1\right)\cdot\boldsymbol{\sigma}_2 \tag{9}$$

The first term is (using the fact that the square of each Pauli matrix is I):

$$\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_1 I = \left(\sigma_{x1}^2 + \sigma_{y1}^2 + \sigma_{z1}^2\right) I \tag{10}$$

$$= 3I^2 \tag{11}$$

$$= 3I \tag{12}$$

The cross product is just a shorthand way of writing the commutation relations. To see this, work out the x component, for example:

$$\left(\boldsymbol{\sigma}_1\times\boldsymbol{\sigma}_1\right)_x = \sigma_{y1}\sigma_{z1} - \sigma_{z1}\sigma_{y1} = 2i\sigma_{x1} \tag{13}$$

We can write this as

$$\left(\boldsymbol{\sigma}_1\times\boldsymbol{\sigma}_1\right) = i\boldsymbol{\sigma}_1 \tag{14}$$

Plugging this into 9 we have

$$\left(\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2\right)^2 = 3I - 2\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2 \tag{15}$$

This gives, from 7

$$\mathbb{P}_1\mathbb{P}_2 = \frac{3}{16}I - \frac{2}{16}\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2 - \frac{3}{16}I + \frac{2}{16}\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2 = 0 \tag{16}$$

A similar calculation shows that

$$\mathbb{P}_2\mathbb{P}_1 = 0 \tag{17}$$

We can also calculate

$$\mathbb{P}_1\mathbb{P}_1 = \left[\frac{3}{4}I + \frac{1}{\hbar^2}\mathbf{S}_1\cdot\mathbf{S}_2\right]\left[\frac{3}{4}I + \frac{1}{\hbar^2}\mathbf{S}_1\cdot\mathbf{S}_2\right] \tag{18}$$

$$= \left[\frac{3}{4}I + \frac{1}{4}\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2\right]\left[\frac{3}{4}I + \frac{1}{4}\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2\right] \tag{19}$$

$$= \frac{9}{16}I + \frac{6}{16}\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2 + \frac{1}{16}\left(\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2\right)^2 \tag{20}$$

$$= \frac{12}{16}I + \frac{4}{16}\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2 \tag{21}$$

$$= \frac{3}{4}I + \frac{1}{4}\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2 \tag{22}$$

$$= \mathbb{P}_1 \tag{23}$$

A similar calculation shows that

$$\mathbb{P}_2\mathbb{P}_2 = \mathbb{P}_2 \tag{24}$$

To find the subspace to which each projection operator projects, we can use the explicit matrix forms in the product basis for the projections. We have

$$\mathbb{P}_1 = \frac{3}{4}I + \frac{1}{\hbar^2}\mathbf{S}_1\cdot\mathbf{S}_2 \tag{25}$$

$$= \frac{3}{4}I + \frac{1}{\hbar^2}\left(\frac{1}{2}S_{1+}S_{2-} + \frac{1}{2}S_{1-}S_{2+} + S_{1z}S_{2z}\right) \tag{26}$$

$$= \frac{3}{4}\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} + \frac{1}{2}\begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} + \tag{27}$$

$$\frac{1}{2}\begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} + \frac{1}{4}\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \tag{28}$$

$$= \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & \frac{1}{2} & 0 \\ 0 & \frac{1}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \tag{29}$$

Similarly

$$\mathbb{P}_2 = \frac{1}{4}I - \frac{1}{\hbar^2}\mathbf{S}_1 \cdot \mathbf{S}_2 \tag{30}$$

$$= \frac{3}{4}I - \frac{1}{\hbar^2}\left(\frac{1}{2}S_{1+}S_{2-} + \frac{1}{2}S_{1-}S_{2+} + S_{1z}S_{2z}\right) \tag{31}$$

$$= \frac{1}{4}\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} - \frac{1}{2}\begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} - \tag{32}$$

$$\frac{1}{2}\begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} - \frac{1}{4}\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \tag{33}$$

$$= \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & -\frac{1}{2} & 0 \\ 0 & -\frac{1}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \tag{34}$$

If we apply these projections to an arbitrary vector V, we have

$$\mathbb{P}_1 V = \mathbb{P}_1 \begin{bmatrix} a \\ b \\ c \\ d \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & \frac{1}{2} & 0 \\ 0 & \frac{1}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} a \\ b \\ c \\ d \end{bmatrix} \tag{35}$$

$$= \begin{bmatrix} a \\ \frac{1}{2}(b+c) \\ \frac{1}{2}(b+c) \\ d \end{bmatrix} \tag{36}$$

$$= a\begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} + \frac{1}{\sqrt{2}}(b+c)\begin{bmatrix} 0 \\ \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \\ 0 \end{bmatrix} + d\begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix} \tag{37}$$

Thus $\mathbb{P}_1$ projects V into the subspace spanned by the basis vectors of the 3-dimensional spin-1 subspace.

For $\mathbb{P}_2$ we have

$$\mathbb{P}_2 V = \mathbb{P}_2 \begin{bmatrix} a \\ b \\ c \\ d \end{bmatrix} = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & -\frac{1}{2} & 0 \\ 0 & -\frac{1}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} a \\ b \\ c \\ d \end{bmatrix} \tag{38}$$

$$= \begin{bmatrix} 0 \\ \frac{1}{2}(b-c) \\ \frac{1}{2}(-b+c) \\ 0 \end{bmatrix} \tag{39}$$

$$= \frac{1}{\sqrt{2}}(b-c) \begin{bmatrix} 0 \\ \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \\ 0 \end{bmatrix} \tag{40}$$

Thus $\mathbb{P}_2$ projects onto the 1-dimensional spin-0 subspace.
In the total-j basis

$$S^2 = (\mathbf{S}_1 + \mathbf{S}_2)^2 = S_1^2 + S_2^2 + 2\mathbf{S}_1 \cdot \mathbf{S}_2 \tag{41}$$

$$\mathbf{S}_1 \cdot \mathbf{S}_2 = \frac{1}{2}\left(S^2 - S_1^2 - S_2^2\right) \tag{42}$$

In both the spin-1 and spin-0 states, the eigenvalues of S_1^2 and S_2^2 are equal to $s_1(s_1+1)\hbar^2 = \frac{3\hbar^2}{4}$. For spin-1, $s=1$ and for the three basis states with $m = \pm 1, 0$, we have, since all operators are diagonal in this space:

$$(\mathbf{S}_1 \cdot \mathbf{S}_2)\,|s=1, m=\pm 1,0\rangle = \frac{1}{2}\left(S^2 - S_1^2 - S_2^2\right)|s=1, m=\pm 1,0\rangle \tag{43}$$

$$= \frac{\hbar^2}{2}\left(s(s+1) - \frac{3}{2}\right) I\,|s=1, m=\pm 1,0\rangle \tag{44}$$

$$= \frac{\hbar^2}{4}\,|s=1, m=\pm 1,0\rangle \tag{45}$$

For the spin-0 state, there is only one basis state with $m=0$, so

$$(\mathbf{S}_1 \cdot \mathbf{S}_2)\,|s=0,m=0\rangle = \frac{1}{2}\left(S^2 - S_1^2 - S_2^2\right)|s=0,m=0\rangle \tag{46}$$

$$= \frac{\hbar^2}{2}\left(s\,(s+1) - \frac{3}{2}\right)|s=0,m=0\rangle \tag{47}$$

$$= -\frac{3\hbar^2}{4}\,|s=0,m=0\rangle \tag{48}$$

Therefore, on any spin-1 state, we have

$$\mathbb{P}_1\,|s=1,m=\pm1,0\rangle = \left(\frac{3}{4}I + \frac{1}{\hbar^2}\mathbf{S}_1 \cdot \mathbf{S}_2\right)|s=1,m=\pm1,0\rangle \tag{49}$$

$$= \left(\frac{3}{4} + \frac{1}{4}\right) I\,|s=1,m=\pm1,0\rangle \tag{50}$$

$$= |s=1,m=\pm1,0\rangle \tag{51}$$

$$\mathbb{P}_2\,|s=1,m=\pm1,0\rangle = \left(\frac{1}{4}I - \frac{1}{\hbar^2}\mathbf{S}_1 \cdot \mathbf{S}_2\right)|s=1,m=\pm1,0\rangle \tag{52}$$

$$= \left(\frac{1}{4} - \frac{1}{4}\right) I\,|s=1,m=\pm1,0\rangle \tag{53}$$

$$= 0 \tag{54}$$

On the spin-0 state

$$\mathbb{P}_1\,|s=0,m=0\rangle = \left(\frac{3}{4}I + \frac{1}{\hbar^2}\mathbf{S}_1 \cdot \mathbf{S}_2\right)|s=0,m=0\rangle \tag{55}$$

$$= \left(\frac{3}{4} - \frac{3}{4}\right) I\,|s=0,m=0\rangle \tag{56}$$

$$= 0 \tag{57}$$

$$\mathbb{P}_2\,|s=0,m=0\rangle = \left(\frac{1}{4}I - \frac{1}{\hbar^2}\mathbf{S}_1 \cdot \mathbf{S}_2\right)|s=0,m=0\rangle \tag{58}$$

$$= \left(\frac{1}{4} + \frac{3}{4}\right) I\,|s=0,m=0\rangle \tag{59}$$

$$= |s=0,m=0\rangle \tag{60}$$

Since the four kets $|s=1,m=\pm1,0\rangle$ and $|s=0,m=0\rangle$ form a basis in the total-j space, any state can be written as a linear combination of them, and thus the projection operator $\mathbb{P}_1$ projects an arbitrary vector onto the $|s=1,m=\pm1,0\rangle$ subspace and $\mathbb{P}_2$ onto the $|s=0,m=0\rangle$ subspace.

PINGBACKS

Pingback: Projection operators for general L + spin-1/2

PROJECTION OPERATORS FOR GENERAL L + SPIN-1/2

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Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 15.2; Exercise 15.2.6.

Post date: 16 Oct 2017

We can generalize the calculation made earlier where we found the projection operators that project an arbitrary vector onto the spin-1 and spin-0 subspaces of the space where two spin-$\frac{1}{2}$ systems are added. Here, we'll consider adding a spin-$\frac{1}{2}$ system to a system with an arbitrary orbital angular momentum $\mathbf{L}$. In our earlier calculation, we found that the projection operators for adding two spin-$\frac{1}{2}$ systems are

$$\mathbb{P}_1 = \frac{3}{4}I + \frac{1}{\hbar^2}\mathbf{S}_1 \cdot \mathbf{S}_2 \tag{1}$$

$$\mathbb{P}_2 = \frac{1}{4}I - \frac{1}{\hbar^2}\mathbf{S}_1 \cdot \mathbf{S}_2 \tag{2}$$

In the more general case, we'll assume that the projection operators have the forms

$$\mathbb{P}_+ = aI + \frac{b}{\hbar^2}\mathbf{L} \cdot \mathbf{S} \tag{3}$$

$$\mathbb{P}_- = cI + \frac{d}{\hbar^2}\mathbf{L} \cdot \mathbf{S} \tag{4}$$

where the constants a, b, c and d are to be determined. The operator $\mathbb{P}_+$ should project a vector onto the $j = l + \frac{1}{2}$ subspace and $\mathbb{P}_-$ should project onto the $j = l - \frac{1}{2}$ subspace. Consider $\mathbb{P}_+$ first. We must therefore have

$$\mathbb{P}_+ \left| l + \frac{1}{2} \right\rangle = \left| l + \frac{1}{2} \right\rangle \tag{5}$$

First, we need a useful identity:

$$\mathbf{J}^2 = (\mathbf{L} + \mathbf{S})^2 = L^2 + S^2 + 2\mathbf{L} \cdot \mathbf{S} \tag{6}$$

$$\mathbf{L} \cdot \mathbf{S} = \frac{1}{2}\left(J^2 - L^2 - S^2\right) \tag{7}$$

Inserting 3 we have

$$\mathbb{P}_+ \left| l+\frac{1}{2} \right\rangle = \left(aI + \frac{b}{\hbar^2}\mathbf{L}\cdot\mathbf{S} \right) \left| l+\frac{1}{2} \right\rangle \tag{8}$$

$$= \left(a + b\left[j\left(j+1\right) - l\left(l+1\right) - s\left(s+1\right) \right] \right) \left| l+\frac{1}{2} \right\rangle \tag{9}$$

$$= \left(a + b\left[\left(l+\frac{1}{2} \right)\left(l+\frac{3}{2} \right) - l\left(l+1\right) - \frac{3}{4} \right] \right) \left| l+\frac{1}{2} \right\rangle \tag{10}$$

$$= \left(a + \frac{bl}{2} \right) \left| l+\frac{1}{2} \right\rangle \tag{11}$$

Operating with $\mathbb{P}_+$ on the state $\left| l-\frac{1}{2} \right\rangle$ must give zero, since this state is orthogonal to $\left| l+\frac{1}{2} \right\rangle$, so

$$\mathbb{P}_+ \left| l-\frac{1}{2} \right\rangle = 0 \tag{12}$$

We therefore have

$$\mathbb{P}_+ \left| l-\frac{1}{2} \right\rangle = \left(aI + \frac{b}{\hbar^2}\mathbf{L}\cdot\mathbf{S} \right) \left| l-\frac{1}{2} \right\rangle \tag{13}$$

$$= \left(a + b\left[j\left(j+1\right) - l\left(l+1\right) - s\left(s+1\right) \right] \right) \left| l-\frac{1}{2} \right\rangle \tag{14}$$

$$= \left(a + b\left[\left(l-\frac{1}{2} \right)\left(l+\frac{1}{2} \right) - l\left(l+1\right) - \frac{3}{4} \right] \right) \left| l-\frac{1}{2} \right\rangle \tag{15}$$

$$= \left(a - \frac{b\left(l+1\right)}{2} \right) \left| l-\frac{1}{2} \right\rangle \tag{16}$$

We thus have the two equations

$$a + \frac{bl}{2} = 1 \tag{17}$$

$$a - \frac{b\left(l+1\right)}{2} = 0 \tag{18}$$

Solving these, we find

$$a = \frac{l+1}{2l+1} \tag{19}$$

$$b = \frac{2}{2l+1} \tag{20}$$

The projection operator is therefore

$$\mathbb{P}_+ = \frac{1}{2l+1}\left[(l+1)\,I + \frac{2}{\hbar^2}\mathbf{L}\cdot\mathbf{S}\right] \tag{21}$$

We can follow the same procedure to find $\mathbb{P}_-$. This yields the same results when we operate on the two states $\left|l+\frac{1}{2}\right\rangle$ and $\left|l-\frac{1}{2}\right\rangle$, with a replaced by c and b by d, but now we require that

$$\mathbb{P}_-\left|l+\frac{1}{2}\right\rangle = 0 \tag{22}$$

$$\mathbb{P}_-\left|l-\frac{1}{2}\right\rangle = \left|l-\frac{1}{2}\right\rangle \tag{23}$$

This gives us the equations

$$c+\frac{dl}{2} = 0 \tag{24}$$

$$c-\frac{d\,(l+1)}{2} = 1 \tag{25}$$

with solutions

$$c = \frac{l}{2l+1} \tag{26}$$

$$d = -\frac{2}{2l+1} \tag{27}$$

Thus the projection operator is

$$\mathbb{P}_- = \frac{1}{2l+1}\left[lI - \frac{2}{\hbar^2}\mathbf{L}\cdot\mathbf{S}\right] \tag{28}$$

As a check we see that 21 and 28 reduce to the correct forms 1 and 2when $l=\frac{1}{2}$.

SYMMETRY OF STATES FORMED FROM TWO EQUAL SPINS

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Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 15.2; Exercise 15.2.7.

Post date: 17 Oct 2017

When we combine two states with angular momenta $\mathbf{J}_1$ and $\mathbf{J}_2$ we get a state with a total angular momentum $\mathbf{J} = \mathbf{J}_1 + \mathbf{J}_2$ where the total angular momentum quantum number (that is, the angular momentum in units of $\hbar$) can take on values from a maximum of $j = j_1 + j_2$ down to either $\frac{1}{2}$ or zero. The general expression uses the Clebsch-Gordan coefficients to write the compound state (in the total-j space) as a linear combination of product states.

Although the calculation of Clebsch-Gordan coefficients can get quite complicated in the general case, we can explore a couple of interesting properties in the case where the two component spins (I'll refer to the angular momenta as spins for brevity, although the argument applies to the addition of angular momenta in general) are equal, so that $j_1 = j_2$.

[Note that in my edition of Shankar's book, there are a couple of typos in exercise 15.2.7, only one of which is corrected in the errata. The problem should ask us to show that states with with $j = 2j_1$ (not $j = 2j_1 - 1$) are symmetric, and states with $j = 2j_1 - 1$ are antisymmetric.]

We'll consider first the case where the z-component is maximum, so that $m = 2j_1$. In this case, we have

$$|2j_1, 2j_1\rangle_t = |j_1 j_1, j_1 j_1\rangle_p \tag{1}$$

The subscript t refers to a total-j ket and p to a product ket. Thus the ket $|2j_1, 2j_1\rangle_t$ is a total-j ket with $j = 2j_1$ and $m = 2j_1$, while $|j_1 j_1, j_1 j_1\rangle_p$ is a product ket where both particles have total spin j_1 and z-component j_1. Clearly if we swap the two particles in the product ket, it remains unchanged so this is a symmetric state. We would like to show that all states with $j = 2j_1$ (that is, for all values of m) are also symmetric.

To see this, we can follow Shankar's procedure of applying the lowering operator $J_- = J_{I-} + J_{II-}$ to the original state. To clarify the notation, I've used roman numerals I and II to refer to the particle number, while the term j_1 just refers to the (common) angular momentum number. It gets a bit confusing since in Shankar's formulas, the two particles were also assumed

to have different angular momenta so he could use the subscripts 1 and 2 to refer both to the particle number and the angular momentum numbers. In our case, the two angular momenta are the same, but there are still two particles that we want to keep track of.

When the lowering operator is applied to 1 we get the state which can be obtained from Shankar's equation 15.2.7 with $j_1 = j_2$:

$$|2j_1, 2j_1 - 1\rangle = \frac{1}{\sqrt{2}} \left(|j_1 \left(j_1 - 1\right), j_1 j_1\rangle + |j_1 j_1, j_1 \left(j_1 - 1\right)\rangle \right) \tag{2}$$

By inspection, the state on the RHS is also symmetric when we swap the two particles. What happens if we carry on applying the lowering operator? To get an idea, consider the possible m_I and m_{II} values for each value of total z-component m.

m	m_I, m_{II}
$2j_1$	j_1
$2j_1 - 1$	j_1, $j_1 - 1$
$2j_1 - 2$	j_1, $j_1 - 1$, $j_1 - 2$
$2j_1 - a$	j_1, $j_1 - 1, \ldots, j_1 - a$

In the last line, we've given the m_I and m_{II} values for an arbitrary value a, where $a = 0, \ldots, j_1$. In each case, the ket $|2j_1, 2j_1 - a\rangle$ is formed from a sum of product kets, where the two particles in each product ket must be chosen so that $m_I + m_{II} = m$. From the first line in the table we get 1 and from the second we get 2. If we apply the lowering operator $J_- = J_{I-} + J_{II-}$ to 2, we can see the following pattern. Note that the two kets on the RHS are swapped versions of each other. If we apply J_{I-} to the first ket on the RHS and J_{II-} to the second ket, we get two kets that are again swapped versions of each other, except now one of the particles has a z-component of j_1 and the other has $j_1 - 2$. These two kets are symmetric with respect to swapping.

Now if we apply J_{I-} to the *second* ket and J_{II-} to the first, we get two kets, in both of which the z-components of the two particles are both equal to $j_1 - 1$. Thus these two kets are again symmetric with respect to each other. (Actually, of course, we can combine them into a single ket of form $|\left(j_1 - 1\right)\left(j_1 - 1\right), \left(j_1 - 1\right)\left(j_1 - 1\right)\rangle$ with some numerical coefficient, but for the purposes of our argument, it's better to keep them as two separate symmetric kets.)

We can see that the same pattern occurs as we continue the lowering process. In each case we apply J_{I-} to one member of a symmetric pair of kets and J_{II-} to the other member of the same pair. This always produces another pair of kets that are also symmetric. Thus the lowering process

retains the symmetric property of the original ket 1 that was at the top of the column.

The lowering operators introduce numerical coefficients since they have the form

$$J_- \left| jmj_1j_2 \right\rangle = \hbar\sqrt{(j+m)\,(j-m+1)}\left| j\,(m-1)\,j_1j_2 \right\rangle \tag{3}$$

However, these coefficients will be the same for each pair of symmetric states. Let's do an explicit example to see how this works. Suppose we look at one symmetric pair in one line of the above table so we have the two kets

$$\left| j_1\,(m-b)\,, j_1b \right\rangle + \left| j_1b, j_1\,(m-b) \right\rangle \tag{4}$$

We assume that these two kets have the same numerical coefficient at this stage. If we look at 2 we see this is true for the case $b = 1$, so we can take this as an anchor step in an inductive proof.

We now apply J_{I-} to the first ket and J_{II-} to the second ket in this pair. This gives

$$J_{I-} \left| j_1\,(m-b)\,, j_1b \right\rangle + J_{II-} \left| j_1b, j_1\,(m-b) \right\rangle = \tag{5}$$

$$\hbar\sqrt{(j_1+m-b)\,(j_1-m+b+1)}\left[\left| j_1\,(m-b-1)\,, j_1b \right\rangle + \left| j_1b, j_1\,(m-b-1) \right\rangle \right] \tag{6}$$

Thus the numerical coefficient is the same for both kets. The other symmetric pair is obtained by swapping the two lowering operators, so we have

$$J_{II-} \left| j_1\,(m-b)\,, j_1b \right\rangle + J_{I-} \left| j_1b, j_1\,(m-b) \right\rangle = \tag{7}$$

$$\hbar\sqrt{(j_1+b)\,(j_1-b+1)}\left[\left| j_1\,(m-b)\,, j_1\,(b-1) \right\rangle + J_{II-} \left| j_1\,(b-1)\,, j_1\,(m-b) \right\rangle \right] \tag{8}$$

This results in another symmetric pair of kets.

Now consider states where $j = 2j_1 - 1$. The top member of this column can be obtained from Shankar's equation 15.2.8 with $j_1 = j_2$:

$$\left| 2j_1-1, 2j_1-1 \right\rangle = \frac{1}{\sqrt{2}}\left(\left| j_1j_1, j_1\,(j_1-1) \right\rangle - \left| j_1\,(j_1-1)\,, j_1j_1 \right\rangle \right) \tag{9}$$

Swapping the two particles on the RHS gives the negative of the original state, so this is an antisymmetric state. We can apply exactly the same argument as above to see that all states with lower values of m are also antisymmetric. In each case, we apply J_{I-} to one member of an antisymmetric

pair and J_{II-} to the other, resulting in another antisymmetric pair with a value of m one lower than before. In this case, however, all states where $m_I = m_{II}$ will cancel out, since such states must be their own negatives. This is just the Pauli exclusion principle for antisymmetric states.

WIGNER-ECKART THEOREM

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Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 15.3.

Post date: 25 Oct 2017

We can write a rank-1 spherical tensor operator T_1^q in terms of a 3-d vector $\mathbf{V}$ as follows:

$$T_1^{\pm 1} = \mp \frac{V_x \pm iV_y}{\sqrt{2}} \tag{1}$$

$$T_1^0 = V_z \tag{2}$$

Shankar provides the example of the position operator R_1^q in spherical coordinates, but (to me, at least) the example needs a bit of clarification. First, we see that R_1^q can be written in terms of the rectangular position coordinates as

$$R_1^{\pm 1} = \mp \frac{x \pm iy}{\sqrt{2}} \tag{3}$$

$$R_1^0 = z \tag{4}$$

We've seen earlier that the spherical harmonics can be written as

$$Y_1^{\pm 1} = \mp \sqrt{\frac{3}{4\pi}} \frac{x \pm iy}{\sqrt{2}r} \tag{5}$$

$$Y_1^0 = \sqrt{\frac{3}{4\pi}} \frac{z}{r} \tag{6}$$

Therefore, we have

$$R_1^q = \sqrt{\frac{4\pi}{3}} r Y_1^q \tag{7}$$

Now suppose we calculate the matrix elements of R_1^q in the basis of angular momentum eigenstates $|\alpha lm\rangle$. Here, we're assuming that the total angular momentum is orbital so $\mathbf{J} = \mathbf{L}$, and α represents quantities that depend on things other than angular momentum. If the potential in the Hamiltonian is spherically symmetric, then the wave function can be written as

the product of a radial function $R_{\alpha l}(r)$ and a spherical harmonic $Y_l^m(\theta,\phi)$. The radial function depends only on r, and its precise form depends on the potential function $V(r)$. The spherical harmonic depends only on the angular coordinates θ and ϕ, and is independent of the potential. Using these facts, we can write the matrix element as

$$\left\langle \alpha_2 l_2 m_2 \left| R_1^q \right| \alpha_1 l_1 m_1 \right\rangle = \int R^*_{\alpha_2 l_2} \left(Y_{l_2}^{m_2}\right)^* \sqrt{\frac{4\pi}{3}} r Y_1^q R_{\alpha_1 l_1} Y_{l_1}^{m_1} r^2 dr\, d\Omega \tag{8}$$

In this equation, I've omitted the explicit functional dependences of the functions on the coordinates to save space, and $d\Omega$ is an increment of solid angle, so $d\Omega = \sin\theta d\theta\, d\phi$. This integral splits into the product of two separate integrals: one over r only and the other over angles only. That is

$$\left\langle \alpha_2 l_2 m_2 \left| R_1^q \right| \alpha_1 l_1 m_1 \right\rangle = \sqrt{\frac{4\pi}{3}} \int R^*_{\alpha_2 l_2} r R_{\alpha_1 l_1} r^2 dr \times \int \left(Y_{l_2}^{m_2}\right)^* Y_1^q Y_{l_1}^{m_1} d\Omega \tag{9}$$

The first integral is known as the *reduced matrix element*, and is written as

$$\left\langle \alpha_2 l_2 \left|\left| R_1 \right|\right| \alpha_1 l_1 \right\rangle \equiv \sqrt{\frac{4\pi}{3}} \int R^*_{\alpha_2 l_2} r R_{\alpha_1 l_1} r^2 dr \tag{10}$$

Notice that this factor is independent of the tensor index q, which appears only in the angular integral. That is, the radial integral is the same for all 3 values of q.

The angular integral is written as

$$\left\langle l_2 m_2 \left| 1 q, l_1 m_1 \right. \right\rangle \tag{11}$$

Shankar claims that this is (up to a numerical factor independent of m_1, m_2 and q) a Clebsch-Gordan coefficient, although he doesn't derive this, so we'll accept it at this point.

This result is a special case of the more general *Wigner-Eckart theorem*, which states that, for any spherical tensor operator T_k^q, its matrix elements can be written as the product of two factors, one of which is the reduced matrix element. That is

$$\left\langle \alpha_2 j_2 m_2 \left| T_k^q \right| \alpha_1 j_1 m_1 \right\rangle = \left\langle \alpha_2 j_2 \left|\left| T_k \right|\right| \alpha_1 j_1 \right\rangle \left\langle j_2 m_2 \left| k q, j_1 m_1 \right. \right\rangle \tag{12}$$

All the dependence of the matrix element on spatial orientation (that is, on θ and ϕ) is contained in the second factor, which can be written in terms of Clebsch-Gordan coefficients.

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SPHERICAL TENSOR OPERATORS; COMMUTATORS

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Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 15.3; Exercise 15.3.1.

Post date: 20 Oct 2017

A *spherical tensor operator* is defined to be an object T_k^q with integer indices q and k. The rank of the tensor is k, and the other index q ranges in integer steps from $-k$ to $+k$, giving T_k^q $2k+1$ components. Its definition includes a requirement that it transform under a rotation according to

$$U\left[R\right]T_k^q U^\dagger\left[R\right]=\sum_{q'}D_{q'q}^{(k)}T_k^{q'} \tag{1}$$

where $D^{(k)}$ is the k-th block in the block diagonal matrix formed from the angular momentum operators J. For a rotation through an angle θ about an axis $\hat{\theta}$, we have

$$D^{(k)}\left[R\left(\boldsymbol{\theta}\right)\right]=\sum_{n=0}^{\infty}\frac{1}{n!}\left(\frac{-i\theta}{\hbar}\right)^n\left(\hat{\boldsymbol{\theta}}\cdot\mathbf{J}^{(k)}\right)^n \tag{2}$$

where $\mathbf{J}^{(k)}$ is the angular momentum vector obtained from the k-th block in each of J_x, J_y and J_z (see Shankar section 12.5 for details).

The series can be written in closed form for some small values of k, but we won't need these forms here.

For a set of angular momentum kets $|kq\rangle$ (Shankar changes the notation here, in that $|kq\rangle$ refers to a state with total angular momentum number k and z component q, rather than the more familiar $|jm\rangle$), the matrix elements of $D^{(k)}$ are

$$D_{q'q}^{(k)}=\left\langle kq'\left|U\left[R\right]\right|kq\right\rangle \tag{3}$$

Note that

$$\left\langle k'q'\left|U\left[R\right]\right|kq\right\rangle=D_{q'q}^{(k)}\delta_{k'k} \tag{4}$$

This follows because a rotation cannot change the total angular momentum of a state, so $U\left[R\right]|kq\rangle$ will always result in a state whose total angular momentum number is also k. From this fact, we can write the rotation of an angular momentum ket as

$$U[R]\,|kq\rangle = \sum_{k'}\sum_{q'} |k'q'\rangle\,\langle k'q'\,|U[R]|\,kq\rangle \tag{5}$$

$$= \sum_{k'}\sum_{q'} |k'q'\rangle\, D^{(k)}_{q'q}\delta_{k'k} \tag{6}$$

$$= \sum_{q'} D^{(k)}_{q'q}\,|kq'\rangle \tag{7}$$

Comparing this result with 1, we see that a passive transformation of the tensor operator T^q_k works in the same way as a rotation of an angular momentum eigenstate $|kq\rangle$.

We can use 1 to work out the commutators of T^q_k with the components of the angular momentum operator $\mathbf{J}$. We use the fact that angular momentum is the generator of rotations and consider an infinitesimal rotation $\delta\boldsymbol{\theta}$ about, say, the x axis. In this case, working to first order in $\delta\theta$:

$$U[R] = I - \frac{i\delta\theta J_x}{\hbar} \tag{8}$$

$$U^\dagger[R] = I + \frac{i\delta\theta J_x}{\hbar} \tag{9}$$

$$U[R]\,T^q_k U^\dagger[R] = \left(I - \frac{i\delta\theta J_x}{\hbar}\right) T^q_k \left(I + \frac{i\delta\theta J_x}{\hbar}\right) \tag{10}$$

$$= T^q_k - \frac{i\delta\theta}{\hbar}\left[J_x, T^q_k\right] \tag{11}$$

On the RHS of 1 we can use 3 to first order in $\delta\theta$:

$$D^{(k)}_{q'q}T^{q'}_k = \left\langle kq' \middle| I - \frac{i\delta\theta J_x}{\hbar} \middle| kq \right\rangle T^{q'}_k \tag{12}$$

$$= \langle kq'\,|kq|\rangle\, T^{q'}_k - \frac{i\delta\theta}{\hbar}\,\langle kq'\,|J_x|\,kq\rangle\, T^{q'}_k \tag{13}$$

$$= T^q_k - \frac{i\delta\theta}{\hbar}\,\langle kq'\,|J_x|\,kq\rangle\, T^{q'}_k \tag{14}$$

Combining the last two results, we have

$$\left[J_x, T^q_k\right] = \sum_{q'} \langle kq'\,|J_x|\,kq\rangle\, T^{q'}_k \tag{15}$$

We could do the same analysis for the y and z components, and we'd get the same result, so we have

$$\left[J_y, T_k^q\right] = \sum_{q'} \left\langle kq' \left| J_y \right| kq \right\rangle T_k^{q'} \tag{16}$$

$$\left[J_z, T_k^q\right] = \sum_{q'} \left\langle kq' \left| J_z \right| kq \right\rangle T_k^{q'} \tag{17}$$

We can simplify the last equation, since the ket $|kq\rangle$ is an eigenket of J_z with eigenvalue $q\hbar$. We therefore have

$$\sum_{q'} \left\langle kq' \left| J_z \right| kq \right\rangle T_k^{q'} = \sum_{q'} \left\langle kq' \left| kq \right. \right\rangle \hbar q T_k^{q'} \tag{18}$$

$$= \hbar q T_k^q \tag{19}$$

To deal with the other two components, we can combine the results in 15 and 16 and use the raising and lowering operators.

$$J_\pm = J_x \pm i J_y \tag{20}$$

$$J_\pm \left| kq \right\rangle = \hbar \sqrt{(k \mp q)(k \pm q + 1)} \left| k, q \pm 1 \right\rangle \tag{21}$$

We have

$$\left[J_\pm, T_k^q\right] = \sum_{q'} \left\langle kq' \left| J_\pm \right| kq \right\rangle T_k^{q'} \tag{22}$$

$$= \hbar \sqrt{(k \mp q)(k \pm q + 1)} \sum_{q'} \left\langle kq' \left| k, q \pm 1 \right. \right\rangle T_k^{q'} \tag{23}$$

$$= \hbar \sqrt{(k \mp q)(k \pm q + 1)} T_k^{q \pm 1} \tag{24}$$

where we've again used the orthogonality of the eigenkets to get the last line.

Example. Suppose we construct a spherical tensor out of the components of a vector operator $\mathbf{V}$ so that we have a rank 1 tensor given by

$$T_1^{\pm 1} = \mp \frac{V_x \pm i V_y}{\sqrt{2}} \tag{25}$$

$$T_1^0 = V_z \tag{26}$$

Vector operators obey the commutation rules

$$[V_i, J_j] = i\hbar \sum_k \varepsilon_{ijk} V_k \tag{27}$$

Applying this gives us, for example

$$\left[T_1^1, J_x\right] = -\frac{1}{\sqrt{2}}\left(\left[V_x, J_x\right] + i\left[V_y, J_x\right]\right) \tag{28}$$
$$= -\frac{1}{\sqrt{2}}\left(0 + \hbar V_z\right) \tag{29}$$
$$= -\hbar\frac{V_z}{\sqrt{2}} \tag{30}$$
$$\left[T_1^1, J_y\right] = -\frac{1}{\sqrt{2}}\left(\left[V_x, J_y\right] + i\left[V_y, J_y\right]\right) \tag{31}$$
$$= -\frac{1}{\sqrt{2}}\left(i\hbar V_z + 0\right) \tag{32}$$
$$= -i\hbar\frac{V_z}{\sqrt{2}} \tag{33}$$

Combining these results, we have

$$\left[T_1^1, J_+\right] = \left[T_1^1, J_x\right] + i\left[T_1^1, J_y\right] \tag{34}$$
$$= -\hbar\frac{V_z}{\sqrt{2}} + \hbar\frac{V_z}{\sqrt{2}} \tag{35}$$
$$= 0 \tag{36}$$

This agrees with 24 with $k = q = 1$.
We also have

$$\left[T_1^1, J_-\right] = \left[T_1^1, J_x\right] - i\left[T_1^1, J_y\right] \tag{37}$$
$$= -\hbar\frac{V_z}{\sqrt{2}} - \hbar\frac{V_z}{\sqrt{2}} \tag{38}$$
$$= -\sqrt{2}\hbar V_z \tag{39}$$
$$= -\sqrt{2}\hbar T_1^0 \tag{40}$$

This also agrees with 24 with $k = q = 1$ (since $\left[T_1^1, J_-\right] = -\left[J_-, T_1^1\right]$).
We can do similar calculations to find that

$$\left[T_1^{-1}, J_+\right] = -\sqrt{2}\hbar T_1^0 \tag{41}$$
$$\left[T_1^{-1}, J_-\right] = 0 \tag{42}$$

Finally, we have

$$\left[T_1^1, J_z\right] = -\frac{1}{\sqrt{2}}\left(\left[V_x, J_z\right] + i\left[V_y, J_z\right]\right) \tag{43}$$

$$= -\frac{1}{\sqrt{2}}\left(-i\hbar V_y - \hbar V_x\right) \tag{44}$$

$$= \frac{\hbar}{\sqrt{2}}\left(V_x + iV_y\right) \tag{45}$$

$$= -\hbar T_1^1 \tag{46}$$

$$\left[J_z, T_1^1\right] = \hbar T_1^1 \tag{47}$$

which is again consistent with 19 with $q = 1$. Similar calculations can be done to verify the other commutation relations.

PINGBACKS

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SPHERICAL TENSOR OPERATORS; A SCALAR OPERATOR

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To leave a comment or report an error, please use the auxiliary blog.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 15.3; Exercise 15.3.2.

Post date: 22 Oct 2017

A spherical tensor operator is defined by the way it transforms under rotation:

$$U\left[R\right]T_k^q U^\dagger\left[R\right] = \sum_{q'} D_{q'q}^{(k)} T_k^{q'} \tag{1}$$

where $D^{(k)}$ is the k-th block in the block diagonal matrix formed from the angular momentum operators J. We can form an operator Ω from two spherical tensor operators:

$$\Omega_k \equiv \sum_q (-1)^q S_k^q T_k^{-q} \tag{2}$$

For $k = 1$ we can write a spherical tensor operator in terms of a 3-d vector operator. We'll use lower-case letters to represent the vector operator, so we have

$$S_1^{\pm 1} = \mp \frac{s_x \pm i s_y}{\sqrt{2}} \tag{3}$$

$$S_1^0 = s_z \tag{4}$$

$$T_1^{\pm 1} = \mp \frac{t_x \pm i t_y}{\sqrt{2}} \tag{5}$$

$$T_1^0 = t_z \tag{6}$$

Plugging these into 2 with $k = 1$ we have

$$\Omega_1 = \frac{1}{2}\left(s_x + i s_y\right)\left(t_x - i t_y\right) + s_z t_z + \frac{1}{2}\left(s_x - i s_y\right)\left(t_x + i t_y\right) \tag{7}$$

$$= s_x t_x + s_y t_y + s_z t_z \tag{8}$$

$$= \mathbf{s} \cdot \mathbf{t} \tag{9}$$

Thus Ω_1 is the scalar product of the two vectors, and is therefore a scalar operator.

To prove this for any k, we can let $\mathbf{\Omega}_k$ operate on an angular momentum eigenket $|jm\rangle$ and then rotate this state, using 1. To simplify things, I'll write the unitary rotation operator $U[R]$ without the explicit R dependence, so it's just U.

$$U\mathbf{\Omega}_k|jm\rangle = U\sum_q (-1)^q S_k^q T_k^{-q}|jm\rangle \tag{10}$$

$$= \sum_q (-1)^q U S_k^q U^\dagger U T_k^{-q} U^\dagger U|jm\rangle \tag{11}$$

$$= \sum_{q,a,b,c} (-1)^q D_{aq}^{(k)} S_k^a D_{-b,-q}^{(k)} T_k^{-b} D_{cm}^{(j)}|jc\rangle \tag{12}$$

Each of the lower indices in $D_{m,m'}^{(k)}$ can take values $-k,\ldots,+k$, so a sum over m is the same as a sum over $-m$. That is

$$UT_k^{-q}U^\dagger = \sum_b D_{b,-q}^{(k)} T_k^b = \sum_b D_{-b,-q}^{(k)} T_k^{-b} \tag{13}$$

We can now use Shankar's hint (which I tried to prove, but couldn't, although it's probably something simple):

$$D_{-b,-q}^{(k)} = (-1)^{b-q}\left(D_{bq}^{(k)}\right)^* \tag{14}$$

Using this, we have

$$U\mathbf{\Omega}_k|jm\rangle = \sum_{q,a,b,c} (-1)^q D_{aq}^{(k)} S_k^a (-1)^{b-q}\left(D_{bq}^{(k)}\right)^* T_k^{-b} D_{cm}^{(j)}|jc\rangle \tag{15}$$

$$= \sum_{a,b,c}\sum_q \left[D_{aq}^{(k)}\left(D_{bq}^{(k)}\right)^*\right](-1)^b S_k^a T_k^{-b} D_{cm}^{(j)}|jc\rangle \tag{16}$$

Because $D_{aq}^{(k)}$ is a unitary matrix (it's the matrix elements of the unitary rotation operator $D_{aq}^{(k)} = \langle ka|U[R]|kq\rangle$) its rows are orthonormal (see Shankar, Theorem 8 in chapter 1), so the sum over q is

$$\sum_q D_{aq}^{(k)}\left(D_{bq}^{(k)}\right)^* = \delta_{ab} \tag{17}$$

Therefore, the rotated state is

$$U\mathbf{\Omega}_k \left|jm\right\rangle = \sum_{a,b,c} \delta_{ab} \left(-1\right)^b S_k^a T_k^{-b} D_{cm}^{(j)} \left|jc\right\rangle \tag{18}$$

$$= \left[\sum_b \left(-1\right)^b S_k^b T_k^{-b}\right] \left[\sum_c D_{cm}^{(j)} \left|jc\right\rangle\right] \tag{19}$$

$$= \mathbf{\Omega}_k U\left[R\right] \left|jm\right\rangle \tag{20}$$

In other words, the operator $\mathbf{\Omega}_k$ is unchanged by rotation, as the same operator operates on the rotated state $U\left[R\right]\left|jm\right\rangle$. Therefore, $\mathbf{\Omega}_k$ is a scalar for all k.

PINGBACKS

Pingback: Wigner-Eckart Theorem - examples

WIGNER-ECKART THEOREM - EXAMPLES

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Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 15.3; Exercise 15.3.3.

Post date: 25 Oct 2017

The Wigner-Eckart theorem says that for any spherical tensor operator T^q_1 we can write its matrix elements in the basis of angular momentum eigenstates $|\alpha lm\rangle$ as a product of two factors:

$$\left\langle \alpha_2 j_2 m_2 \left| T^q_k \right| \alpha_1 j_1 m_1 \right\rangle = \left\langle \alpha_2 j_2 \left|\left| T_k \right|\right| \alpha_1 j_1 \right\rangle \left\langle j_2 m_2 \left| k q, j_1 m_1 \right. \right\rangle \tag{1}$$

where the first factor on the RHS is the reduced matrix element, and is independent of m_1, m_2 and the tensor index q. Our earlier example went through the calculation for the position operator R^q_1, and this involved integrals over spatial coordinates. The theorem also applies to cases where the matrix elements depend only on angular momentum parameters.

First, we'll look at the rank-1 tensor J^q_1 which represents total angular momentum. The tensor components are

$$J^{\pm 1}_1 = \mp \frac{J_x \pm i J_y}{\sqrt{2}} = \mp \frac{J_\pm}{\sqrt{2}} \tag{2}$$

$$J^0_1 = J_z \tag{3}$$

where $J_\pm$ are the usual raising and lowering operators.

According to 1, we can write the matrix elements as

$$\left\langle \alpha_2 j_2 m_2 \left| J^q_1 \right| \alpha_1 j_1 m_1 \right\rangle = \left\langle \alpha_2 j_2 \left|\left| J_1 \right|\right| \alpha_1 j_1 \right\rangle \left\langle j_2 m_2 \left| 1 q, j_1 m_1 \right. \right\rangle \tag{4}$$

Since the factor $\left\langle \alpha_2 l_2 \left|\left| J_1 \right|\right| \alpha_1 l_1 \right\rangle$ does not depend on q, the equation must be true for the case $q = 0$, so the LHS becomes

$$\left\langle \alpha_2 j_2 m_2 \left| J^0_1 \right| \alpha_1 j_1 m_1 \right\rangle = \left\langle \alpha_2 j_2 m_2 \left| J_z \right| \alpha_1 j_1 m_1 \right\rangle \tag{5}$$

$$= m_1 \hbar \left\langle \alpha_2 j_2 m_2 \left| \alpha_1 j_1 m_1 \right. \right\rangle \tag{6}$$

$$= m_1 \hbar \delta_{\alpha_2 \alpha_1} \delta_{j_2 j_1} \delta_{m_2 m_1} \tag{7}$$

where the δs arise because the kets are orthonormal. Now suppose that we take $m_1 = m_2 = j_1 = j$, and we use the hint given by Shankar that

$$\langle jj\,|jj,10\rangle = \sqrt{\frac{j}{j+1}} \tag{8}$$

Then, from 4 we have

$$\langle \alpha_2 j_2 \,||J_1||\, \alpha_1 j_1\rangle = \frac{\left\langle \alpha_2 j_2 j \left| J_1^0 \right| \alpha_1 j j\right\rangle}{\langle jj\,|jj,10\rangle} \tag{9}$$

$$= \hbar j \delta_{\alpha_2\alpha_1}\delta_{j_2 j}\sqrt{\frac{j+1}{j}} \tag{10}$$

$$= \sqrt{j\,(j+1)}\hbar\delta_{\alpha_2\alpha_1}\delta_{j_2 j} \tag{11}$$

Now suppose we consider a more general case where the tensor operator is $\mathbf{J}\cdot\mathbf{A}$, where $\mathbf{A}$ is some arbitrary vector. We've seen earlier that the scalar product of two vectors can be written as

$$\mathbf{J}\cdot\mathbf{A} = \sum_{q=\pm 1,0} (-1)^q J_1^q A_1^{-q} \tag{12}$$

where the tensors in the sum on the RHS are formed the same way as in 2. Writing out this sum gives the hint in Shankar's question, which is that we can write the scalar product as

$$\mathbf{J}\cdot\mathbf{A} = J_z A_z + \frac{1}{2}\left(J_- A_+ + J_+ A_-\right) \tag{13}$$

In what follows, we'll also need the fact that

$$J_\pm^\dagger = J_\mp \tag{14}$$

$$J_z^\dagger = J_z \tag{15}$$

and that

$$J_\pm\,|\alpha,j,m\rangle = \hbar\sqrt{(j\mp m)\,(j\pm m+1)}\,|\alpha,j,m\pm 1\rangle \tag{16}$$

Now let's take the matrix element of $\mathbf{J}\cdot\mathbf{A}$, although this time things are made a bit easier since we take $j_2 = j_1 = j$, so the total angular momentum is the same in all matrix elements. We have

$$\left\langle \alpha' jm' \left| \mathbf{J}\cdot\mathbf{A} \right| \alpha jm \right\rangle = \left\langle \alpha' jm' \left| J_z A_z \right| \alpha jm \right\rangle + \tag{17}$$

$$\frac{1}{2}\left(\left\langle \alpha' jm' \left| J_- A_+ \right| \alpha jm \right\rangle + \left\langle \alpha' jm' \left| J_+ A_- \right| \alpha jm \right\rangle \right) \tag{18}$$

$$= \left\langle J_z \alpha' jm' \left| A_z \right| \alpha jm \right\rangle + \tag{19}$$

$$\frac{1}{2}\left(\left\langle J_+ \alpha' jm' \left| A_+ \right| \alpha jm \right\rangle + \left\langle J_- \alpha' jm' \left| A_- \right| \alpha jm \right\rangle \right) \tag{20}$$

$$= m'\hbar \left\langle \alpha' jm' \left| A_z \right| \alpha jm \right\rangle + \tag{21}$$

$$\frac{\hbar}{2}\left(\sqrt{(j-m')(j+m'+1)} \left\langle \alpha' j, m'+1 \left| A_+ \right| \alpha jm \right\rangle + \right. \tag{22}$$

$$\left. \sqrt{(j+m')(j-m'+1)} \left\langle \alpha' j, m'-1 \left| A_- \right| \alpha jm \right\rangle \right) \tag{23}$$

From 2, we have that $A_+ = -\sqrt{2}A_1^1$, $A_- = \sqrt{2}A_1^{-1}$ and $A_z = A_1^0$, so we have

$$\left\langle \alpha' jm' \left| \mathbf{J}\cdot\mathbf{A} \right| \alpha jm \right\rangle = m'\hbar \left\langle \alpha' jm' \left| A_1^0 \right| \alpha jm \right\rangle + \tag{24}$$

$$\frac{\hbar}{\sqrt{2}}\left(-\sqrt{(j-m')(j+m'+1)} \left\langle \alpha' j, m'+1 \left| A_1^1 \right| \alpha jm \right\rangle + \right. \tag{25}$$

$$\left. \sqrt{(j+m')(j-m'+1)} \left\langle \alpha' j, m'-1 \left| A_1^{-1} \right| \alpha jm \right\rangle \right) \tag{26}$$

However, from 1 we know that

$$\left\langle \alpha' jm' \left| A_1^q \right| \alpha jm \right\rangle = \left\langle \alpha' j \left|\left| A_1 \right|\right| \alpha j \right\rangle \left\langle jm' \left| 1q, jm \right. \right\rangle \tag{27}$$

where the first factor is the same for all q. Therefore, we can write 24 as

$$\left\langle \alpha' jm' \left| \mathbf{J}\cdot\mathbf{A} \right| \alpha jm \right\rangle = c \left\langle \alpha' j \left|\left| A_1 \right|\right| \alpha j \right\rangle \tag{28}$$

where

$$c = m'\hbar \left\langle jm' \right| 10, jm \left\rangle + \right. \tag{29}$$

$$\frac{\hbar}{\sqrt{2}} \left(\sqrt{(j+m')(j-m'+1)} \left\langle j, m'-1 \right| 1, -1, jm \left\rangle - \right. \right. \tag{30}$$

$$\left. \sqrt{(j-m')(j+m'+1)} \left\langle j, m'+1 \right| 11, jm \left\rangle \right. \right) \tag{31}$$

which is independent of α and α'.

To work out c explicitly, we need to find the bracket terms in its expression. We can do this by going back to 9 with $j_1 = j_2 = j$. We have

$$\left\langle jm' \left| J_1^q \right| jm \right\rangle = \left\langle j \left|\left| J_1 \right|\right| j \right\rangle \left\langle jm' \right| 1q, jm \left\rangle \right. \tag{32}$$

From 11 we have

$$\left\langle jm' \right| 1q, jm \left\rangle = \frac{\left\langle jm' \left| J_1^q \right| jm \right\rangle}{\hbar\sqrt{j(j+1)}} \right. \tag{33}$$

We can work out the matrix elements $\left\langle jm' \left| J_1^q \right| jm \right\rangle$ by using 2 and the raising and lowering operators. We get

$$\left\langle jm' \left| 10, jm \right.\right\rangle = \frac{\langle jm' | J_z | jm \rangle}{\hbar\sqrt{j\,(j+1)}} \tag{34}$$

$$= \frac{m\hbar}{\hbar} \frac{\langle jm' | jm \rangle}{\sqrt{j\,(j+1)}} \tag{35}$$

$$= \frac{m}{\sqrt{j\,(j+1)}} \delta_{mm'} \tag{36}$$

$$\left\langle j, m'-1 \left| 1-1, jm \right.\right\rangle = \frac{1}{\sqrt{2}} \frac{\langle j, m'-1 | J_- | jm \rangle}{\hbar\sqrt{j\,(j+1)}} \tag{37}$$

$$= \frac{1}{\sqrt{2}} \frac{\langle J_+ j, m'-1 | jm \rangle}{\hbar\sqrt{j\,(j+1)}} \tag{38}$$

$$= \frac{\sqrt{(j-m'+1)\,(j+m')}}{\sqrt{2}\sqrt{j\,(j+1)}} \left\langle jm' \left| jm \right.\right\rangle \tag{39}$$

$$= \frac{\sqrt{(j-m+1)\,(j+m)}}{\sqrt{2}\sqrt{j\,(j+1)}} \delta_{mm'} \tag{40}$$

$$\left\langle j, m'+1 \left| 11, jm \right.\right\rangle = -\frac{1}{\sqrt{2}} \frac{\langle j, m'+1 | J_+ | jm \rangle}{\hbar\sqrt{j\,(j+1)}} \tag{41}$$

$$= -\frac{1}{\sqrt{2}} \frac{\langle J_- j, m'+1 | jm \rangle}{\hbar\sqrt{j\,(j+1)}} \tag{42}$$

$$= -\frac{\sqrt{(j+m'+1)\,(j-m')}}{\sqrt{2}\sqrt{j\,(j+1)}} \left\langle jm' \left| jm \right.\right\rangle \tag{43}$$

$$= -\frac{\sqrt{(j+m+1)\,(j-m)}}{\sqrt{2}\sqrt{j\,(j+1)}} \delta_{mm'} \tag{44}$$

Putting everything together, we have

$$c = \frac{\hbar\delta_{mm'}}{\sqrt{j\,(j+1)}} \left[m^2 + \frac{1}{2}\,(j-m+1)\,(j+m) + \frac{1}{2}\,(j+m+1)\,(j-m) \right] \tag{45}$$

$$= \frac{\hbar\delta_{mm'}}{\sqrt{j\,(j+1)}} \left(j^2 + j \right) \tag{46}$$

$$= \hbar\sqrt{j\,(j+1)}\delta_{mm'} \tag{47}$$

We can combine these results to get an expression for the matrix elements of A^q_1. From 27, 28, 33 and 47 we have

$$\left\langle \alpha' jm' \left| A_1^q \right| \alpha jm \right\rangle = \left\langle \alpha' j \left|\left| A_1 \right|\right| \alpha j \right\rangle \left\langle jm' \left| 1q, jm \right. \right\rangle \tag{48}$$

$$= \frac{1}{c} \left\langle \alpha' jm' \left| \mathbf{J} \cdot \mathbf{A} \right| \alpha jm \right\rangle \left\langle jm' \left| 1q, jm \right. \right\rangle \tag{49}$$

$$= \frac{\left\langle \alpha' jm' \left| \mathbf{J} \cdot \mathbf{A} \right| \alpha jm \right\rangle}{\hbar^2 j \left(j+1 \right)} \left\langle jm' \left| J_1^q \right| jm \right\rangle \tag{50}$$

PINGBACKS

Pingback: Wigner-Eckart Theorem - adding orbital and spin angular momenta

WIGNER-ECKART THEOREM - ADDING ORBITAL AND SPIN ANGULAR MOMENTA

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 15.3; Exercise 15.3.4 - 15.3.5.

Post date: 28 Oct 2017

The Wigner-Eckart theorem says that for any spherical tensor operator T_1^q we can write its matrix elements in the basis of angular momentum eigenstates $|\alpha lm\rangle$ as a product of two factors:

$$\left\langle \alpha_2 j_2 m_2 \left| T_k^q \right| \alpha_1 j_1 m_1 \right\rangle = \left\langle \alpha_2 j_2 \left|| T_k \right|| \alpha_1 j_1 \right\rangle \left\langle j_2 m_2 \left| k q, j_1 m_1 \right. \right\rangle \tag{1}$$

where the first factor on the RHS is the reduced matrix element, and is independent of m_1, m_2 and the tensor index q.

We can apply this to the case where we have a particle such as a proton or electron with both orbital and spin angular momentum. Such a particle has a magnetic moment

$$\boldsymbol{\mu} = \gamma_1 \mathbf{J}_1 + \gamma_2 \mathbf{J}_2 \tag{2}$$

Here γ_i are the gyromagnetic ratios for the two angular momenta. Suppose we want to find $\langle \boldsymbol{\mu} \rangle$ for a particle in a state $|jm, j_1 j_2\rangle$, where this ket represents a state with the two component momenta j_1 and j_2 and total angular momentum j with z component m. [This is different from the notation that Shankar uses in most of Chapter 15, where $|j_1 m_1, j_2 m_2\rangle$ represents a state with the two components j_1 and j_2 and their corresponding z components.] We can use the formula derived earlier

$$\left\langle \alpha' j m' \left| A_1^q \right| \alpha j m \right\rangle = \frac{\left\langle \alpha' j m' \left| \mathbf{J} \cdot \mathbf{A} \right| \alpha j m \right\rangle}{\hbar^2 j\,(j+1)} \left\langle j m' \left| J_1^q \right| j m \right\rangle \tag{3}$$

We can work out 2 by applying this formula to each momentum component separately. As we're concerned only with angular momentum we can omit α (since it represents other parameters) and set $m' = m$. The notation can be a bit confusing, since in this problem, the subscript 1 or 2 represents a label for a particular angular momentum and not the rank of a tensor. With $\mathbf{A} = \mathbf{J}_1$ we have

$$\langle jm, j_1 j_2 | J_{1i} | jm, j_1 j_2 \rangle = \frac{\langle jm, j_1 j_2 | \mathbf{J} \cdot \mathbf{J}_1 | jm, j_1 j_2 \rangle}{\hbar^2 j (j+1)} \langle jm, j_1 j_2 | J_i | jm, j_1 j_2 \rangle \tag{4}$$

The subscript i represents the component x, y or z. We can workout the middle matrix element using

$$\mathbf{J} \cdot \mathbf{J}_1 = J_1^2 + \mathbf{J}_2 \cdot \mathbf{J}_1 \tag{5}$$

$$= J_1^2 + \frac{1}{2}\left(J^2 - J_1^2 - J_2^2\right) \tag{6}$$

$$= \frac{1}{2}\left(J^2 + J_1^2 - J_2^2\right) \tag{7}$$

Therefore

$$\langle jm, j_1 j_2 | \mathbf{J} \cdot \mathbf{J}_1 | jm, j_1 j_2 \rangle = \frac{\hbar^2}{2}\left(j (j+1) + j_1 (j_1+1) - j_2 (j_2+1)\right) \tag{8}$$

Applying the same calculation for $\mathbf{J} \cdot \mathbf{J}_2$ we have

$$\langle jm, j_1 j_2 | \mathbf{J} \cdot \mathbf{J}_2 | jm, j_1 j_2 \rangle = \frac{\hbar^2}{2}\left(j (j+1) + j_2 (j_2+1) - j_1 (j_1+1)\right) \tag{9}$$

We also have

$$\langle jm, j_1 j_2 | J_z | jm, j_1 j_2 \rangle = m\hbar \tag{10}$$

From the raising and lowering operators we have

$$J_x = \frac{1}{2}\left(J_+ + J_-\right) \tag{11}$$

$$J_y = \frac{1}{2i}\left(J_+ - J_-\right) \tag{12}$$

Because kets with different m values are orthogonal and $J_\pm$ raises or lowers the m value, we have

$$\langle jm, j_1 j_2 | J_\pm | jm, j_1 j_2 \rangle = 0 \tag{13}$$

Therefore

$$\langle jm, j_1 j_2 | J_{x,y} | jm, j_1 j_2 \rangle = 0 \tag{14}$$

Putting these into 2 gives

$$\langle \mu_x \rangle = \langle \mu_y \rangle = 0 \tag{15}$$

$$\langle \mu_z \rangle = \frac{\hbar^2}{2\hbar^2 j\left(j+1\right)} \left[\gamma_1 \left(j\left(j+1\right) + j_1\left(j_1+1\right) - j_2\left(j_2+1\right)\right) + \right. \tag{16}$$

$$\left. \gamma_2 \left(j\left(j+1\right) + j_2\left(j_2+1\right) - j_1\left(j_1+1\right)\right)\right] \hbar m \tag{17}$$

$$= \frac{\hbar m}{2} \left[\gamma_1 + \gamma_2 + \left(\gamma_1 - \gamma_2\right) \frac{j_1\left(j_1+1\right) - j_2\left(j_2+1\right)}{j\left(j+1\right)}\right] \tag{18}$$

For a proton in the state ${}^2P_{1/2}$, the orbital angular momentum is $j_1 = 1$ (from the P), the spin is $j_2 = \frac{1}{2}$ (from $2S+1=2$) and the total angular momentum is $j = \frac{1}{2}$ (from the subscript). The orbital gyromagnetic ratio is (Shankar, eqn 14.4.7)

$$\gamma_1 = \frac{e}{2Mc} \tag{19}$$

The spin gyromagnetic ratio is (Shankar, p. 391):

$$\gamma_2 = 5.6 \frac{e}{2Mc} \tag{20}$$

Plugging these into 18 we get

$$\langle \mu_z \rangle = 0.53 m \frac{e\hbar}{2Mc} \tag{21}$$

The z component of total angular momentum can take values of $\pm\frac{1}{2}$ for $j = \frac{1}{2}$, so we have

$$\langle \mu_z \rangle = \pm 0.267 \frac{e\hbar}{2Mc} \tag{22}$$

where $\frac{e\hbar}{2Mc}$ is the nuclear Bohr magneton.

For an electron in the state ${}^2P_{1/2}$ everything is the same except that the spin gyromagnetic ratios are

$$\gamma_1 = -\frac{e}{2m_e c} \tag{23}$$

$$\gamma_2 = -\frac{e}{m_e c} \tag{24}$$

Plugging these into 18 gives

$$\langle \mu_z \rangle = \pm \frac{1}{3} \frac{e\hbar}{2m_e c} \tag{25}$$

where $\frac{e\hbar}{2m_e c}$ is electron Bohr magneton.

Finally, we can note a condition of the matrix elements of a general spherical tensor T_k^q, which we can see from 1. If $j_1 = j_2 = j$ and $m_1 = m_2 = m$ we have (disregarding α):

$$\left\langle jm \left| T_k^q \right| jm \right\rangle = \langle j \, || T_k || \, j \rangle \, \langle jm \, | kq, jm \rangle \tag{26}$$

The factor $\langle jm \, | kq, jm \rangle$ is a Clebsch-Gordan coefficient (up to a numerical factor), which means that it must be possible to form the angular momentum in the bra by adding the two angular momenta in the ket. This gives the condition that

$$|k - j| \leq j \leq k + j \tag{27}$$

If $k > j$ this gives the condition

$$0 \leq k \leq 2j \tag{28}$$

Any values of $k > 2j$ give a zero Clebsch-Gordan coefficient, so $\left\langle jm \left| T_k^q \right| jm \right\rangle = 0$ for $k > 2j$.

VARIATIONAL PRINCIPLE AND THE HARMONIC OSCILLATOR

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 16.1; Exercise 16.1.1.

Post date: 30 Oct 2017

We've covered the variational principle before while studying Griffiths's book, but Shankar provides a few new examples which are worth going through. In this example, we look at the harmonic oscillator and use the trial function

$$\psi = Ae^{-\alpha x^2} \tag{1}$$

where A is the normalization constant and α is the parameter to be varied in an attempt to get the best estimate for the ground state energy. [Of course, we already know that the exact ground state wave function has this form, so this exercise can be viewed more as a demonstration that the variational principle can give the exact answer if the right form of trial function is used.]

First we find A from the condition

$$\int_{-\infty}^{\infty} \psi^2 dx = A^2 \int_{-\infty}^{\infty} e^{-2\alpha x^2} dx = 1 \tag{2}$$

This is a standard Gaussian integral, but I've used Maple to do the integrals here. We have

$$\int_{-\infty}^{\infty} e^{-2\alpha x^2} dx = \sqrt{\frac{\pi}{2\alpha}} \tag{3}$$

so

$$A = \left(\frac{2\alpha}{\pi}\right)^{1/4} \tag{4}$$

We can now apply the variational principle. We must find

$$\langle \psi | H | \psi \rangle = \sqrt{\frac{2\alpha}{\pi}} \int_{-\infty}^{\infty} e^{-\alpha x^2} \left(-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + \frac{1}{2} m\omega^2 x^2 e^{-\alpha x^2} \right) dx \tag{5}$$

The first term in the integrand is

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = -\frac{\hbar^2\alpha}{m}\left(2\alpha x^2 - 1\right)e^{-\alpha x^2} \tag{6}$$

Thus

$$\langle E\rangle = \langle\psi|H|\psi\rangle = \sqrt{\frac{2\alpha}{\pi}}\int_{-\infty}^{\infty} e^{-2\alpha x^2}\left[-\frac{\hbar^2\alpha}{m}\left(2\alpha x^2-1\right)+\frac{1}{2}m\omega^2x^2\right]dx \tag{7}$$

$$= \sqrt{\frac{2\alpha}{\pi}}\left[\left(\frac{1}{2}m\omega^2 - \frac{2\hbar^2\alpha^2}{m}\right)\int_{-\infty}^{\infty} x^2e^{-2\alpha x^2}dx + \right. \tag{8}$$

$$\left.\frac{\hbar^2\alpha}{m}\int_{-\infty}^{\infty} e^{-2\alpha x^2}dx\right] \tag{9}$$

$$= \frac{\hbar^2\alpha}{2m} + \frac{m\omega^2}{8\alpha} \tag{10}$$

where I used Maple to do the integrals and simplify the result to get the last line. If you want to do them by hand, the two integrals are standard Gaussian integrals so you should be able to do them by looking them up in tables.

We now find the optimum value of α by differentiating:

$$\frac{d\langle E\rangle}{d\alpha} = \frac{\hbar^2}{2m} - \frac{m\omega^2}{8\alpha^2} = 0 \tag{11}$$

Solving, we find

$$\alpha_0 = \frac{m\omega}{2\hbar} \tag{12}$$

(There is also a negative root, but we know $\alpha > 0$ to prevent the wave function blowing up at infinity.)

Substituting into 10 we get the energy as

$$E_0 = \frac{1}{2}\hbar\omega \tag{13}$$

which is the exact ground state energy.

VARIATIONAL PRINCIPLE AND THE INFINITE SQUARE WELL

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 16.1; Exercise 16.1.2.

Post date: 31 Oct 2017

Although we're looking at the variational principle, the example in this post isn't technically an application of this, as there isn't anything to vary. However, the idea behind the variational principle is that if we take *any* wave function ψ then, for a given Hamiltonian H, the ground state energy E_0 is bounded by

$$E_0 \leq \frac{\langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle} \tag{1}$$

Given this, then we don't need to vary a parameter in the wave function in order to get an upper bound on the ground state energy. As an example, suppose we look at the infinite square well. The exercise in Shankar uses the square well centred on the origin, so that

$$V(x) = \begin{cases} 0 & -a < x < a \\ \infty & \text{otherwise} \end{cases} \tag{2}$$

We know that the exact normalized ground state wave function is

$$\psi_1(x) = \frac{1}{\sqrt{a}} \cos\left(\frac{\pi x}{2a}\right) \tag{3}$$

and the corresponding ground state energy is

$$E_1 = \frac{\pi^2 \hbar^2}{8ma^2} \tag{4}$$

Suppose we didn't know this, but guessed that the wave function was peaked at $x = 0$ and went to 0 at $x = \pm a$. We might then try a parabolic function such as

$$\psi = (x + a)(x - a) = x^2 - a^2 \tag{5}$$

Although ψ actually has a minimum at $x = 0$, we could convert it into a function with a maximum at $x = 0$ by taking the negative, which amounts

to multiplying by a phase factor of $e^{i\pi}$, so has no effect on physical measurements.

In this case, 1 gives us

$$\langle \psi | \psi \rangle = \int_{-a}^{a} \left(x^2 - a^2\right)^2 dx \tag{6}$$

$$= \frac{16}{15} a^5 \tag{7}$$

$$\langle \psi | H | \psi \rangle = -\frac{\hbar^2}{2m} \int_{-a}^{a} \left(x^2 - a^2\right) \frac{d^2}{dx^2} \left(x^2 - a^2\right) dx \tag{8}$$

$$= -\frac{\hbar^2}{m} \int_{-a}^{a} \left(x^2 - a^2\right) dx \tag{9}$$

$$= \frac{4\hbar^2 a^3}{3m} \tag{10}$$

The ground state energy estimate is then

$$E_{1,est} \leq \frac{5\hbar^2}{4ma^2} \tag{11}$$

Comparing with the exact answer 4 we see that

$$\frac{E_{1,est}}{E_1} = \frac{10}{\pi^2} \approx 1.013 \tag{12}$$

Thus the estimate of E_1 using this parabolic wave function is actually not too bad.

The fact that $\frac{d^2\psi}{dx^2}$ is discontinuous at the boundaries $x = \pm a$ doesn't affect the energy since $\psi = 0$ at the boundaries, so the particle is never found there.

VARIATIONAL PRINCIPLE AND THE DELTA FUNCTION WELL

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 16.1; Exercise 16.1.3.

Post date: 2 Nov 2017

Here we'll apply the variational principle to the delta function well, with potential

$$V = -aV_0\delta(x) \tag{1}$$

where a and V_0 are positive constants. As we've seen earlier, there is a single bound state with energy

$$E = -\frac{ma^2V_0^2}{2\hbar^2} \tag{2}$$

[In the earlier treatment, based on Griffiths's book, $V = -\alpha\delta(x)$ for a positive constant α.] The exact wave function has a discontinuous derivatve at $x = 0$, and decays exponentially on both sides of $x = 0$. To apply the variational principle, we'll use a Gaussian as a trial function, so that

$$\psi(x) = Ae^{-bx^2} \tag{3}$$

for some constants A and b. From normalization, we can find A:

$$\int_{-\infty}^{\infty}\psi^2 dx = A^2\int_{-\infty}^{\infty}e^{-2bx^2}dx = 1 \tag{4}$$

Evaluating the Gaussian integral we have

$$\int_{-\infty}^{\infty}e^{-2bx^2}dx = \sqrt{\frac{\pi}{2b}} \tag{5}$$

This gives

$$A = \left(\frac{2b}{\pi}\right)^{1/4} \tag{6}$$

To apply the variational principle, we need to work out the integral

$$\langle\psi|H|\psi\rangle = \sqrt{\frac{2b}{\pi}}\int_{-\infty}^{\infty} e^{-bx^2}\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} - aV_0\delta(x)\right)e^{-bx^2}dx \tag{7}$$

We calculate the derivative:

$$\frac{d^2}{dx^2}e^{-bx^2} = 2b\left(2bx^2-1\right)e^{-bx^2} \tag{8}$$

We therefore have (using Maple to integrate the first term; the delta function integral is easy)

$$\langle H\rangle = \langle\psi|H|\psi\rangle = \frac{\hbar^2}{2m}b - a\sqrt{\frac{2b}{\pi}}V_0 \tag{9}$$

We now want the value of b that minimizes the energy, so we take the derivative

$$\frac{d\langle H\rangle}{db} = \frac{\hbar^2}{2m} - \frac{aV_0}{\sqrt{2\pi}}b^{-1/2} = 0 \tag{10}$$

$$b_0 = \frac{2a^2V_0^2m^2}{\pi\hbar^4} \tag{11}$$

Substituting $b = b_0$ into 9 we get

$$E_0 = -\frac{ma^2V_0^2}{\pi\hbar^2} \tag{12}$$

Comparing this with 2 we see that the variational estimate is

$$E = \frac{\pi}{2}E_0 \approx 1.57E_0 \tag{13}$$

Note that E_0 still provides an *upper* bound on E since the energy is negative. In this case, the Gaussian estimate isn't that good.

VARIATIONAL PRINCIPLE AND THE HARMONIC OSCILLATOR (QUARTIC WAVE FUNCTION)

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To leave a comment or report an error, please use the auxiliary blog.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 16.1; Exercise 16.1.4.

Post date: 3 Nov 2017

Here we'll apply the variational principle again to the harmonic oscillator, this time with potential

$$\psi(x) = \begin{cases} (x-a)^2(x+a)^2 & x \leq |a| \\ 0 & |x| > a \end{cases} \tag{1}$$

Here a is the parameter to be varied, and we can see that it controls the width of the trial wave function as well as its height. We first find the normalization constant

$$N \equiv \langle \psi | \psi \rangle = \int_{-a}^{a} (x-a)^4 (x+a)^4 \, dx \tag{2}$$

$$= \frac{256}{315} a^9 \tag{3}$$

where I used Maple to do and simplify the integral. If you want to do it by hand, it's probably easiest to use the substitution $u = x - a$ before multiplying out the factors in the integrand.

The energy estimate is then obtained by minimizing

$$E = \frac{\langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle} \tag{4}$$

where the Hamiltonian contains the harmonic oscillator potential:

$$H = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2} m\omega^2 x^2 \tag{5}$$

To calculate $\langle \psi | H | \psi \rangle$ requires integrating a sixth-degree polynomial which is straightforward but very tedious to do by hand if you like (which is probably why the exercise is marked as 'optional' in Shankar), but again I used Maple to get

$$\frac{d^2\psi}{dx^2} = 12x^2 - 4a^2 \tag{6}$$

$$\langle\psi|H|\psi\rangle = \int_{-a}^{a} (x-a)^2 (x+a)^2 \left[-\frac{\hbar^2}{2m}\left(12x^2 - 4a^2\right) + \right. \tag{7}$$

$$\left. \frac{1}{2} m\omega^2 x^2 (x-a)^2 (x+a)^2 \right] dx \tag{8}$$

$$= \frac{128}{3465}\left(a^{11} m\omega^2 + 33\frac{\hbar^2 a^7}{m}\right) \tag{9}$$

The expression to minimize is therefore

$$E = \frac{128}{3465}\left(a^{11} m\omega^2 + 33\frac{\hbar^2 a^7}{m}\right) \times \frac{315}{256a^9} \tag{10}$$

$$= \frac{1}{22}\left(a^2 m\omega^2 + \frac{33\hbar^2}{m} a^{-2}\right) \tag{11}$$

Taking the derivative, we need to solve

$$\frac{dE}{da} = \frac{1}{11}\left(am\omega^2 - \frac{33\hbar^2}{m} a^{-3}\right) = 0 \tag{12}$$

This gives an optimum value for a:

$$a_0 = 33^{1/4}\sqrt{\frac{\hbar}{m\omega}} \tag{13}$$

Substituting into 11 we get the estimate of the ground state energy

$$E_0 = \frac{\sqrt{33}}{11}\hbar\omega \simeq 0.522\hbar\omega \tag{14}$$

The exact ground state energy for the harmonic oscillator is $\frac{1}{2}\hbar\omega$ so this estimate is reasonably good.

This answer agrees with the back-of-the-book answer in Shankar, since

$$\frac{\sqrt{33}}{11} = \frac{1}{2}\frac{\sqrt{4\times 33}}{11} = \frac{1}{2}\frac{\sqrt{12\times 11}}{11} = \frac{1}{2}\sqrt{\frac{12}{11}} \tag{15}$$

VARIATIONAL PRINCIPLE AND L=1 STATES OF THE HYDROGEN ATOM

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To leave a comment or report an error, please use the auxiliary blog.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 16.1; Exercise 16.1.5.

Post date: 6 Nov 2017

Here we'll apply the variational principle to the hydrogen atom. In the problem, Shankar asks us to look at the $l = 1$ states but does not specify the principal quantum number n, so I'll assume he wants us to solve the problem for the lowest value of n for which we can have an $l = 1$ state, which is $n = 2$.

To review, the wave function for hydrogen is given as

$$\begin{aligned}
\psi_{nlm}(r,\theta,\phi) &= R_{nl}(r)\,Y_l^m(\theta,\phi) && (1)\\
u_{nl}(\rho) &= \rho^{l+1}e^{-\rho}v_{nl}(\rho) && (2)\\
u_{nl}(r) &\equiv rR_{nl}(r) && (3)\\
\rho &= \kappa r && (4)\\
\rho_0 &= \frac{me^2}{2\pi\epsilon_0\hbar^2\kappa} && (5)\\
\kappa &= \frac{\sqrt{-2mE}}{\hbar} && (6)
\end{aligned}$$

The solution was expressed as a series:

$$v_{nl}(\rho) = \sum_{j=0}^{\infty} c_j\rho^j \tag{7}$$

with the coefficients c_j satisfying a recursion relation:

$$c_{j+1} = \frac{2(j+l+1)-\rho_0}{(j+1)(j+2(l+1))}c_j \tag{8}$$

To keep the wave function finite as $r \to \infty$, the series for v_{nl} must terminate, which gives rise to the quantization condition $n = j + l + 1$. If we specify n and l, then we get the maximum value of $j_{max} = n - l - 1$ that appears in the series 7. If we take $n = 2$ and $l = 1$, then $j_{max} = 0$, which means that v_{21} is a constant. The wave function therefore has the form

$$\psi_{21m}(r,\theta,\phi) = R_{21}(r)\,Y_1^m(\theta,\phi) \tag{9}$$

$$= \frac{u_{21}(r)}{r} Y_1^m(\theta,\phi) \tag{10}$$

$$= Are^{-ar} Y_1^m(\theta,\phi) \tag{11}$$

for constants A (determined by normalization) and a. Since the quantum number m (for the z component of angular momentum) appears only in the form $e^{im\phi}$ in the spherical harmonic $Y_1^m(\theta,\phi)$, it will disappear when we calculate matrix elements.

The trial function given by 11 incorporates the required limiting behaviour of the wave function, since it behaves as r as $r \to 0$ and as e^{-ar} as $r \to \infty$. The number of nodes in the wave function is determined by the degree of the polynomial v_{nl} and since this is constant, there are no nodes. (If we wanted to solve the system for, say, $n = 3$ and $l = 1$, then $j_{max} = 1$ in 7 and we would have a single node.)

To apply the variational principle, we first need to find $\langle\psi|\psi\rangle$. Since the spherical harmonics are normalized already and are the only place where the angular variables occur, we can ignore them in what follows and just concentrate on the radial bits. Our trial function is therefore

$$R = Are^{-ar} \tag{12}$$

Therefore

$$\langle\psi|\psi\rangle = \int_0^\infty \left(Are^{-ar}\right)^2 r^2 dr \tag{13}$$

$$= \frac{3A^2}{4a^5} \tag{14}$$

where as usual I'm using Maple to do the integrals.

The function $R(r)$ satisfies the radial equation which is

$$-\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + \left(\frac{\hbar^2}{2m}\frac{l(l+1)}{r^2} + V(r)\right)R = ER \tag{15}$$

In our case, $l = 1$ and $V = -\frac{e^2}{r}$ so we have

$$-\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + \left(\frac{\hbar^2}{m}\frac{1}{r^2} - \frac{e^2}{r}\right)R = ER \tag{16}$$

If we call the operator on the LHS H_R then the matrix element is

$$\langle H_R \rangle = \langle R | H_R | R \rangle \tag{17}$$

The derivative term is (Maple again):

$$-\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) = -\frac{\hbar^2}{2m}A\frac{e^{-ar}}{r}\left(a^2r^2 - 4ar + 2\right) \tag{18}$$

Therefore (again, remember that the angular integral comes out to 1):

$$\langle \psi | H_R | \psi \rangle = A^2 \int_0^\infty re^{-ar}\left[-\frac{\hbar^2}{2m}\frac{e^{-ar}}{r}\left(a^2r^2 - 4ar + 2\right) + \right. \tag{19}$$

$$\left.\left(\frac{\hbar^2}{m}\frac{1}{r^2} - \frac{e^2}{r}\right)re^{-ar}\right]r^2dr \tag{20}$$

$$= \frac{3}{8}A^2\frac{a\hbar^2 - me^2}{ma^4} \tag{21}$$

Our estimate for the energy is therefore

$$\langle E \rangle = \frac{\langle \psi | H_R | \psi \rangle}{\langle \psi | \psi \rangle} \tag{22}$$

$$= \frac{\left(\hbar^2 a - me^2\right)a}{2m} \tag{23}$$

To find the bound on the energy, we take the derivative and solve

$$\frac{d\langle E \rangle}{da} = \frac{\hbar^2 a}{m} - \frac{e^2}{2} = 0 \tag{24}$$

$$a_0 = \frac{me^2}{2\hbar^2} \tag{25}$$

Plugging this back into 23 we find

$$E_0 \leq -\frac{me^4}{8\hbar^2} \tag{26}$$

This is, in fact, the exact answer for $n = 2$, which isn't terribly surprising, since our choice for the trial function is in fact the correct form of the exact equation.

DIRAC EQUATION: DERIVATION

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Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 20, Exercise 20.1.1.

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The Dirac equation arose out of the need for a quantum mechanical wave equation that treats position and time on an equal basis. The first attempt at such an equation resulted in the Klein-Gordon equation, in which both time and position occur as second derivatives. However, the wave function in this equation is a scalar, meaning that it does not incorporate spin, which requires the wave function to have at least two components (in the case of spin-$\frac{1}{2}$; more components for higher spin).

Dirac began with the relativistic equation for the energy of a particle, which is

$$E = \sqrt{p^2c^2 + m^2c^4} \tag{1}$$

where p is the momentum and m is the rest mass. The usual quantum mechanical prescription for converting the energy to an operator therefore requires replacing the numerical momentum p by its operator equivalent P, and doing this results in a square root containing an operator. It's not obvious how this can be handled.

Dirac's solution was essentially to turn the problem on its head. Rather than trying to find the square root of an existing quantity, he postulated that the quantity inside the square root is the perfect square of an expression that is linear in the momentum. That is, he proposed

$$P^2c^2 + m^2c^4 = \left(c\alpha_x P_x + c\alpha_y P_y + c\alpha_z P_z + \beta mc^2\right)^2 \tag{2}$$

$$= \left(c\boldsymbol{\alpha}\cdot\mathbf{P} + \beta mc^2\right)^2 \tag{3}$$

The problem is then to find the quantities α_i and β. We can do this by substituting

$$\mathbf{P} = P_x\hat{\mathbf{x}} + P_y\hat{\mathbf{y}} + P_z\hat{\mathbf{z}} \tag{4}$$

on the LHS of 3 and then matching terms. The LHS becomes

$$LHS = P^2c^2 + m^2c^4 = \mathbf{P}\cdot\mathbf{P}c^2 + m^2c^4 \tag{5}$$
$$= \left(P_x^2 + P_y^2 + P_z^2\right)c^2 + m^2c^4 \tag{6}$$

The RHS becomes

$$RHS = c^2 \sum_{i=x,y,z} \alpha_i^2 P_i^2 + c^2\left[\left(\alpha_x\alpha_y + \alpha_y\alpha_x\right)P_xP_y + \right. \tag{7}$$
$$\left.\left(\alpha_x\alpha_z + \alpha_z\alpha_x\right)P_xP_z + \left(\alpha_y\alpha_z + \alpha_z\alpha_y\right)P_yP_z\right] + \tag{8}$$
$$mc^3 \sum_{i=x,y,z} \left(\alpha_i\beta + \beta\alpha_i\right)P_i + \beta^2m^2c^4 \tag{9}$$

Notice that this expansion assumes that $\boldsymbol{\alpha}$ and β commute with $\mathbf{P}$, since we've factored out the terms involving P_i. This is equivalent to assuming that $\boldsymbol{\alpha}$ and β do not depend on position, since the $\mathbf{P}$ operator contains derivatives with respect to position. For a free particle, this is reasonable, since such a particle is not localized anywhere in space. Note also that we do *not* assume that the α_is and β commute with each other, which is why we've written out the terms with these objects in a particular order.

In fact, if we require the LHS equal the RHS above, the α_is and β *cannot* commute. This is so because all the terms on the RHS except for the first and last terms must be zero. That is

$$\left[\alpha_i, \alpha_j\right]_+ = \alpha_i\alpha_j + \alpha_j\alpha_i = 0 \text{ if } i \neq j \tag{10}$$
$$\left[\alpha_i, \beta\right]_+ = \alpha_i\beta + \beta\alpha_i = 0 \tag{11}$$
$$\alpha_i^2 = \beta^2 = 1 \tag{12}$$

where $[]_+$ denotes an anticommutator.

Thus the α_is and β cannot be just numbers (real or complex), as all numbers commute. We *can* find $\boldsymbol{\alpha}$ and β if we take them to be matrices. Since $c\boldsymbol{\alpha}\cdot\mathbf{P} + \beta mc^2$ is to represent the Hamiltonian, it must be hermitian and, since $\mathbf{P}$ is hermitian (it's the momentum, which is observable), then $\boldsymbol{\alpha}$ and β must also be hermitian.

To find them, we recall some properties of hermitian matrices. For hermitian matrices that satisfy

$$M^iM^j + M^jM^i = 2\delta^{ij}I \tag{13}$$

we found that their eigenvalues are ± 1, they have zero trace and must be even-dimensional.

Our first thought is that the α_is and β are 2×2 matrices. This would be especially nice since it would then imply that the wave function ψ has

two components which is just what we need to describe particles such as the electron with spin-$\frac{1}{2}$. However, we know that any 2×2 matrix can be written as a linear combination of the Pauli matrices and the 2×2 unit matrix and that there is no non-zero matrix that commutes with all three Pauli matrices. Thus there is no way to satisfy both 10 and 11 with 2×2 matrices. We are therefore forced to try the next simplest type of even-dimensional matrices, which are 4×4.

The most commonly used such matrices are given by

$$\boldsymbol{\alpha} = \begin{bmatrix} 0 & \boldsymbol{\sigma} \\ \boldsymbol{\sigma} & 0 \end{bmatrix} \tag{14}$$

$$\beta = \begin{bmatrix} I & 0 \\ 0 & -I \end{bmatrix} \tag{15}$$

where $\boldsymbol{\sigma}$ represents the vector of 3 Pauli matrices, 0 represents a 2×2 zero matrix and I is the 2×2 unit matrix.

These aren't the only matrices that satisfy the conditions, since we can apply a unitary transformation with a unitary operator S. For example if we transform as follows:

$$\alpha_i' = S^\dagger \alpha_i S \tag{16}$$

$$\beta' = S^\dagger \beta S \tag{17}$$

then we have, since $S^\dagger = S^{-1}$:

$$\left[\alpha_i', \alpha_j'\right]_+ = \alpha_i' \alpha_j' + \alpha_j' \alpha_i' \tag{18}$$

$$= S^\dagger \alpha_i S S^\dagger \alpha_j S + S^\dagger \alpha_j S S^\dagger \alpha_i S \tag{19}$$

$$= S^\dagger \alpha_i \alpha_j S + S^\dagger \alpha_j \alpha_i S \tag{20}$$

$$= S^\dagger \left[\alpha_i, \alpha_j\right]_+ S \tag{21}$$

$$= 0 \tag{22}$$

Putting everything together, we get the Dirac equation

$$\boxed{i\hbar \frac{\partial \left|\psi\right\rangle}{\partial t} = \left(c\boldsymbol{\alpha} \cdot \mathbf{P} + \beta mc^2\right) \left|\psi\right\rangle} \tag{23}$$

In this equation, since $\boldsymbol{\alpha}$ and β are 4×4 matrices, the wave function $|\psi\rangle$ must be a 4-component vector. We'll see later how to make this consistent with a wave function describing a 2-component object such as an electron.

Finally, we can show that the Dirac equation still allows us to interpret $\psi^\dagger \psi$ as a probability density, provided we define the probability current

appropriately. Conservation of probability requires the probability density ρ satisfies the continuity equation

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{j} = 0 \tag{24}$$

where $\mathbf{j}$ is the probability current. Starting with

$$\rho = \psi^\dagger \psi \tag{25}$$

we have (note that since ψ is now a vector, we need to maintain the correct order of terms):

$$\frac{\partial \rho}{\partial t} = \frac{\partial \psi^\dagger}{\partial t}\psi + \psi^\dagger \frac{\partial \psi}{\partial t} \tag{26}$$

$$= \frac{1}{-i\hbar}\left[\left(c\boldsymbol{\alpha}^\dagger \cdot \mathbf{P}^\dagger + \beta^\dagger mc^2\right)\right]\psi^\dagger + \psi^\dagger \frac{1}{i\hbar}\left[\left(c\boldsymbol{\alpha}\cdot\mathbf{P} + \beta mc^2\right)\right]\psi \tag{27}$$

Since $\boldsymbol{\alpha}$ and β are hermitian, we have, using $\mathbf{P} = -i\hbar\nabla$ and $\mathbf{P}^\dagger = i\hbar\nabla$:

$$\frac{\partial \rho}{\partial t} = \frac{1}{-i\hbar}\left[\left(i\hbar c\boldsymbol{\alpha}\cdot\nabla + \beta mc^2\right)\psi^\dagger\right]\psi + \psi^\dagger \frac{1}{i\hbar}\left[\left(-i\hbar c\boldsymbol{\alpha}\cdot\nabla + \beta mc^2\right)\psi\right] \tag{28}$$

$$= -c\left(\boldsymbol{\alpha}\cdot\nabla\psi^\dagger\right)\psi - \psi^\dagger c\left(\boldsymbol{\alpha}\cdot\nabla\psi\right) - \frac{1}{i\hbar}\beta mc^2\psi^\dagger\psi + \frac{1}{i\hbar}\beta mc^2\psi^\dagger\psi \tag{29}$$

$$= -c\left(\boldsymbol{\alpha}\cdot\nabla\psi^\dagger\right)\psi - \psi^\dagger c\left(\boldsymbol{\alpha}\cdot\nabla\psi\right) \tag{30}$$

$$= -c\nabla\left(\psi^\dagger\boldsymbol{\alpha}\psi\right) \tag{31}$$

We can therefore identify as the probability current

$$\mathbf{j} = c\psi^\dagger\boldsymbol{\alpha}\psi \tag{32}$$

PINGBACKS

Pingback: Dirac equation: gamma matrices and
Pingback: Dirac equation: set of independent matrices
Pingback: Dirac equation: linear independence of matrices
Pingback: Dirac equation: nonuniqueness of solutions
Pingback: Gamma matrices in Dirac-Pauli representation
Pingback: Lagrangian for the Dirac field
Pingback: Hermitian Lagrangian for the Dirac field

PHYSICS

Principles of Quantum Mechanics

Shankar's *Principles of Quantum Mechanics* is a great book, although not recommended as the first textbook for beginners. Griffiths' *Introduction to Quantum Mechanics* is much more approachable.

Here is the official Errata, which is unfortunately but not surprisingly incomplete.

Solutions to most problems can be found here and here. Some are however missing and can be found below.

Chapter 5 - Simple Problems in One Dimension

Solutions

Exercise 5.4.1

If we replace x by $x+a$ in (5.1.15) and p_0 by $\hbar k_0$, we get the following wave function.

$$\psi(x,t) = e^{ik_0(x+a-\frac{\hbar k_0 t}{2m})} \frac{e^{\frac{-(x+a-\frac{\hbar k_0 t}{m})^2}{2\Delta^2(1+\frac{i\hbar t}{m\Delta^2})}}}{\pi^{\frac{1}{4}}(\Delta+\frac{i\hbar t}{m\Delta})^{\frac{1}{2}}}$$

It describes a particle of mass m. At $t=0$, it has mean position $\langle X\rangle = -a$ and $\Delta X = \frac{\Delta}{\sqrt{2}}$. Through its whole evolution, $\langle P\rangle = p_0$ and the evelope, as described by the Gaussian function, moves at a group velocity of $\frac{p_0}{m}$.

The wave function above is obtained from the following calculation.

$$\psi(x,t) = (\frac{\Delta^2}{4\pi^3})^{\frac{1}{4}} \int_{-\infty}^{\infty} e^{\frac{-i\hbar {k_1}^2 t}{2m}} e^{\frac{-(k_1-k_0)^2\Delta^2}{2}} e^{ik_1(x+a)} \mathrm{d}k_1$$

The last term in (5.4.15) is as follows.

$$* = (\frac{\Delta^2}{4\pi^3})^{\frac{1}{4}} \int_{-\infty}^{\infty} e^{\frac{-i\hbar {k_1}^2 t}{2m}} e^{\frac{-(k_1-k_0)^2\Delta^2}{2}} e^{ik_1 a} \frac{C}{A} e^{i({k_1}^2-\frac{2mV_0}{\hbar^2})^{\frac{1}{2}}x} \theta(x) \mathrm{d}k_1$$

Due to the second exponential in the integrand, only k_1 close to k_0 has a real impact on the result, therefore we can take the following approximation.

- $\frac{C}{A}$, which depends on k_1 can be replaced by $\frac{C_0}{A_0}$, its value at $k_1 = k_0$.
- Expand the factor $({k_1}^2 - \frac{2mV_0}{\hbar^2})^{\frac{1}{2}}$ and keep just the first derivative in the Taylor series.

To simply notations, we define $k_2 \equiv ({k_0}^2 - \frac{2mV_0}{\hbar^2})^{\frac{1}{2}}$, $\gamma \equiv \frac{k_2}{k_0} < 1$, and $k_1' = \frac{k_1}{\gamma}$.

The Taylor expansion, up to the first derivative, is then $k_2 + \frac{k_0}{k_2}(k_1 - k_0) = k_2 + \frac{k_1 - k_0}{\gamma}$, and we have the following.

$$
\begin{aligned}
* &= \frac{C_0}{A_0}\theta(x)(\frac{\Delta^2}{4\pi^3})^{\frac{1}{4}}\int_{-\infty}^{\infty} e^{\frac{-i\hbar {k_1}^2 t}{2m}} e^{\frac{-(k_1-k_0)^2\Delta^2}{2}} e^{ik_1 a} e^{ik_2 x} e^{i\frac{k_1-k_0}{\gamma}x}\,\mathrm{d}k_1 \\
&= \frac{C_0}{A_0}\theta(x)e^{i(k_2-\frac{k_0}{\gamma})x}(\frac{\Delta^2}{4\pi^3})^{\frac{1}{4}}\int_{-\infty}^{\infty} e^{\frac{-i\hbar {k_1}^2 t}{2m}} e^{\frac{-(k_1-k_0)^2\Delta^2}{2}} e^{ik_1 a} e^{i\frac{k_1}{\gamma}x}\,\mathrm{d}k_1 \\
&= \gamma^{\frac{1}{2}}\frac{C_0}{A_0}\theta(x)e^{i(k_2-\frac{k_0}{\gamma})x}(\frac{(\gamma\Delta)^2}{4\pi^3})^{\frac{1}{4}}\int_{-\infty}^{\infty} e^{\frac{-i\hbar {k_1'}^2 t}{2\frac{m}{\gamma^2}}} e^{\frac{-(k_1'-\frac{k_0}{\gamma})^2(\gamma\Delta)^2}{2}} e^{ik_1'(x+\gamma a)}\,\mathrm{d}k_1' \\
&= \gamma^{\frac{1}{2}}\frac{C_0}{A_0}\theta(x)e^{i(k_2-\frac{k_0}{\gamma})x}\triangle
\end{aligned}
$$

Compare $\triangle$ to the calculation for the original Gaussian packet, we can see it has exactly the same form, with $\Delta \to \Delta' \equiv \gamma\Delta$, $m \to m' \equiv \frac{m}{\gamma^2}$, $k_0 \to k_0' \equiv \frac{k_0}{\gamma}$, $a \to a' \equiv \gamma a$, and $k_1 \to k_1'$. From here we can already derive the transmission coefficient T.

$$
T = \gamma|\frac{C_0}{A_0}|^2\int_{-\infty}^{\infty}\theta^2(x)|\triangle|^2\mathrm{d}x = \gamma|\frac{C_0}{A_0}|^2
$$

This is exactly the same result as in (5.4.21). Note $\theta(x)$ can be effectively ignored with $t \to \infty$ since $\triangle$ represents a particle moving towards $+x$ at $\frac{\hbar k_0'}{m'} = \frac{\hbar\gamma k_0}{m} = \frac{\hbar k_2}{m}$. This is also what we would expect from classical mechanics.

Although we could stop here, it is beneficial to continue the derivation a bit.

$$
\begin{aligned}
* &= \gamma^{\frac{1}{2}}\frac{C_0}{A_0}\theta(x)e^{i(k_2-\frac{k_0}{\gamma})x}\triangle \\
&= \gamma^{\frac{1}{2}}\frac{C_0}{A_0}\theta(x)e^{i(k_2-\frac{k_0}{\gamma})x}e^{ik_0'(x+a'-\frac{\hbar k_0' t}{2m'})}\frac{e^{\frac{-(x+a'-\frac{\hbar k_0' t}{m'})^2}{2\Delta'^2(1+\frac{i\hbar t}{m'\Delta'^2})}}}{\pi^{\frac{1}{4}}(\Delta'+\frac{i\hbar t}{m'\Delta'})^{\frac{1}{2}}} \\
&= \gamma^{\frac{1}{2}}\frac{C_0}{A_0}\theta(x)e^{i(k_2-\frac{k_0}{\gamma}+k_0')x}e^{ik_0(a-\frac{\hbar k_0 t}{2m})}\frac{e^{\frac{-(x+a'-\frac{\hbar k_2 t}{m})^2}{2\Delta'^2(1+\frac{i\hbar t}{m\Delta^2})}}}{\pi^{\frac{1}{4}}(\Delta'+\frac{i\hbar\gamma t}{m\Delta})^{\frac{1}{2}}} \\
&= \gamma^{\frac{1}{2}}\frac{C_0}{A_0}\theta(x)e^{ik_2 x}e^{ik_0(a-\frac{\hbar k_0 t}{2m})}\frac{e^{\frac{-(x+a'-\frac{\hbar k_2 t}{m})^2}{2\Delta'^2(1+\frac{i\hbar t}{m\Delta^2})}}}{\pi^{\frac{1}{4}}(\Delta'+\frac{i\hbar\gamma t}{m\Delta})^{\frac{1}{2}}}
\end{aligned}
$$

From the term $e^{ik_2 x}$, it can be clearly seen that $\langle P\rangle = \hbar k_2$, again exactly as what we would expect from classical mechanics.

Exercise 5.4.3

We have the following Hamiltonian.

$$
H = \frac{P^2}{2m} - fX
$$

In momentum space, $X \to i\hbar\frac{\partial}{\partial p}$ and $P \to p$. We have thus the following differential equation.

$$
\frac{p^2}{2m}\psi_E(p) - i\hbar f\frac{\mathrm{d}\psi_E(p)}{\mathrm{d}p} = E\psi_E(p)
$$

Its general solution is $\psi_E(p) = Ce^{-\frac{ip^3}{6\hbar m f}+\frac{iEp}{\hbar f}}$, where C can be any constant.

Its normalization requires the following.

$$
\langle E|E'\rangle = |C|^2\int_{-\infty}^{\infty} e^{\frac{i(E'-E)}{\hbar f}p}\mathrm{d}p = |C|^2 2\pi\hbar f\delta(E'-E) = \delta(E'-E)
$$

We have used Eq. (1.10.26) in the derivation above.

And therefore we can set $C = \frac{1}{\sqrt{2\pi\hbar f}}$ and $\psi_E(p) = \frac{1}{\sqrt{2\pi\hbar f}}e^{-\frac{ip^3}{6\hbar m f}+\frac{iEp}{\hbar f}}$.

Now we have the following.

$$
\begin{aligned}
U(p,t;p',0) &= \langle p|U(t)|p'\rangle \\
&= \int_{-\infty}^{\infty} \langle p|E\rangle e^{-\frac{iE}{\hbar}t}\langle E|p'\rangle \mathrm{d}E \\
&= \int_{-\infty}^{\infty} \psi_E(p) e^{-\frac{iE}{\hbar}t}\psi_E^*(p)\mathrm{d}E \\
&= \frac{1}{2\pi\hbar f}\int_{-\infty}^{\infty} e^{-\frac{ip^3}{6\hbar m f}} e^{\frac{iEp}{\hbar f}} e^{-\frac{iE}{\hbar}t} e^{\frac{ip'^3}{6\hbar m f}} e^{-\frac{iEp'}{\hbar f}}\,\mathrm{d}E \\
&= \frac{1}{2\pi\hbar f} e^{\frac{i(p'^3-p^3)}{6\hbar m f}} \int_{-\infty}^{\infty} e^{i\frac{p-p'-ft}{\hbar f}E}\mathrm{d}E \\
&= \delta(p-p'-ft) e^{\frac{i(p'^3-p^3)}{6mhf}}
\end{aligned}
$$

Here we have used Eq. (1.10.26) again.

In coordinate space it is as follows.

$$
\begin{aligned}
U(x,t;x',0) &= \langle x|U(t)|x'\rangle \\
&= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \langle x|p><p|U(t)|p'\rangle\langle p'|x'\rangle \mathrm{d}p\mathrm{d}p' \\
&= \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{ipx/\hbar}\delta(p-p'-ft) e^{\frac{i(p'^3-p^3)}{6mhf}} e^{-ip'x'/\hbar}\mathrm{d}p\mathrm{d}p' \\
&= \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} e^{ifptx/\hbar} e^{i(p-ft)(x-x')/\hbar} e^{\frac{i(-3p^2ft+3pf^2t^2-f^3t^3)}{6mhf}}\mathrm{d}p \\
&= \frac{e^{ifptx'/\hbar}e^{-i\frac{f^2t^3}{6mh}}}{2\pi\hbar}\int_{-\infty}^{\infty} e^{-\frac{i(p^2t-pft^2)}{2m\hbar}+\frac{ip(x-x')}{\hbar}}\mathrm{d}p \\
&= \frac{e^{ifptx'/\hbar}e^{-i\frac{f^2t^3}{6mh}}}{2\pi\hbar}\int_{-\infty}^{\infty} e^{-\frac{it}{2m\hbar}p^2} e^{-2\frac{-i(ft^2+2m(x-x'))}{4m\hbar}p}\mathrm{d}p \\
&= \frac{e^{ifptx'/\hbar}e^{-i\frac{f^2t^3}{6mh}}}{2\pi\hbar}\left(\frac{2\pi m\hbar}{it}\right)^{\frac{1}{2}} e^{i\frac{(ft^2+2m(x-x'))^2}{8m\hbar t}} \\
&= \left(\frac{m}{2\pi\hbar it}\right)^{\frac{1}{2}} e^{\frac{i}{\hbar}\left(ftx'-\frac{f^2t^3}{6m}+\frac{(ft^2+2m(x-x'))^2}{8mt}\right)} \\
&= \left(\frac{m}{2\pi\hbar it}\right)^{\frac{1}{2}} e^{\frac{i}{\hbar}\left(ftx'-\frac{f^2t^3}{6m}+\frac{f^2t^3}{8m}+\frac{m(x-x')^2}{2t}+\frac{ft(x-x')}{2}\right)} \\
&= \left(\frac{m}{2\pi\hbar it}\right)^{\frac{1}{2}} e^{\frac{i}{\hbar}\left(\frac{m(x-x')^2}{2t}+\frac{1}{2}ft(x+x')-\frac{f^2t^3}{24m}\right)}
\end{aligned}
$$

Chapter 18 - Time-Dependent Perturbation Theory

Errata

Page 476, Eq. (18.2.12): $\mathscr{H}$ should be $\mathscr{E}$.

Page 489, Eq. (18.3.27): The last factor in the integrand of the second term on the right hand side should be $e^{-iE_i^0(t'-t_0)/\hbar}$.

Page 506, Eq. (18.5.31): If we want to pedantic, it should be $\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \frac{8\pi c}{|\boldsymbol{A_0}|^2\omega^2}\hbar\omega R_{i\to\mathrm{d}\Omega}/\mathrm{d}\Omega$.

Page 509, Eq. (18.5.42): The claim that $|\nabla\times\boldsymbol{A}|^2 = -\boldsymbol{A}\cdot\nabla^2\boldsymbol{A}$ is valid when $\nabla\cdot\boldsymbol{A}=0$ is by itself wrong. A counter-example is $\boldsymbol{A}=\boldsymbol{A_0}\cos(i\boldsymbol{kr})$, where $\boldsymbol{A_0}$ and $\boldsymbol{k}$ are mutually perpendicular. We can see that the left hand side will have a $\sin^2(i\boldsymbol{kr})$ term, while the right hand side will have a $\cos^2(i\boldsymbol{kr})$ term.

If we apply, to $-\boldsymbol{A}\cdot\nabla^2\boldsymbol{A}$, first $\nabla^2\boldsymbol{A} = \nabla(\nabla\cdot\boldsymbol{A}) - \nabla\times(\nabla\times\boldsymbol{A})$, keeping in mind $\nabla\cdot\boldsymbol{A}=0$, and then $\boldsymbol{Y}\cdot(\nabla\times\boldsymbol{X}) = \boldsymbol{X}\cdot(\nabla\times\boldsymbol{Y}) + \nabla\cdot(\boldsymbol{X}\times\boldsymbol{Y})$, where we set $\boldsymbol{Y}=\boldsymbol{A}$ and $\boldsymbol{X}=\nabla\times\boldsymbol{A}$, we get

$$
|\nabla\times\boldsymbol{A}|^2 = -\boldsymbol{A}\cdot\nabla^2\boldsymbol{A} + \nabla\cdot(\boldsymbol{A}\times(\nabla\times\boldsymbol{A})).
$$

The extra term, however, is negligible in an integral over an infinite volume V, when both $\boldsymbol{A}$ and $\nabla\times\boldsymbol{A}$ are finite, because we can apply Gauss' theorem and the integral becomes

$\int_{\partial V} \boldsymbol{A} \times (\nabla \times \boldsymbol{A}) \mathrm{d}\boldsymbol{S}$, which grows at $V^{2/3}$, and its per volume contribution becomes zero as V approaches infinity.

Page 514, Eq. (18.5.60): $\boldsymbol{k}^-$ should be $\boldsymbol{k}$.

Page 518, Eq. (18.5.81): $e^{i\boldsymbol{kr}}$ should be $e^{-i\boldsymbol{kr}}$. Idem for the equation immediately below.

Notes

Below are some useful vector calculus identies for electromagnetism.

$$\nabla(\nabla \cdot \boldsymbol{A}) - \nabla \times (\nabla \times \boldsymbol{A}) = \nabla^2 \boldsymbol{A}$$

$$\nabla \cdot (\nabla^2 \boldsymbol{A}) = \nabla^2 (\nabla \cdot \boldsymbol{A})$$

$$\nabla \cdot (\boldsymbol{A} \times \boldsymbol{B}) = \boldsymbol{B} \cdot (\nabla \times \boldsymbol{A}) - \boldsymbol{A} \cdot (\nabla \times \boldsymbol{B})$$

$$(\boldsymbol{A} \times \boldsymbol{B}) \cdot (\boldsymbol{C} \times \boldsymbol{D}) = (\boldsymbol{A} \cdot \boldsymbol{C})(\boldsymbol{B} \times \boldsymbol{D}) - (\boldsymbol{B} \cdot \boldsymbol{C})(\boldsymbol{A} \times \boldsymbol{D})$$

Page 482, Eq. (18.2.35)

It would seem that $P_{i \to f} \to \infty$ as $t \to \infty$, when $\omega_{fi} = \omega$. But keep in mind that the first-order calculation is reliable only if $|d_f(t)| \ll 1 (f \neq i)$. (See the discussion underneath Eq. (18.2.9).)

Page 483, Eq. (18.2.42)

We will apply *Fermi's golden rule* to *time-independent* perturbation when we study spontaneous emissions. It is valid because we can simply set $\omega = 0$ and all the derivation will still follow.

Page 494, Exercise 18.4.3, (4): It is easy to show $\nabla^2 \Lambda = 0$. Its solution is unique when its boundary value is fixed. Hence the uniqueness of A when $|A| \to 0$ at spatial infinity. A proof of the uniqueness of solutions to Laplace's equation with fixed boundary conditions can be found here.

Page 501, Footnote

Note that $\boldsymbol{A} = \boldsymbol{A_0} e^{i\boldsymbol{kr}}$.

Page 505, Eq. (18.5.24)

Strictly speaking, there should also be an extra term $\frac{m}{p_f} \delta\{p_f + [2m(E_i^0 + \hbar\omega)]^{1/2}\}$ on the right hand side. But this term will become irrelevant in Eq. (18.5.25), where we are only interested in $p_f \in [0, \infty]$ for the integral.

Page 505, Eq. (18.5.25)

Note $R_{i \to d\Omega} = \int_0^\infty R_{i \to f}(\boldsymbol{p_f}) p_f^2 \mathrm{d}p_f \mathrm{d}\Omega$.

Page 508, Note ‡

Those who want to derive Maxwell's equations from the Lagrangian without reading Goldsteins' wonderful book *Classical Mechanics*, only need to know the Euler–Lagrange equation for a continuous field is $\partial_t \frac{\partial \mathscr{L}}{\partial(\partial_t \phi)} + \partial_x \frac{\partial \mathscr{L}}{\partial(\partial_x \phi)} = \frac{\partial \mathscr{L}}{\partial \phi}$, where $\mathscr{L}$ is the Lagrangian density and ϕ is the scalar field. For three dimensions, add ∂_y and ∂_z terms on the left hand side. For a vector field, simply treat each vector componnent as a scalar field.

Page 509, Eq. (18.5.6)

See the previous note.

Page 512, Eq. (18.5.51)

Some hard work to derive these equalities can be found below.

First we can derive $\boldsymbol{a}(\boldsymbol{k})$ from Eq. (18.5.44) and Eq. (18.5.46).

$$\boldsymbol{a}(\boldsymbol{k}) = \frac{1}{2(2\pi)^3}\int [\boldsymbol{A}(\boldsymbol{r}) + \frac{4\pi i c}{k}\boldsymbol{\Pi}(\boldsymbol{r})]e^{-i\boldsymbol{k}\boldsymbol{r}}\mathrm{d}^3\boldsymbol{r}$$

Multiplying $\boldsymbol{\varepsilon}((\boldsymbol{k}\lambda_0))$ on both sides of Eq. (18.5.48) and then dropping the subscript 0, we get

$$a(\boldsymbol{k}\lambda) = \frac{\boldsymbol{\varepsilon}(\boldsymbol{k}\boldsymbol{\lambda})}{2(2\pi)^2}\int [\frac{\sqrt{\omega}}{c}\boldsymbol{A}(\boldsymbol{r}) + \frac{4\pi i c}{\sqrt{\omega}}\boldsymbol{\Pi}(\boldsymbol{r})]e^{-i\boldsymbol{k}\boldsymbol{r}}\mathrm{d}^3\boldsymbol{r}.$$

In the continuous system that interests us now, the Poisson bracket is defined as

$$\{X, Y\} = \sum_i \int \frac{\partial X}{\partial A_i(\boldsymbol{r})}\frac{\partial Y}{\partial \Pi_i(\boldsymbol{r})} - \frac{\partial Y}{\partial A_i(\boldsymbol{r})}\frac{\partial X}{\partial \Pi_i(\boldsymbol{r})}\mathrm{d}^3\boldsymbol{r},$$

where $\boldsymbol{r}$ is a continuous index rather than an independent variable.

Differentiating $a(\boldsymbol{k}\lambda)$ over $A_i(\boldsymbol{r})$ or $\Pi_i(\boldsymbol{r})$ gives us

$$\frac{\partial a(\boldsymbol{k}\lambda)}{\partial A_i(\boldsymbol{r})} = \frac{\boldsymbol{\varepsilon}(\boldsymbol{k}\boldsymbol{\lambda})\cdot\boldsymbol{\varepsilon}_i}{2(2\pi)^2}\frac{\sqrt{\omega}}{c}e^{-i\boldsymbol{k}\boldsymbol{r}},$$

$$\frac{\partial a(\boldsymbol{k}\lambda)}{\partial \Pi_i(\boldsymbol{r})} = \frac{\boldsymbol{\varepsilon}(\boldsymbol{k}\boldsymbol{\lambda})\cdot\boldsymbol{\varepsilon}_i}{2(2\pi)^2}\frac{4\pi i c}{\sqrt{\omega}}e^{-i\boldsymbol{k}\boldsymbol{r}},$$

where we have used the fact that $\boldsymbol{A}(\boldsymbol{r}) = \sum_i A_i(\boldsymbol{r})\boldsymbol{\varepsilon}_i$.

Now we have

$$\begin{aligned}
&\{a(\boldsymbol{k}\lambda), a(\boldsymbol{k}'\lambda')\}\\
&= \sum_i \int \frac{\partial a(\boldsymbol{k}\lambda)}{\partial A_i(\boldsymbol{r})}\frac{\partial a(\boldsymbol{k}'\lambda')}{\partial \Pi_i(\boldsymbol{r})} - \frac{\partial a(\boldsymbol{k}'\lambda')}{\partial A_i(\boldsymbol{r})}\frac{\partial a(\boldsymbol{k}\lambda)}{\partial \Pi_i(\boldsymbol{r})}\mathrm{d}^3\boldsymbol{r}\\
&= \sum_i \frac{[\boldsymbol{\varepsilon}(\boldsymbol{k}\boldsymbol{\lambda})\cdot\boldsymbol{\varepsilon}_i][\boldsymbol{\varepsilon}(\boldsymbol{k}'\boldsymbol{\lambda}')\cdot\boldsymbol{\varepsilon}_i]i}{2(2\pi)^3}(\sqrt{\frac{\omega}{\omega'}} - \sqrt{\frac{\omega'}{\omega}})\int e^{-i\boldsymbol{k}\boldsymbol{r}}e^{-i\boldsymbol{k}'\boldsymbol{r}}\mathrm{d}^3\boldsymbol{r}\\
&= \frac{\boldsymbol{\varepsilon}(\boldsymbol{k}\boldsymbol{\lambda})\cdot\boldsymbol{\varepsilon}(\boldsymbol{k}'\boldsymbol{\lambda}')i}{2}(\sqrt{\frac{\omega}{\omega'}} - \sqrt{\frac{\omega'}{\omega}})\delta^3(\boldsymbol{k}+\boldsymbol{k}')\\
&= 0.
\end{aligned}$$

We have last equality because $\omega = \omega'$ when $\boldsymbol{k} = -\boldsymbol{k}'$.

Similarly we have $\{a^*(\boldsymbol{k}\lambda), a^*(\boldsymbol{k}'\lambda')\} = 0$.

And finally we have

$$\begin{aligned}
&\{a(\boldsymbol{k}\lambda), a^*(\boldsymbol{k}'\lambda')\}\\
&= \sum_i \int \frac{\partial a(\boldsymbol{k}\lambda)}{\partial A_i(\boldsymbol{r})}\frac{\partial a^*(\boldsymbol{k}'\lambda')}{\partial \Pi_i(\boldsymbol{r})} - \frac{\partial a^*(\boldsymbol{k}'\lambda')}{\partial A_i(\boldsymbol{r})}\frac{\partial a(\boldsymbol{k}\lambda)}{\partial \Pi_i(\boldsymbol{r})}\mathrm{d}^3\boldsymbol{r}\\
&= \sum_i \frac{[\boldsymbol{\varepsilon}(\boldsymbol{k}\boldsymbol{\lambda})\cdot\boldsymbol{\varepsilon}_i][\boldsymbol{\varepsilon}(\boldsymbol{k}'\boldsymbol{\lambda}')\cdot\boldsymbol{\varepsilon}_i](-i)}{2(2\pi)^3}(\sqrt{\frac{\omega}{\omega'}} + \sqrt{\frac{\omega'}{\omega}})\int e^{-i\boldsymbol{k}\boldsymbol{r}}e^{i\boldsymbol{k}'\boldsymbol{r}}\mathrm{d}^3\boldsymbol{r}\\
&= \frac{\boldsymbol{\varepsilon}(\boldsymbol{k}\boldsymbol{\lambda})\cdot\boldsymbol{\varepsilon}(\boldsymbol{k}'\boldsymbol{\lambda}')(-i)}{2}(\sqrt{\frac{\omega}{\omega'}} + \sqrt{\frac{\omega'}{\omega}})\delta^3(\boldsymbol{k}-\boldsymbol{k}')\\
&= -i\delta_{\lambda\lambda'}\delta^3(\boldsymbol{k}-\boldsymbol{k}').
\end{aligned}$$

Page 513, Eq. (18.5.54)

Below is the derivation.

From Eq. (18.5.41), we have

$$\mathscr{H} = 2\pi c^2\int |\boldsymbol{\Pi}|^2\mathrm{d}^3\boldsymbol{r} + \frac{1}{8\pi}\int |\nabla\times\boldsymbol{A}|^2\mathrm{d}^3\boldsymbol{r}.$$

The first term can be calculated as follows.

$$
\begin{aligned}
&2\pi c^2 \int |\boldsymbol{\Pi}|^2 \mathrm{d}^3\boldsymbol{r} \\
=& \frac{2\pi c^2}{16\pi^2 c^2} \int \left\{ \int k[\boldsymbol{a}^*(\boldsymbol{k}) e^{-i\boldsymbol{k}\boldsymbol{r}} - \boldsymbol{a}(\boldsymbol{k}) e^{i\boldsymbol{k}\boldsymbol{r}}] \mathrm{d}^3\boldsymbol{k} \right\} \left\{ \int k'[\boldsymbol{a}(\boldsymbol{k}') e^{i\boldsymbol{k}'\boldsymbol{r}} - \boldsymbol{a}^*(\boldsymbol{k}') e^{-i\boldsymbol{k}'\boldsymbol{r}}] \mathrm{d}^3\boldsymbol{k}' \right\} \mathrm{d}^3\boldsymbol{r} \\
=& \frac{1}{8\pi} \int\int\int kk'[\boldsymbol{a}^*(\boldsymbol{k}) e^{-i\boldsymbol{k}\boldsymbol{r}} - \boldsymbol{a}(\boldsymbol{k}) e^{i\boldsymbol{k}\boldsymbol{r}}][\boldsymbol{a}(\boldsymbol{k}') e^{i\boldsymbol{k}'\boldsymbol{r}} - \boldsymbol{a}^*(\boldsymbol{k}') e^{-i\boldsymbol{k}'\boldsymbol{r}}] \mathrm{d}^3\boldsymbol{r} \mathrm{d}^3\boldsymbol{k} \mathrm{d}^3\boldsymbol{k}' \\
=& \frac{(2\pi)^3}{8\pi} \int\int kk'[\boldsymbol{a}^*(\boldsymbol{k})\boldsymbol{a}(\boldsymbol{k}')\delta^3(\boldsymbol{k}-\boldsymbol{k}') - \boldsymbol{a}^*(\boldsymbol{k})\boldsymbol{a}^*(\boldsymbol{k}')\delta^3(\boldsymbol{k}+\boldsymbol{k}') - \boldsymbol{a}(\boldsymbol{k})\boldsymbol{a}(\boldsymbol{k}')\delta^3(\boldsymbol{k}+\boldsymbol{k}') + \boldsymbol{a}(\boldsymbol{k})\boldsymbol{a}^*(\boldsymbol{k}')\delta^3(\boldsymbol{k}-\boldsymbol{k}')] \\
=& 2\pi^2 \int k^2 \boldsymbol{a}^*(\boldsymbol{k})\boldsymbol{a}(\boldsymbol{k}) \mathrm{d}^3\boldsymbol{k} - 2\pi^2 \int k^2 \Re[\boldsymbol{a}(\boldsymbol{k})\boldsymbol{a}(-\boldsymbol{k})] \mathrm{d}^3\boldsymbol{k}
\end{aligned}
$$

The second term can be calculated as follows.

$$
\begin{aligned}
&\frac{1}{8\pi} \int |\nabla \times \boldsymbol{A}|^2 \mathrm{d}^3\boldsymbol{r} \\
=& \frac{1}{8\pi} \int \left\{ \int [-i\boldsymbol{k} \times \boldsymbol{a}^*(\boldsymbol{k}) e^{-i\boldsymbol{k}\boldsymbol{r}} + i\boldsymbol{k} \times \boldsymbol{a}(\boldsymbol{k}) e^{i\boldsymbol{k}\boldsymbol{r}}] \mathrm{d}^3\boldsymbol{k} \right\} \left\{ \int [i\boldsymbol{k}' \times \boldsymbol{a}(\boldsymbol{k}') e^{i\boldsymbol{k}'\boldsymbol{r}} - i\boldsymbol{k}' \times \boldsymbol{a}^*(\boldsymbol{k}') e^{-i\boldsymbol{k}'\boldsymbol{r}}] \mathrm{d}^3\boldsymbol{k}' \right\} \mathrm{d}^3\boldsymbol{r} \\
=& \frac{1}{8\pi} \int\int\int [(\boldsymbol{k}\cdot\boldsymbol{k}')(\boldsymbol{a}^*(\boldsymbol{k})\cdot\boldsymbol{a}(\boldsymbol{k}')) - (\boldsymbol{a}^*(\boldsymbol{k})\cdot\boldsymbol{k}')(\boldsymbol{k}\cdot\boldsymbol{a}(\boldsymbol{k}'))] e^{-i(\boldsymbol{k}-\boldsymbol{k}')\boldsymbol{r}} \mathrm{d}^3\boldsymbol{r} \mathrm{d}^3\boldsymbol{k} \mathrm{d}^3\boldsymbol{k}' - \\
&\frac{1}{8\pi} \int\int\int [(\boldsymbol{k}\cdot\boldsymbol{k}')(\boldsymbol{a}^*(\boldsymbol{k})\cdot\boldsymbol{a}^*(\boldsymbol{k}')) - (\boldsymbol{a}^*(\boldsymbol{k})\cdot\boldsymbol{k}')(\boldsymbol{k}\cdot\boldsymbol{a}^*(\boldsymbol{k}'))] e^{-i(\boldsymbol{k}+\boldsymbol{k}')\boldsymbol{r}} \mathrm{d}^3\boldsymbol{r} \mathrm{d}^3\boldsymbol{k} \mathrm{d}^3\boldsymbol{k}' - \\
&\frac{1}{8\pi} \int\int\int [(\boldsymbol{k}\cdot\boldsymbol{k}')(\boldsymbol{a}(\boldsymbol{k})\cdot\boldsymbol{a}(\boldsymbol{k}')) - (\boldsymbol{a}(\boldsymbol{k})\cdot\boldsymbol{k}')(\boldsymbol{k}\cdot\boldsymbol{a}(\boldsymbol{k}'))] e^{i(\boldsymbol{k}+\boldsymbol{k}')\boldsymbol{r}} \mathrm{d}^3\boldsymbol{r} \mathrm{d}^3\boldsymbol{k} \mathrm{d}^3\boldsymbol{k}' + \\
&\frac{1}{8\pi} \int\int\int [(\boldsymbol{k}\cdot\boldsymbol{k}')(\boldsymbol{a}(\boldsymbol{k})\cdot\boldsymbol{a}^*(\boldsymbol{k}')) - (\boldsymbol{a}(\boldsymbol{k})\cdot\boldsymbol{k}')(\boldsymbol{k}\cdot\boldsymbol{a}^*(\boldsymbol{k}'))] e^{i(\boldsymbol{k}-\boldsymbol{k}')\boldsymbol{r}} \mathrm{d}^3\boldsymbol{r} \mathrm{d}^3\boldsymbol{k} \mathrm{d}^3\boldsymbol{k}' \\
=& 2\pi^2 \int k^2 \boldsymbol{a}^*(\boldsymbol{k})\boldsymbol{a}(\boldsymbol{k}) \mathrm{d}^3\boldsymbol{k} + 2\pi^2 \int k^2 \Re[\boldsymbol{a}(\boldsymbol{k})\boldsymbol{a}(-\boldsymbol{k})] \mathrm{d}^3\boldsymbol{k}
\end{aligned}
$$

Combining the two terms above, and substituting $\boldsymbol{a}(\boldsymbol{k})$ using Eq. (18.5.48), we have

$$
\begin{aligned}
\mathscr{H} &= 4\pi^2 \int k^2 \boldsymbol{a}^*(\boldsymbol{k})\boldsymbol{a}(\boldsymbol{k}) \mathrm{d}^3\boldsymbol{k} \\
&= \int \frac{c^2k^2}{\omega} \sum_{\lambda=1}^{2} \boldsymbol{a}^*(\boldsymbol{k}\lambda)\boldsymbol{a}(\boldsymbol{k}\lambda) \mathrm{d}^3\boldsymbol{k} \\
&= \sum_{\lambda=1}^{2} \int \omega \boldsymbol{a}^*(\boldsymbol{k}\lambda)\boldsymbol{a}(\boldsymbol{k}\lambda) \mathrm{d}^3\boldsymbol{k}.
\end{aligned}
$$

Page 515, Eq. (18.5.67)

Below is the derivation. (When applying $\boldsymbol{A} \times (\boldsymbol{B} \times \boldsymbol{C}) = (\boldsymbol{A}\cdot\boldsymbol{C})\boldsymbol{B} - (\boldsymbol{A}\cdot\boldsymbol{B})\boldsymbol{C}$, we will omit the last term since we know they will be later eliminated through $\delta^3(\boldsymbol{k} \pm \boldsymbol{k}')$ and $\boldsymbol{a}(\boldsymbol{k})\cdot\boldsymbol{k} = 0$ any way.)

$$
\begin{aligned}
\mathscr{P} &= \frac{1}{4\pi c} \int (\boldsymbol{E} \times \boldsymbol{B}) \mathrm{d}^3\boldsymbol{r} \\
&= -\int (\boldsymbol{\Pi} \times (\nabla \times \boldsymbol{A})) \mathrm{d}^3\boldsymbol{r} \\
&= -\frac{1}{4\pi i c} \int \left(\int k[\boldsymbol{a}(\boldsymbol{k}) e^{i\boldsymbol{k}\boldsymbol{r}} - \boldsymbol{a}^*(\boldsymbol{k}) e^{-i\boldsymbol{k}\boldsymbol{r}}] \mathrm{d}^3\boldsymbol{k} \right) \times \left(\nabla \times \int [\boldsymbol{a}(\boldsymbol{k}') e^{i\boldsymbol{k}'\boldsymbol{r}} + \boldsymbol{a}^*(\boldsymbol{k}') e^{-i\boldsymbol{k}'\boldsymbol{r}}] \mathrm{d}^3\boldsymbol{k}' \right) \mathrm{d}^3\boldsymbol{r} \\
&= -\frac{1}{4\pi c} \int\int\int k \left[\boldsymbol{a}(\boldsymbol{k}) e^{i\boldsymbol{k}\boldsymbol{r}} - \boldsymbol{a}^*(\boldsymbol{k}) e^{-i\boldsymbol{k}\boldsymbol{r}} \right] \times \left[\boldsymbol{k}' \times \boldsymbol{a}(\boldsymbol{k}') e^{i\boldsymbol{k}'\boldsymbol{r}} - \boldsymbol{k}' \times \boldsymbol{a}^*(\boldsymbol{k}') e^{-i\boldsymbol{k}'\boldsymbol{r}} \right] \mathrm{d}^3\boldsymbol{r} \mathrm{d}^3\boldsymbol{k} \mathrm{d}^3\boldsymbol{k}' \\
&= -\frac{1}{4\pi c} \int\int\int k \left[(\boldsymbol{a}(\boldsymbol{k})\cdot\boldsymbol{a}(\boldsymbol{k}'))\boldsymbol{k}' e^{i(\boldsymbol{k}+\boldsymbol{k}')\boldsymbol{r}} - (\boldsymbol{a}(\boldsymbol{k})\cdot\boldsymbol{a}^*(\boldsymbol{k}'))\boldsymbol{k}' e^{i(\boldsymbol{k}-\boldsymbol{k}')\boldsymbol{r}} - (\boldsymbol{a}^*(\boldsymbol{k})\cdot\boldsymbol{a}(\boldsymbol{k}'))\boldsymbol{k}' e^{-i(\boldsymbol{k}-\boldsymbol{k}')\boldsymbol{r}} + (\boldsymbol{a}^*(\boldsymbol{k}) \right. \\
&= \frac{4\pi^2}{c} \int k \left[(\boldsymbol{a}(\boldsymbol{k})\cdot\boldsymbol{a}^*(\boldsymbol{k}))\boldsymbol{k} + \Re[\boldsymbol{a}(\boldsymbol{k})\cdot\boldsymbol{a}(-\boldsymbol{k})]\boldsymbol{k} \right] \mathrm{d}^3\boldsymbol{k}
\end{aligned}
$$

The second term in the integrand does not matter because it will be cancelled when we take $\boldsymbol{k} = -\boldsymbol{k}$. Therefore,

$$\begin{aligned}\mathscr{P} &= \frac{4\pi^2}{c}\int k\left(\boldsymbol{a}(\boldsymbol{k})\cdot\boldsymbol{a}^*(\boldsymbol{k})\right)\boldsymbol{k}\mathrm{d}^3\boldsymbol{k}\\ &= \sum_{\lambda=1}^{2}\int \frac{kc}{\omega}(a(\boldsymbol{k}\lambda)a^*(\boldsymbol{k}\lambda))\,\boldsymbol{k}\mathrm{d}^3\boldsymbol{k}\\ &= \sum_{\lambda=1}^{2}\int (a(\boldsymbol{k}\lambda)a^*(\boldsymbol{k}\lambda))\,\boldsymbol{k}\mathrm{d}^3\boldsymbol{k}.\end{aligned}$$

The quantization of the classical result above is to replace $a(\boldsymbol{k}\lambda)a^*(\boldsymbol{k}\lambda)$ by $\hbar\frac{a(\boldsymbol{k}\lambda)a^\dagger(\boldsymbol{k}\lambda)+a^\dagger(\boldsymbol{k}\lambda)a(\boldsymbol{k}\lambda)}{2}$, and we we have

$$\begin{aligned}\boldsymbol{P} &= \sum_{\lambda=1}^{2}\int \hbar\frac{a(\boldsymbol{k}\lambda)a^\dagger(\boldsymbol{k}\lambda)+a^\dagger(\boldsymbol{k}\lambda)a(\boldsymbol{k}\lambda)}{2}\boldsymbol{k}\mathrm{d}^3\boldsymbol{k}\\ &= \sum_{\lambda=1}^{2}\int \hbar\left(a^\dagger(\boldsymbol{k}\lambda)a(\boldsymbol{k}\lambda)+\frac{1}{2}\right)\boldsymbol{k}\mathrm{d}^3\boldsymbol{k}.\end{aligned}$$

Again, the $\frac{1}{2}$ does not matter because it will be cancelled when we take $\boldsymbol{k}=-\boldsymbol{k}$. Therefore,

$$\boldsymbol{P} = \sum_{\lambda=1}^{2}\int \left(a^\dagger(\boldsymbol{k}\lambda)a(\boldsymbol{k}\lambda)\right)\hbar\boldsymbol{k}\mathrm{d}^3\boldsymbol{k}.$$

Page 517, discussion about photon's spin

Recall that an infinitesimal rotation around the z axis is $I-i\mathrm{d}\theta S_z/\hbar$. Invariance under such a rotation requires that $s_z=0$.

Page 520, Eq. (18.5.89)

The equation at the bottom of the previous page sums over all directions but not both polarizations. One needs to multiply it by 2 to count for both $\lambda=1$ and $\lambda=2$ and get the factor $(\frac{2}{3})^8$.

Solutions

Chapter 21 - Path Integrals: Part Invariance

This is probably the most interesting chapter of the whole book. Unfortunately there are no solutions available online, except here.

Errata

Page 598, Eq. (21.1.82)

The left-hand side should be $e^{iS/\hbar}$ instead of just S.

Page 631, Eq. (21.2.82)

It should be $\ln\lambda_0$ instead of just λ_0.

Notes

Page 602, Eqs. (21.1.102) and (21.1.103)

The factor C is missing in the Hamiltonian. But it does not matter in further calculations, because both the numerator and the denominator in Eq. (21.1.107) would be scaled by C^2 and the result would be the same.

Page 604, Eq. (21.1.111)

The mathematically inclined should notice that there is no guarantee that each $\boldsymbol{f}$ can be mapped to a unique f_0. (For example, we can simply set $\boldsymbol{f}$ to be a constant for any point in parameter space.) But it does not really matter due to the argument under Eq. (21.1.112).

Page 631, Eqs. (21.2.88), (21.2.89), and (21.2.90)

Strictly speaking, we should have

$$T = e^{-H\tau/\hbar},$$

$$H = -\frac{\hbar}{\tau} K^* \sigma_1,$$

and

$$f = -\frac{\tau}{\hbar} E_0 = K^*.$$

Solutions

Exercise 21.1.1

The answer is exactly the same as the derivation leading to Eq. (5.1.10). The only difference is that for some unknown reason, the definition of $|p\rangle$ here as in Eq. (21.1.14) is unnormalized and misses a factor of $\frac{1}{\sqrt{2\pi\hbar}}$. As a consequence, the resolution of identity as in Eq. (21.1.13) has an extra factor correspondingly.

Exercise 21.1.2

There isn't anything new compared to Exercise (12.3.8). The commutation rules for (Q', P') can be derived similarly to those of (Q, P).

Exercise 21.1.3

From Eq. (21.1.39), we have

$$\frac{\partial}{\partial x} = \frac{\partial}{\partial z} + \frac{\partial}{\partial z^*},$$

and

$$\frac{\partial}{\partial y} = i\frac{\partial}{\partial z} - i\frac{\partial}{\partial z^*}.$$

In the coordinate representation, using both the equalities above and the definition of ω_0, we have

$$\begin{aligned}
a &= \sqrt{\frac{\mu\omega_0}{2\hbar}} Q + \frac{iP}{\sqrt{2\mu\omega_0\hbar}} \\
&= \sqrt{\frac{c}{2\hbar qB}}(-i\hbar\frac{\partial}{\partial x} + qyB/2c) + \sqrt{\frac{c}{2\hbar qB}}(\hbar\frac{\partial}{\partial y} - iqBx/2c) \\
&= \sqrt{\frac{c}{2\hbar qB}}(-i\hbar\frac{\partial}{\partial x} + \hbar\frac{\partial}{\partial y}) + \sqrt{\frac{c}{2\hbar qB}}(-iqBx/2c + qyB/2c) \\
&= -i\sqrt{\frac{2\hbar c}{qB}}\frac{\partial}{\partial z^*} - \frac{i}{2}\sqrt{\frac{qB}{2\hbar c}}(x + iy) \\
&= -i\sqrt{\frac{2\hbar c}{qB}}(\frac{\partial}{\partial z^*} + \frac{qB}{4\hbar c}z),
\end{aligned}$$

from which Eqs. (21.1.38) and (21.1.41) follow.

The probability density is concentrated at radius r_m that maximizes

$$r_m \psi^*_{0,m}\psi_{0,m} = r_m^{2m+1} e^{-\frac{qBr_m^2}{2\hbar c}}.$$

Setting its derivative to zero gives us

$$r_m = \sqrt{\frac{(2m+1)\hbar c}{qB}} \approx \sqrt{\frac{2m\hbar c}{qB}}$$

for large m.

By requiring $r_m \leq R$, we get Eq. (21.1.43).

Exercise 21.1.4

It is easy to show from Eq. (21.1.47) that

$$\boldsymbol{v} \cdot \boldsymbol{\nabla} V = \dot{x}\frac{\partial V}{\partial x} + \dot{y}\frac{\partial V}{\partial y} = 0.$$

Hence $\boldsymbol{v}$ and $\boldsymbol{\nabla} V$ are orthogonal, and the motion is on contours of constant V.

Exercise 21.1.5

Trivial.

Exercise 21.1.6

Eq. (21.1.49) is antisymmetric, because when we switch z_i and z_j, the following happen.

- $(z_i - z_j)$ switches sign;
- Any term involving z_k, where $k < \min(i, j)$ or $k > \max(i, j)$, keeps its original sign;
- Any term involving z_k, where $\min(i, j) < k < \max(i, j)$, switches its sign.

The first case takes place once, while the last one takes place twice with each k. In total there are an odd number of sign switchings.

For the three particle case, Eq. (21.1.49) gives us

$$\begin{aligned}
&(z_2 - z_1)(z_3 - z_1)(z_3 - z_2) \\
=\ & z_2 z_3 z_3 - z_2 z_3 z_2 - z_2 z_1 z_3 + z_2 z_1 z_2 - z_1 z_3 z_3 + z_1 z_3 z_2 + z_1 z_1 z_3 - z_1 z_1 z_2 \\
=\ & z_1^0 z_2^1 z_3^2 - z_1^0 z_2^2 z_3^1 + z_1^1 z_2^2 z_3^0 - z_1^1 z_2^0 z_3^2 + z_1^2 z_2^0 z_3^1 - z_1^2 z_2^1 z_3^0,
\end{aligned}$$

which is exactly the same as what Eq. (10.3.36) would give us.

Exercise 21.1.7

First of all, it should be noted that both $\psi(R', \varepsilon)$ and $\psi(R' + \eta, 0)$ in Eq. (21.1.74) refer to the wave functions of the nucleus.

Eq. (21.1.74) is obtained by treating Eq. (21.1.71), which includes the $\langle n(R')|n(R'+\eta)\rangle$ term, as $U(R', \varepsilon; R, 0)$ and then apply Eq. (5.1.12), except that

- $V(R)$ is taken to be 0 everywhere;
- E_n, the extra potential from the electron, is ignored.

All odd powers of η in the product of Eq. (21.1.76) and Eq. (21.1.76) can be ignored, because any symmetric integral of an odd function is 0. Eq. (21.1.74) is thus simplied as follows.

$$\begin{aligned}
&\psi(R, \varepsilon) \\
=\ & \sqrt{\frac{m}{2\pi\hbar i\varepsilon}} \int_{-\infty}^{\infty} e^{im\eta^2/2\hbar\varepsilon} \langle n(R)|n(R+\eta)\rangle \psi(R+\eta, 0) \mathrm{d}\eta \\
=\ & \sqrt{\frac{m}{2\pi\hbar i\varepsilon}} \int_{-\infty}^{\infty} e^{im\eta^2/2\hbar\varepsilon} \psi(R, 0) \mathrm{d}\eta + \\
& \sqrt{\frac{m}{2\pi\hbar i\varepsilon}} \int_{-\infty}^{\infty} e^{im\eta^2/2\hbar\varepsilon} \eta^2 \left(\frac{1}{2}\frac{\partial^2 \psi}{\partial R^2} + \langle n|\partial n\rangle \frac{\partial \psi}{\partial R} + \frac{1}{2}\langle n|\partial^2 n\rangle \psi(R, 0) \right) \mathrm{d}\eta \\
=\ & \psi(R, 0) + \frac{i\hbar\varepsilon}{m} \left(\frac{1}{2}\frac{\partial^2 \psi}{\partial R^2} + \langle n|\partial n\rangle \frac{\partial \psi}{\partial R} + \frac{1}{2}\langle n|\partial^2 n\rangle \psi(R, 0) \right)
\end{aligned}$$

This directly leads to Eq. (21.1.78).

Exercise 21.1.8

Substituting Eqs. (21.1.80) and (21.1.81) into Eq. (21.1.79) and using $\langle n|\partial n\rangle = -\langle \partial n|n\rangle$, we have, in the coordinate basis,

$$
\begin{aligned}
& H\psi(R) \\
= & \frac{1}{2m}\left(-i\hbar\frac{\partial}{\partial R}-i\hbar\langle n|\partial n\rangle\right)^2\psi(R)+\frac{\hbar^2}{2m}[\langle\partial n|\partial n\rangle-\langle\partial n|n\rangle\langle n|\partial n\rangle]\,\psi(R) \\
= & -\frac{\hbar^2}{2m}\left(\frac{\partial^2\psi(R)}{\partial R^2}+\frac{\partial\left(\langle n|\partial n\rangle\psi(R)\right)}{\partial R}+\langle n|\partial n\rangle\frac{\partial\psi(R)}{\partial R}+\langle n|\partial n\rangle^2\psi(R)\right)+\frac{\hbar^2}{2m}[\langle\partial n|\partial n\rangle-\langle\partial n|n\rangle\langle n|\partial n\rangle]\,\psi(R) \\
= & -\frac{\hbar^2}{2m}\left(\frac{\partial^2\psi(R)}{\partial R^2}+\frac{\partial\langle n|\partial n\rangle}{\partial R}\psi(R)+2\langle n|\partial n\rangle\frac{\partial\psi(R)}{\partial R}\right)+\frac{\hbar^2}{2m}\langle\partial n|\partial n\rangle\psi(R) \\
= & -\frac{\hbar^2}{2m}\left(\frac{\partial^2\psi(R)}{\partial R^2}+\left(\langle\partial n|\partial n\rangle+\langle n|\partial^2 n\rangle\right)\psi(R)+2\langle n|\partial n\rangle\frac{\partial\psi(R)}{\partial R}-\langle\partial n|\partial n\rangle\psi(R)\right) \\
= & -\frac{\hbar^2}{2m}\left(\frac{\partial^2\psi(R)}{\partial R^2}+\langle n|\partial^2 n\rangle\psi(R)+2\langle n|\partial n\rangle\frac{\partial\psi(R)}{\partial R}\right),
\end{aligned}
$$

consistent with Eq. (21.1.78).

Exercise 21.1.9

By taking the derivative of $\langle n|n\rangle=1$, we have

$$\langle n|\partial n\rangle+\langle\partial n|n\rangle=0,$$

and by taking its derivative again, we have

$$\langle n|\partial^2 n\rangle+\langle\partial^2 n|n\rangle+2\langle\partial n|\partial n\rangle=0.$$

These two relationships will be used in further derivation.

It is obvious that a Taylor series per Eq. (21.1.77) will lead to a result containing $A^n(R')$ rather than $A^n(\frac{R+R'}{2})$.

Instead, we have the following. Note that $|n\rangle$, $|\partial n\rangle$, and $|\partial^2 n\rangle$ without any parameter R are all meant to be taken at $\frac{R+R'}{2}$. Also, all higher order terms than $(R'-R)^2$ are ignored.

$$
\begin{aligned}
& \langle n(R')|n(R)\rangle \\
= & \left(\langle n|+\frac{R'-R}{2}\langle\partial n|+\frac{(R'-R)^2}{8}\langle\partial^2 n|\right)\left(|n\rangle+\frac{R-R'}{2}|\partial n\rangle+\frac{(R-R')^2}{8}|\partial^2 n\rangle\right) \\
= & I+\frac{R'-R}{2}(\langle\partial n|n\rangle-\langle n|\partial n\rangle)+\frac{(R'-R)^2}{8}(-2\langle\partial n|\partial n\rangle+\langle\partial^2 n|n\rangle+\langle n|\partial^2 n\rangle) \\
= & I-(R'-R)\langle n|\partial n\rangle-\frac{(R'-R)^2}{2}\langle\partial n|\partial n\rangle \\
= & e^{-(R'-R)\langle n|\partial n\rangle-\frac{(R'-R)^2}{2}\langle n|\partial n\rangle^2-\frac{(R'-R)^2}{2}\langle\partial n|\partial n\rangle} \\
= & e^{-(R'-R)\langle n|\partial n\rangle-\frac{(R'-R)^2}{2}\langle\partial n|(I-|n\rangle\langle n|)|\partial n\rangle}
\end{aligned}
$$

Combined with the factor from Eq. (21.1.72), we get Eq. (21.1.82), as desired.

Exercise 21.1.10

Compared to Eq. (21.1.79), I plays the role of m, and ϕ plays the role of R. Therefore the factor $2m$ in Eq. (21.1.81) should be replaced by $2I=1$ here.

The calculations themselves are trivial and is omitted here.

Exercise 21.1.11

The downward spinor can be chosen as $|\theta\phi\rangle=\begin{bmatrix}-\sin\frac{\theta}{2}\\ i\cos\frac{\theta}{2}e^{i\phi}\end{bmatrix}$. (See Eq. (14.3.28b).)

Correspondingly, we have

$$A^-(\phi)=i\hbar\langle\theta\phi|\frac{\partial}{\partial\phi}|\theta\phi\rangle=-\hbar\cos^2\frac{\theta}{2},$$

$$\Phi=\frac{\hbar^2\sin^2\theta}{4}.$$

Eq. (21.1.91) becomes

$$E^-=\lambda^2+BC,$$

and Eq. (21.1.93) becomes

$$\lambda = m\hbar - A^- = \left(m + \cos^2\frac{\theta}{2}\right)\hbar.$$

Finally Eq. (21.1.94) becomes

$$E^- = \left(m + \cos^2\frac{\theta}{2}\right)^2\hbar^2 + BC.$$

Exercise 21.1.12

Its solution is exactly the same as that to Exercise 21.1.8.

Exercise 21.1.13

Let's first calculate $\mathscr{B}^\uparrow$. Note here $\uparrow$ is taken to be the direction of $\boldsymbol{R}$.

$$\begin{aligned}
&\mathscr{B}_k^\uparrow \\
=& \frac{1}{2}\epsilon_{ijk}F_{ij}^\uparrow \\
=& \frac{1}{2}\epsilon_{ijk}\frac{i\hbar}{4R^2}(\langle\uparrow|\sigma_i|\downarrow\rangle\langle\downarrow|\sigma_j|\uparrow\rangle - \langle\uparrow|\sigma_j|\downarrow\rangle\langle\downarrow|\sigma_i|\uparrow\rangle) \\
=& \frac{1}{2}\epsilon_{ijk}\frac{i\hbar}{4R^2}\sum_{m=\uparrow,\downarrow}(\langle\uparrow|\sigma_i|m\rangle\langle m|\sigma_j|\uparrow\rangle - \langle\uparrow|\sigma_j|m\rangle\langle m|\sigma_i|\uparrow\rangle) \\
=& \frac{1}{2}\epsilon_{ijk}\frac{i\hbar}{4R^2}\langle\uparrow|[\sigma_i,\sigma_j]|\uparrow\rangle \\
=& -\frac{\hbar}{2R^2}\langle\uparrow|\sigma_k|\uparrow\rangle
\end{aligned}$$

So the only non-zero component is $\mathscr{B}_z^\uparrow = -\frac{\hbar}{2R^2}$ and therefore we have

$$\mathscr{B}^\uparrow = -\hbar\frac{\hat{\boldsymbol{R}}}{2R^2}.$$

The sign is simply reversed for the $\downarrow$ state.

Exercise 21.1.14

Note that there is no reason why we have to use Cartesian coordinates in *parameter space*. In fact, we can also use spherical coordinates. Then we have

$$\begin{aligned}
r &= \sqrt{B_1^2 + B_2^2} \\
\theta &= \arctan\frac{B_2}{B_1} \\
\phi &= \phi' + \frac{\pi}{2},
\end{aligned}$$

where ϕ' is the azimuthal angle in *real space*.

A^+, expressed as a ϕ-derivative, is exactly the same in both real space and parameter space, and so is the line integral. (However, the vector $\boldsymbol{A}^+$ are certainly different in both spaces. In real space, its magnitude has a factor of $\frac{1}{r}$, where r is the radius of the circle. In parameter space, on the other hand, it has a factor of $\frac{1}{B_2}$.)

Exercise 21.1.15

Note that the magnitude of $\boldsymbol{A}$ is indeed $\frac{1}{B_2}\cdot i\hbar\langle\theta\phi|\frac{\partial}{\partial\phi}|\theta\phi\rangle$. The factor $\frac{1}{B_2}$ is there because $\mathrm{d}\boldsymbol{R} = B_2\mathrm{d}\phi\boldsymbol{e}_\phi$.

Around the south pole, the line integral is

$$A(2\pi R\sin\theta) = -2\pi\hbar\sin^2\frac{\pi}{2} = -2\pi\hbar.$$

The singularity around the north pole can be shown similarly.

Exercise 21.1.16

Below is the derivation.

$$\begin{aligned}
&\int \frac{\mathrm{d}x\mathrm{d}y}{\pi}|z\rangle\langle z|e^{-z^*z} \\
=&\int \frac{\mathrm{d}x\mathrm{d}y}{\pi}\sum_{n,m}\frac{z^n}{\sqrt{n!}}\frac{z^{*m}}{\sqrt{m!}}|n\rangle\langle m|e^{-z^*z} \\
=&\sum_{n,m}\int \frac{r\mathrm{d}r\mathrm{d}\theta}{\pi}\frac{r^{n+m}e^{i\theta(n-m)}}{\sqrt{n!}\sqrt{m!}}|n\rangle\langle m|e^{-r^2} \\
=&\sum_{n,m}\frac{|n\rangle\langle m|}{\pi\sqrt{n!}\sqrt{m!}}\int_0^\infty r^{n+m+1}e^{-r^2}\mathrm{d}r\int_0^{2\pi}e^{i\theta(n-m)}\mathrm{d}\theta
\end{aligned}$$

Note that the integral on θ will be zero unless $m=n$. We have thus

$$\begin{aligned}
&\int \frac{\mathrm{d}x\mathrm{d}y}{\pi}|z\rangle\langle z|e^{-z^*z} \\
=&\sum_{n}\frac{2\pi|n\rangle\langle n|}{\pi n!}\int_0^\infty r^{2n+1}e^{-r^2}\mathrm{d}r \\
=&\sum_{n}\frac{|n\rangle\langle n|}{n!} \\
=&I.
\end{aligned}$$

Exercise 21.1.17

$$\begin{aligned}
&a^2a^\dagger \\
=&[a^2,a^\dagger]+a^\dagger a^2 \\
=&a[a,a^\dagger]+[a,a^\dagger]a+a^\dagger a^2 \\
=&a^\dagger a^2+2a
\end{aligned}$$

Exercise 21.1.18

From

$$\begin{aligned}
&0 \\
=&(a-z)|z\rangle \\
=&(\sqrt{\frac{m\omega}{2\hbar}}x-z)\psi_z(x)+i\sqrt{\frac{1}{2m\omega\hbar}}(-i\hbar)\frac{\partial\psi_z(x)}{\partial x} \\
=&(\sqrt{\frac{m\omega}{2\hbar}}x-z)\psi_z(x)+\sqrt{\frac{\hbar}{2m\omega}}\frac{\partial\psi_z(x)}{\partial x}
\end{aligned}$$

we have

$$\ln\psi_z(x)=-\frac{m\omega}{2\hbar}x^2+\sqrt{\frac{2m\omega}{\hbar}}zx+C',$$

or equivalently,

$$\psi_z(x)=Ce^{-\frac{m\omega}{2\hbar}x^2}e^{\sqrt{\frac{2m\omega}{\hbar}}zx}.$$

For the normalization, we have

$$\begin{aligned}
&\langle z'|z\rangle \\
=&C(z')^*C(z)\int_{-\infty}^{\infty}e^{-\frac{m\omega}{\hbar}x^2}e^{\sqrt{\frac{2m\omega}{\hbar}}(z'^*+z)x}\mathrm{d}x \\
=&C(z')^*C(z)\sqrt{\frac{\pi\hbar}{m\omega}}e^{\frac{(z'^*+z)^2}{2}} \\
=&e^{z'^*z}
\end{aligned}$$

One obvious (though non-unique) solution is

$$C(z)=(\frac{m\omega}{\pi\hbar})^{1/4}e^{-z^2/2}.$$

Set $z=\sqrt{\frac{m\omega}{2\hbar}}x_0+i\sqrt{\frac{1}{2m\omega\hbar}}p_0$, we have

$$
\begin{aligned}
&\psi_z(x) \\
&= (\frac{m\omega}{\pi\hbar})^{1/4} e^{-z^2/2} e^{-\frac{m\omega}{2\hbar}x^2} e^{\sqrt{\frac{2m\omega}{\hbar}}zx} \\
&= (\frac{m\omega}{\pi\hbar})^{1/4} e^{-\frac{m\omega}{4\hbar}{x_0}^2} e^{\frac{1}{4m\omega\hbar}{p_0}^2} e^{-\frac{ip_0x_0}{2\hbar}} e^{-\frac{m\omega}{2\hbar}x^2} e^{\frac{m\omega}{\hbar}x_0x} e^{\frac{ip_0x}{\hbar}} \\
&= (\frac{m\omega}{\pi\hbar})^{1/4} e^{\frac{m\omega}{4\hbar}{x_0}^2} e^{\frac{1}{4m\omega\hbar}{p_0}^2} e^{\frac{ip_0x_0}{2\hbar}} e^{\frac{ip_0(x-x_0)}{\hbar}} e^{-\frac{m\omega}{2\hbar}(x-x_0)^2} \\
&= (\frac{m\omega}{\pi\hbar})^{1/4} e^{\frac{r^2}{2}} e^{\frac{ip_0x_0}{2\hbar}} e^{\frac{ip_0(x-x_0)}{\hbar}} e^{-\frac{m\omega}{2\hbar}(x-x_0)^2},
\end{aligned}
$$

where r is the magnitude of z.

At time t, $|z\rangle \to |ze^{-i\omega t}\rangle$, and we can easily see that

- r_0 and p_0 behaves as in a classical oscillator of angular velocity ω;
- $\psi_z(x)$ behaves like a Gaussian packet oscillating at angular velocity ω.

Exercise 21.1.19

Substituting Eqs. (21.1.151) and (21.1.152) into the exponent in Eq. (21.1.143), we have

$$
\begin{aligned}
&{z_f}^* z_f + \frac{i}{\hbar}\int_0^t [i\hbar z^* \frac{\mathrm{d}z}{\mathrm{d}t} - H(z^*, z)]\mathrm{d}t \\
&= {z_f}^* z_f + \frac{i}{\hbar}\int_0^t [i\hbar(-i\omega){z_f}^* e^{i\omega(t-T)} z_i e^{-i\omega t} - \hbar\omega {z_f}^* z_i e^{i\omega(t-T)} e^{i\omega t}]\mathrm{d}t \\
&= {z_f}^* z_f.
\end{aligned}
$$

Exercise 21.1.20

Trivial.

Exercise 21.1.21

First note that we do not need to care about the prefactor, which has no dependence on x_1 or x_2, because $V(x)$ is quadratic. (See the discussion under Eq. (8.6.11).)

There are a few ways the solve this problem.

The most obvious, but also most tedious, is to substitute z_i, ${z_i}^*$, z_f, ${z_f}^*$ by x_i, y_i, x_f, y_f, and eliminate the latter one by one.

An easier way is to realize that one could simply take the partial derivatives of the exponent on each of the four variables, i.e. x_i, y_i, x_f, y_f, and solve them simulatenously.

Finally, one can also treat x_i, y_i, x_f, y_f as functions of z_i, ${z_i}^*$, z_f, ${z_f}^*$, which are considered *independent* variables. After all, variables like x_i, y_i are not required to be real when we solve the simulatenous equations in the previous approach. It should be noted that now z_i and ${z_i}^*$ are no longer complex conjugates to each other. The chain rule implies then that the partial derivative of the exponent on z_i (or ${z_i}^*$, etc.), being a linear combination of the partial derivaties on x_i and y_i, must also vanish.

Below is the derivation using the last approach.

$$
\begin{aligned}
&\langle x_2|U(T)|x_1\rangle \\
&= \int \frac{\mathrm{d}x_f \mathrm{d}y_f \mathrm{d}x_i \mathrm{d}y_i}{\pi^2} \langle x_2|z_f\rangle e^{-{z_f}^* z_f} \langle z_f|U(T)|z_i\rangle e^{-{z_i}^* z_i} \langle z_i|x_1\rangle \\
&= \frac{1}{\pi^2}\sqrt{\frac{m\omega}{\pi\hbar}} e^{-\frac{m\omega}{2\hbar}({x_1}^2+{x_2}^2)} \int e^{-\frac{{z_f}^2}{2}} e^{\sqrt{\frac{2m\omega}{\hbar}}z_f x_2} e^{-{z_f}^* z_f} e^{z_i {z_f}^* e^{-i\omega T}} e^{-\frac{{z_i}^{*2}}{2}} e^{\sqrt{\frac{2m\omega}{\hbar}}{z_i}^* x_1} e^{-{z_i}^* z_i} \mathrm{d}x_f \mathrm{d}y_f \mathrm{d}x_i \mathrm{d}y_i.
\end{aligned}
$$

(It is clear that neither x_1 nor x_2 appears in any quandratic terms of x_i, y_i, x_f, y_f. Therefore they will not appear in any prefactor in the result of the Gaussian integrals. This is consistent with the claim made in the very beginning.)

Let us denote the exponent as E, The simulatenous equations are

$$
\begin{aligned}
\frac{\partial E}{\partial z_f} &= -z_f + \sqrt{\frac{2m\omega}{\hbar}}\, x_2 - {z_f}^* = 0, \\
\frac{\partial E}{\partial {z_i}^*} &= -{z_i}^* + \sqrt{\frac{2m\omega}{\hbar}}\, x_1 - z_i = 0, \\
\frac{\partial E}{\partial {z_f}^*} &= -z_f + z_i e^{-i\omega T} = 0, \\
\frac{\partial E}{\partial z_i} &= -{z_i}^* + {z_f}^* e^{-i\omega T} = 0.
\end{aligned}
$$

The solution is

$$
\begin{aligned}
z_i &= \sqrt{\frac{2m\omega}{\hbar}}\, \frac{-x_2 + x_1 e^{i\omega T}}{2i \sin \omega T}, \\
{z_f}^* &= \sqrt{\frac{2m\omega}{\hbar}}\, \frac{-x_1 + x_2 e^{i\omega T}}{2i \sin \omega T}, \\
{z_i}^* &= \sqrt{\frac{2m\omega}{\hbar}}\, \frac{x_2 - x_1 e^{-i\omega T}}{2i \sin \omega T}, \\
z_f &= \sqrt{\frac{2m\omega}{\hbar}}\, \frac{x_1 - x_2 e^{-i\omega T}}{2i \sin \omega T}.
\end{aligned}
$$

Substituting these back into the original integral, we have

$$
\begin{aligned}
&\langle x_2 | U(T) | x_1 \rangle \\
&= \frac{1}{\pi^2} \sqrt{\frac{m\omega}{\pi\hbar}}\, e^{-\frac{m\omega}{2\hbar}({x_1}^2 + {x_2}^2)}\, C(T) e^{-\frac{{z_f}^2 + {z_i}^{*2}}{2}}\, e^{\sqrt{\frac{2m\omega}{\hbar}}(z_f x_2 + {z_i}^* x_1)}\, e^{-({z_f}^* z_f + {z_i}^* z_i)}\, e^{z_i {z_f}^* e^{-i\omega T}} \\
&= \frac{1}{\pi^2} \sqrt{\frac{m\omega}{\pi\hbar}}\, e^{-\frac{m\omega}{2\hbar}({x_1}^2 + {x_2}^2)}\, C(T) e^{-\frac{m\omega}{2\hbar \sin^2 \omega T}\left\{\left[-\frac{({x_1}^2 + {x_2}^2)(1 + e^{-2i\omega T})}{2} + 2x_1 x_2 e^{-i\omega T}\right] + \left[4ix_1 x_2 \sin \omega T - 2i({x_1}^2 + {x_2}^2) e^{-i\omega T} \sin \omega T\right] + \left[2({x_1}^2 + {x_2}^2) - 4x_1 x_2\right.\right.} \\
&= \frac{1}{\pi^2} \sqrt{\frac{m\omega}{\pi\hbar}}\, e^{-\frac{m\omega}{2\hbar}({x_1}^2 + {x_2}^2)}\, C(T) e^{-\frac{m\omega}{2\hbar \sin^2 \omega T}\left[-({x_1}^2 + {x_2}^2)(\sin^2 \omega T + i \sin \omega T \cos \omega T) + 2ix_1 x_2 \sin \omega T\right]} \\
&= \frac{1}{\pi^2} \sqrt{\frac{m\omega}{\pi\hbar}}\, C(T) e^{\frac{im\omega}{2\hbar \sin \omega T}\left[({x_1}^2 + {x_2}^2) \cos \omega T - 2x_1 x_2\right]},
\end{aligned}
$$

consistent with the answer to Exercise (8.6.2).

Exercise 21.2.1

From Exercise (8.6.3), we have

$$
A(t) = \sqrt{\frac{m\omega}{2\pi i \hbar \sin \omega t}}.
$$

Substituting $\tau = it$, we have

$$
A(\tau) = \sqrt{\frac{m\omega}{2\pi \hbar \sinh \omega \tau}}.
$$

Taking the limit $\tau \to \infty$, we have

$$
\lim_{\tau \to \infty} A(\tau) = \sqrt{\frac{m\omega}{\pi\hbar}}\, e^{-\frac{\omega\tau}{2}}.
$$

Comparing it to Eqs. (21.2.14) and (21.2.15), we can easily read that ground state is

$$
\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega x^2}{2\hbar}},
$$

and

$$
E_0 = \frac{\hbar\omega}{2}.
$$

Exercise 21.2.2

We have

$$
\begin{aligned}
& T|\theta\rangle \\
&= \frac{1}{\sqrt{N}} \sum_{n=1}^{N} e^{in\theta} T|n\rangle \\
&= \frac{1}{\sqrt{N}} \sum_{n=1}^{N} e^{in\theta} |n+1\rangle \\
&= \frac{1}{\sqrt{N}} \sum_{n=2}^{N+1} e^{-i\theta} e^{in\theta} |n\rangle \\
&= e^{-i\theta} \frac{1}{\sqrt{N}} \sum_{n=1}^{N} e^{in\theta} |n\rangle \\
&= e^{-i\theta} |\theta\rangle.
\end{aligned}
$$

Therefore the eigenvalue is $e^{-i\theta}$.

As $T^N = I$, we have $N\theta = 2k\pi$ and $\theta = \frac{2k\pi}{N}$, where k is any integer. However, k and $k+N$ would give the same $|\theta\rangle$. Therefore the complete set of eigenstates is

$$
|\theta = \frac{2k\pi}{N} >, k = 0, 1, \dots N-1.
$$

Further, we have

$$
\begin{aligned}
& H|\theta\rangle \\
&= \frac{1}{\sqrt{N}} \sum_{n=1}^{N} e^{in\theta} H|n\rangle \\
&= \frac{1}{\sqrt{N}} \sum_{n=1}^{N} e^{in\theta} \sum_{m=1}^{N} \left[E_0 |m\rangle\langle m| - t(|m\rangle\langle m+1| + |m+1\rangle\langle m|) \right] |n\rangle \\
&= \frac{1}{\sqrt{N}} \sum_{n=1}^{N} e^{in\theta} \left[E_0 |n\rangle\langle n| - t(|n-1\rangle\langle n| + |n+1\rangle\langle n|) \right] |n\rangle \\
&= \frac{1}{\sqrt{N}} \sum_{n=1}^{N} e^{in\theta} \left[E_0 |n\rangle - t(|n-1\rangle + |n+1\rangle) \right] \\
&= \frac{1}{\sqrt{N}} \left[E_0 \sum_{n=1}^{N} e^{in\theta} |n\rangle - t(\sum_{n=1}^{N} e^{in\theta} |n-1\rangle + \sum_{n=1}^{N} e^{in\theta} |n+1\rangle) \right] \\
&= \frac{1}{\sqrt{N}} \left[E_0 \sum_{n=1}^{N} e^{in\theta} |n\rangle - t(e^{i\theta} \sum_{n=1}^{N} e^{in\theta} |n\rangle + e^{-i\theta} \sum_{n=1}^{N} e^{in\theta} |n\rangle) \right] \\
&= (E_0 - 2t\cos\theta) \sum_{n=1}^{N} \frac{1}{\sqrt{N}} e^{in\theta} |n\rangle \\
&= (E_0 - 2t\cos\theta) |\theta\rangle.
\end{aligned}
$$

For $N = 2$, we have eigenstates $|\theta = 0\rangle$ and $|\theta = \pi\rangle$, with energy levels $E_0 - 2t$ and $E_0 + 2t$, respectively.

Exercise 21.2.3

From Eq. (21.2.15) and Exercise (21.2.1), we have

$$
U(x, x', \tau) = \sqrt{\frac{m\omega}{2\pi\hbar \sinh\omega\tau}} \exp(-\frac{m\omega}{2\hbar \sinh\omega\tau} [(x^2 + {x'}^2)\cosh\omega\tau - 2xx']).
$$

Therefore,

$$
\begin{aligned}
&Z \\
&= \sqrt{\frac{m\omega}{2\pi\hbar\sinh\omega\tau}} \int_{-\infty}^{\infty} \exp\left(-\frac{m\omega x^2}{\hbar\sinh\omega\tau}(\cosh\omega\tau - 1)\right) \mathrm{d}x \\
&= \sqrt{\frac{m\omega}{2\pi\hbar\sinh\omega\tau}} \sqrt{\frac{\pi\hbar\sinh\omega\tau}{m\omega(\cosh\omega\tau - 1)}} \\
&= \frac{e^{-\frac{\omega\tau}{2}}}{1 - e^{-\omega\tau}} \\
&= e^{-\frac{\omega\tau}{2}} \sum_{n=0}^{\infty} e^{-\omega\tau n} \\
&= \sum_{n=0}^{\infty} e^{-\beta\hbar\omega(n+1/2)}.
\end{aligned}
$$

Exercise 21.2.4

$$
\lambda \approx \frac{\hbar}{p} \approx \frac{\hbar}{\sqrt{mkT}} = \sqrt{\frac{\beta}{m}}\hbar
$$

Exercise 21.2.5

$$
\begin{aligned}
&Z \\
&= \sum_{s_0=-}^{+} \langle s_0 | T^N | s_0 \rangle \\
&= {T^N}_{--} + {T^N}_{++} \\
&= \mathrm{Tr} T^N.
\end{aligned}
$$

Exercise 21.2.6

From Eq. (21.2.85), we have

$$
K^* = \ln\sqrt{\frac{1 + e^{-2K}}{1 - e^{-2K}}},
$$

and

$$
\ln\cosh K^* = \ln\sqrt{\frac{1}{1 - e^{-4K}}},
$$

and finally

$$
f = K^* - \ln\cosh K^* = \ln\left(\sqrt{\frac{1 + e^{-2K}}{1 - e^{-2K}}}\sqrt{1 - e^{-4K}}\right) = \ln(1 + e^{-2K}).
$$

Exercise 21.2.7

Simply notice that in the low temperature limit, where $K^* \to 0$, $K^* \approx \tanh K^* = e^{-2K}$.

Exercise 21.2.8

If we ignore hs_N, which clearly does not matter in the limit $N \to \infty$, we have

$$
Z = \sum_{s_i=\pm 1} \exp\left[\sum_{i=0}^{N-1} K(s_i s_{i+1} - 1) + h s_i\right] = \sum_{s_i=\pm 1} \prod_{i=0}^{N-1} e^{K(s_i s_{i+1} - 1)} e^{h s_i}.
$$

Clearly, Z will remain the same if we simultaneously switch the sign of every s_i in the sum. But this is also equivalent to changing h to $-h$. Hence $Z(h) = Z(-h)$.

We can re-write Eq. (21.2.73) as

$$
Z = \sum_{s_i, s_i'} T_{s_N' s_{N-1}} \cdots T_{s_2' s_1} M_{s_1 s_1'} T_{s_1' s_0} M_{s_0 s_0'},
$$

which is clearly a matrix product. Note that to get the orignal Eq. (21.2.73), we only need to set each $M_{s_i s_i'}$ to the identity matrix $\delta_{s_i s_i'}$. In our current case, we simply need to set

$$M_{++} = e^h, M_{--} = e^{-h}, M_{+-} = M_{-+} = 0,$$

or equivalently

$$M = e^{h\sigma_3}.$$

If we combine T and M and re-label is as T, we have

$$T = e^{K^*\sigma_1} e^{h\sigma_3} \equiv T_k T_h,$$

where as before, $e^{K^*\sigma_1}$ should really be understood as $\frac{e^{K^*\sigma_1}}{\cosh K^*}$.

T is not Hermitian because σ_1 and σ_3 do not commute.

Notice that except for the end points, we can also write Z as

$$Z = \sum_{s_i=\pm 1} \exp\left[\sum_{i=0}^{N-1} \frac{h}{2} s_i + K(s_i s_{i+1} - 1) + \frac{h}{2} s_{i+1}\right] = \sum_{s_i=\pm 1} \prod_{i=0}^{N-1} e^{\frac{h}{2} s_i} e^{K(s_i s_{i+1} - 1)} e^{\frac{h}{2} s_i}.$$

Following the same derivation, we get

$$T = e^{\frac{h}{2}\sigma_3} e^{K^*\sigma_1} e^{\frac{h}{2}\sigma_3} = {T_h}^{1/2} T_k {T_h}^{1/2},$$

which is Hermitian.

From now on, we will always include the prefactor $\cosh K^*$. We have

$$T = \begin{bmatrix} e^h & \tanh K^* \\ \tanh K^* & e^{-h} \end{bmatrix},$$

with eigenvalues $\cosh h \pm \sqrt{\sinh^2 h + \tanh^2 K^*}$ and (non-normalized) eigenvectors

$$\begin{bmatrix} \tanh K^* \\ -\sinh h \pm \sqrt{\sinh^2 h + \tanh^2 K^*} \end{bmatrix}.$$

There is degeneracy only if $\sinh^2 h = \tanh^2 K^* = 0$ or $h = K^* = 0$. Also note that λ_0 and $|0\rangle$ correspond to the $+$ case because K in the partition function is actually positive, contrary to the usual convention.

It is then straightforward to calculate that, after normalizing $|0\rangle$,

$$\langle s \rangle = \langle 0|\sigma_3|0\rangle = \sinh h \frac{\sqrt{\sinh^2 h + \tanh^2 K^*} - \sinh h}{\tanh^2 K^* - \sinh\sqrt{\sinh^2 h + \tanh^2 K^*} + \sinh^2 h},$$

which can be easily shown to be equal to

$$\frac{\partial f}{\partial h} = \frac{\partial \ln \lambda_0}{\partial h}.$$

Exercise 21.2.9

With periodic boundary conditions, we have

$$\begin{aligned} &\langle s_j s_i \rangle \\ &= \frac{\langle 0|T^{N-j}\sigma_3 T^{j-i}\sigma_3 T^i|0\rangle + \langle 1|T^{N-j}\sigma_3 T^{j-i}\sigma_3 T^i|1\rangle}{\langle 0|T^N|0\rangle + \langle 1|T^N|1\rangle} \\ &= \frac{{\lambda_0}^{N-j+i}\langle 1|T^{j-i}|1\rangle + {\lambda_1}^{N-j+i}\langle 0|T^{j-i}|0\rangle}{{\lambda_0}^N + {\lambda_1}^N} \\ &= \frac{{\lambda_0}^{N-j+i}{\lambda_1}^{j-i} + {\lambda_1}^{N-j+i}{\lambda_0}^{j-i}}{{\lambda_0}^N + {\lambda_1}^N} \\ &\approx (\frac{\lambda_1}{\lambda_0})^{j-i} + (\frac{\lambda_1}{\lambda_0})^{N-(j-i)}, \end{aligned}$$

from which it is obvious that the answer is invariant under $j - i \leftrightarrow N - (j - i)$ and that only the first term is needed as long as $j - i$ is much smaller than N.

Exercise 21.2.10

We will use the actual T in the derivation below, instead of first dropping the prefactor $\cosh K^*$ and then recovering it. Note that the corresponding eigenvalues are then $e^{\pm K^*}/\cosh K^*$. Also, at least in the derivation itself, we will use m and n instead of i and j, to avoid confusion with the imaginery number i.

We will also use the following identities.

$$\begin{aligned}\sinh(a+b) &= \sinh a \cosh b + \cosh a \sinh b \\ \cosh(a+b) &= \cosh a \cosh b + \sinh a \sinh b\end{aligned}$$

From Eq. (21.2.84), we have

$$T = \frac{e^{K^*\sigma_1}}{\cosh K^*}.$$

Therefore we have

$$T^m = \frac{e^{mK^*\sigma_1}}{\cosh^m K^*} = \frac{\cosh mk^*(I + \tanh mK^*\sigma_1)}{\cosh^m K^*},$$

and

$$\begin{aligned}&T^{-m}\sigma_3 T^m \\ &= \cosh^2 mK^*(I - \tanh mK^*\sigma_1)\sigma_3(I + \tanh mK^*\sigma_1) \\ &= \cosh^2 mK^*(I - \tanh mK^*\sigma_1)(\sigma_3 + i\tanh mK^*\sigma_2) \\ &= \cosh^2 mK^*(\sigma_3 + i\tanh mK^*\sigma_2 + i\tanh mK^*\sigma_2 + \tanh^2 mK^*\sigma_3) \\ &= \cosh 2mK^*(\sigma_3 + i\tanh 2mK^*\sigma_2).\end{aligned}$$

Now we have

$$\begin{aligned}&\sigma_3(n)\sigma_3(m) \\ &= \cosh 2nK^* \cosh 2mK^*(\sigma_3 + i\tanh 2nK^*\sigma_2)(\sigma_3 + i\tanh 2mK^*\sigma_2) \\ &= \cosh 2nK^* \cosh 2mK^* \left[(1 - \tanh 2mK^* \tanh 2nK^*)I + (\tanh 2mK^* - \tanh 2nK^*)\sigma_1\right] \\ &= \cosh 2(m-n)K^* \left[I + \tanh 2(m-n)K^*\sigma_1\right] \\ &= (T\cosh K^*)^{2(m-n)}\end{aligned}$$

No matter whether we set $|s_0\rangle$ to $+$ or $-$ (or $\uparrow$ or $\downarrow$), the relationship below holds. (The sum of s_N is also over the two values $+$ and $-$.)

$$\sum_{s_N} |s_N\rangle = (I + \sigma_1)|s_0\rangle$$

Now we have, fixing s_0 at one end but leaving s_N open at the other, and keeping in mind that $|0\rangle$ and $|1\rangle$ are the eigenvectors of σ_1 with eigenvalues ± 1,

$$\begin{aligned}&\langle s_j s_i\rangle \\ &= \frac{\sum_{s_N}\langle s_N|T^N\sigma_3(j)\sigma_3(i)|s_0\rangle}{\sum_{s_N}\langle s_N|T^N|s_0\rangle} \\ &= \frac{\langle s_0|(I+\sigma_1)T^N(T\cosh K^*)^{2(i-j)}|s_0\rangle}{\langle s_0|(I+\sigma_1)T^N|s_0\rangle} \\ &= \frac{\langle s_0|(I+\sigma_1)|0\rangle{\lambda_0}^N e^{2(i-j)K^*}\langle 0|s_0\rangle + \langle s_0|(I+\sigma_1)|1\rangle{\lambda_1}^N e^{-2(i-j)K^*}\langle 1|s_0\rangle}{\langle s_0|(I+\sigma_1)|0\rangle{\lambda_0}^N\langle 0|s_0\rangle + \langle s_0|(I+\sigma_1)|1\rangle{\lambda_1}^N\langle 1|s_0\rangle} \\ &= \frac{2\langle s_0|0\rangle{\lambda_0}^N e^{2(i-j)K^*}\langle 0|s_0\rangle}{2\langle s_0|0\rangle{\lambda_0}^N\langle 0|s_0\rangle} \\ &= e^{-2(j-i)K^*}.\end{aligned}$$

Noticing that $\tanh K^* = e^{-2K} \iff \tanh K = e^{-2K^*}$, we see that the result above is consistent with Eq. (21.2.69).

Contact Me

Your name

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