

Lecture 11, February 13, 2006

Solved Homework

We are asked to find $\langle T \rangle$ for the first harmonic oscillator wave function

$$\Psi_0(x) = \left(\frac{\sqrt{k\mu}}{\pi\hbar} \right)^{1/4} e^{-\sqrt{k\mu}x^2/2\hbar}$$

So, for $\langle T \rangle_{n=0}$ we have

$$\langle T \rangle_{n=0} = \int_{-\infty}^{\infty} \left(\frac{\sqrt{k\mu}}{\pi\hbar} \right)^{1/4} e^{-\sqrt{k\mu}x^2/2\hbar} \left(-\frac{\hbar^2}{2\mu} \frac{d^2}{dx^2} \right) \left(\frac{\sqrt{k\mu}}{\pi\hbar} \right)^{1/4} e^{-\sqrt{k\mu}x^2/2\hbar} dx$$

We need to evaluate the second derivative. It is

$$\begin{aligned} \frac{d^2}{dx^2} e^{-\sqrt{k\mu}x^2/2\hbar} &= \frac{d}{dx} \left[\frac{d}{dx} \left(e^{-\sqrt{k\mu}x^2/2\hbar} \right) \right] \\ &= \frac{d}{dx} \left[-\frac{x\sqrt{k\mu}}{\hbar} e^{-\sqrt{k\mu}x^2/2\hbar} \right] \\ &= -\frac{\sqrt{k\mu}}{\hbar} e^{-\sqrt{k\mu}x^2/2\hbar} + \frac{x^2 k\mu}{\hbar^2} e^{-\sqrt{k\mu}x^2/2\hbar} \end{aligned}$$

Thus,

$$\langle T \rangle_{n=0} = -\frac{\hbar^2}{2\mu} \left(\frac{\sqrt{k\mu}}{\pi\hbar} \right)^{1/2} \left[\begin{array}{l} \left(\frac{k\mu}{\hbar^2} \right) \int_{-\infty}^{\infty} x^2 e^{-\sqrt{k\mu}x^2/\hbar} dx \\ - \left(\frac{\sqrt{k\mu}}{\hbar} \right) \int_{-\infty}^{\infty} e^{-\sqrt{k\mu}x^2/\hbar} dx \end{array} \right]$$

We've already evaluated the two integrals in previous work. Using the appropriate formulae provides

$$\begin{aligned}
\langle T \rangle_{n=0} &= -\frac{\hbar^2}{2\mu} \left(\frac{\sqrt{k\mu}}{\pi\hbar} \right)^{1/2} \left[\begin{array}{c} \left(\frac{k\mu}{\hbar^2} \right) \left(\frac{\hbar}{2\sqrt{k\mu}} \right) \left(\frac{\pi\hbar}{\sqrt{k\mu}} \right)^{1/2} \\ - \left(\frac{\sqrt{k\mu}}{\hbar} \right) \left(\frac{\pi\hbar}{\sqrt{k\mu}} \right)^{1/2} \end{array} \right] \\
&= -\frac{\hbar^2}{2\mu} \left(\frac{\sqrt{k\mu}}{\pi\hbar} \right)^{1/2} \left[- \left(\frac{\sqrt{k\mu}}{2\hbar} \right) \left(\frac{\pi\hbar}{\sqrt{k\mu}} \right)^{1/2} \right] \\
&= \frac{\hbar}{4} \sqrt{\frac{k}{\mu}}
\end{aligned}$$

Recall from our last homework that

$$\langle x^2 \rangle_{n=0} = \left(\frac{\hbar}{2\sqrt{k\mu}} \right)$$

The expectation value of the potential energy $\langle V \rangle$ is simply $(k/2)\langle x^2 \rangle$, or

$$\begin{aligned}
\frac{1}{2}k\langle x^2 \rangle_{n=0} &= \frac{k}{2} \left(\frac{\hbar}{2\sqrt{k\mu}} \right) \\
&= \frac{\hbar}{4} \sqrt{\frac{k}{\mu}}
\end{aligned}$$

This completes the proof that $\langle T \rangle = \langle V \rangle$ for the $n = 0$ state of the QMHO. It is similarly straightforward, if increasingly tedious, to prove this for the first excited state, and indeed for *any* state.

Angular Momentum

Angular momentum is a vector quantity, defined as the cross product of the position vector and the momentum vector. In cartesian coordinates, it is most easily expressed as the determinant

$$\mathbf{L} = \begin{vmatrix} \mathbf{i} & \mathbf{j} & \mathbf{k} \\ x & y & z \\ p_x & p_y & p_z \end{vmatrix} \quad (11-1)$$

where x , y , and z are the components of the position vector (i.e., the coefficients multiplying the unit vectors \mathbf{i} , \mathbf{j} , and \mathbf{k} , respectively) and p_x , p_y , and p_z are the

components of the momentum vector. A 3×3 determinant may be evaluated by Cramer's rule (no relation to your enthusiastic instructor, as far as I know...), which states that the determinant is equal to the sum of the three down-right wraparound multiplications minus the sum of the three up-right wraparound multiplications. That is

$$\begin{vmatrix} \mathbf{i} & \mathbf{j} & \mathbf{k} \\ x & y & z \\ p_x & p_y & p_z \end{vmatrix} = yp_z \mathbf{i} + zp_x \mathbf{j} + xp_y \mathbf{k} - yp_x \mathbf{k} - zp_y \mathbf{i} - xp_z \mathbf{j} \quad (11-2)$$

$$= (yp_z - zp_y) \mathbf{i} + (zp_x - xp_z) \mathbf{j} + (xp_y - yp_x) \mathbf{k}$$

Thus, the components of \mathbf{L} , namely, L_x , L_y , and L_z , are the terms in parentheses preceding the corresponding unit vectors. In the absence of a torque on a system, angular momentum is a conserved quantity, just as linear momentum is conserved in the absence of a force on a system.

The magnitude of the angular momentum is (as for any vector quantity) $|\mathbf{L}|^2$ (typically also written L^2 , since it is just a number). From eq. 11-2, that implies

$$L^2 = L_x^2 + L_y^2 + L_z^2 \quad (11-3)$$

In a quantum mechanical system, the discussion thus far continues to apply, except that the momentum components themselves are the operators

$$p_q = -i\hbar \frac{\partial}{\partial q} \quad (11-4)$$

where q is either x , y , or z .

Let us now consider the commutation properties for any two components of the angular momentum. We'll take L_x and L_y as an example. For an arbitrary function f we have

$$\begin{aligned}
[L_x, L_y]f &= \left[\begin{aligned} &(-i\hbar)\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)(-i\hbar)\left(z\frac{\partial f}{\partial x} - x\frac{\partial f}{\partial z}\right) \\ &-(-i\hbar)\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right)(-i\hbar)\left(y\frac{\partial f}{\partial z} - z\frac{\partial f}{\partial y}\right) \end{aligned} \right] \\
&= -\hbar^2 \left[\begin{aligned} &\left(y\frac{\partial f}{\partial x} + yz\frac{\partial^2 f}{\partial x\partial z} - xy\frac{\partial^2 f}{\partial z^2} - z^2\frac{\partial^2 f}{\partial x\partial y} + xz\frac{\partial^2 f}{\partial y\partial z}\right) \\ &\left(-yz\frac{\partial^2 f}{\partial x\partial z} + z^2\frac{\partial^2 f}{\partial x\partial y} + xy\frac{\partial^2 f}{\partial z^2} - x\frac{\partial f}{\partial y} - xz\frac{\partial^2 f}{\partial y\partial z}\right) \end{aligned} \right] \quad (11-5) \\
&= -\hbar^2 \left(y\frac{\partial}{\partial x} - x\frac{\partial}{\partial y} \right) f \\
&= i\hbar L_z f
\end{aligned}$$

So, the commutator is not zero, but instead involves the operator L_z . By symmetry of the operators, it should be clear that

$$\begin{aligned}
[L_x, L_y] &= i\hbar L_z \\
[L_y, L_z] &= i\hbar L_x \\
[L_z, L_x] &= i\hbar L_y
\end{aligned} \quad (11-6)$$

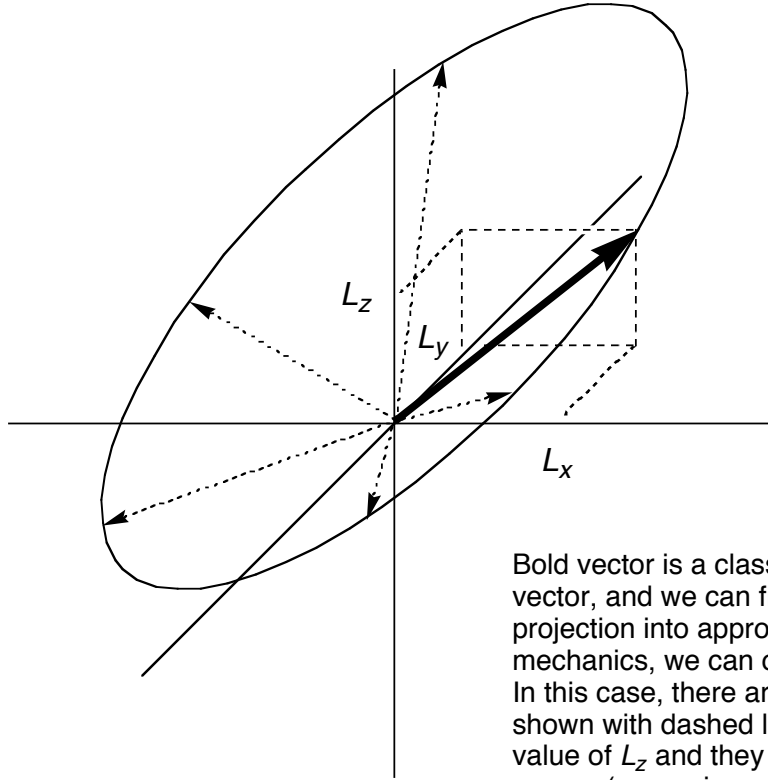
So, from the uncertainty principle, we see that *we can never know more than one component of the angular momentum to perfect accuracy*. In three dimensions, this is equivalent to saying that we can know the angular momentum only to within a circle defining the base of a cone having height equal to the one component we can know. Below is an illustration of this point for the arbitrary case of saying we can know only the z component.

What about the total magnitude of the angular momentum? Can we know it in addition to any one component? To evaluate that, we need to compute the commutator of any one component with L^2 . This one we can do symbolically given our prior results

$$\begin{aligned}
[L^2, L_z] &= [L_x^2 + L_y^2 + L_z^2, L_z] \\
&= [L_x^2, L_z] + [L_y^2, L_z] + [L_z^2, L_z]
\end{aligned} \quad (11-7)$$

To go further, it is helpful to prove a quick property of commutators of a product of two operators with another operator. Note that

$$[AA, B] = AAB - BAA \quad (11-8)$$



Bold vector is a classical angular momentum vector, and we can find its components by projection into appropriate planes. In quantum mechanics, we can only know *one* component. In this case, there are many other vectors (here shown with dashed lines) having the same value of L_z and they define the circular base of a cone (appearing as an ellipse here only because of our perspective).

and that

$$\begin{aligned} [A, B]A + A[A, B] &= ABA - BAA + AAB - ABA \\ &= AAB - BAA \end{aligned} \quad (11-9)$$

Comparing eqs. 11-8 and 11-9 shows us how to continue with equation 11-7

$$\begin{aligned} [L_x^2, L_z] + [L_y^2, L_z] + [L_z^2, L_z] &= [L_x, L_z]L_x + L_x[L_x, L_z] + [L_y, L_z]L_y \\ &\quad + L_y[L_y, L_z] + [L_z, L_z]L_z + L_z[L_z, L_z] \\ &= -i\hbar L_y L_x - i\hbar L_x L_y + i\hbar L_x L_y + i\hbar L_y L_x \quad (11-10) \\ &\quad + 0 \cdot L_z + L_z \cdot 0 \\ &= 0 \end{aligned}$$

Since the commutator is zero, we can simultaneously know both the total angular momentum, and a single component of the angular momentum, but that is all we can know precisely.

Eigenvalues of the Angular Momentum Operators

We can learn a remarkable amount about the angular momentum eigenvalues of a QM system with knowledge only of its commutation relationships, i.e., without knowing the eigenfunctions. To do this, we need to define two new operators, called raising and lowering operators and indicated by "+" and "-" subscripts, respectively. The definitions are

$$L_+ = L_x + iL_y \quad \text{and} \quad L_- = L_x - iL_y \quad (11-11)$$

Let us say that we have an eigenfunction Ψ of L_z and L^2 such that

$$L_z \Psi = m_l \hbar \Psi \quad \text{and} \quad L^2 \Psi = l(l+1)\hbar^2 \Psi \quad (11-12)$$

We will see at the end why we chose those particular names/forms for the eigenvalues, but for now we will just accept them. Now consider the raising operator applied to the first part of eq. 11-12. We see

$$\begin{aligned} L_+ L_z \Psi &= L_+ m_l \hbar \Psi \\ &= m_l \hbar L_+ \Psi \end{aligned} \quad (11-13)$$

Let us evaluate that equation in a somewhat different way

$$\begin{aligned} L_+ L_z \Psi &= (L_z L_+ + L_+ L_z - L_z L_+) \Psi \\ &= (L_z L_+ + [L_+, L_z]) \Psi \\ &= (L_z L_+ + [L_x + iL_y, L_z]) \Psi \\ &= (L_z L_+ - i\hbar L_y - \hbar L_x) \Psi \\ &= (L_z L_+ - \hbar L_+) \Psi \end{aligned} \quad (11-14)$$

Equating the results from eqs. 11-13 and 11-14 gives, after rearrangement

$$L_z L_+ \Psi = (m_l + 1)\hbar L_+ \Psi \quad (11-15)$$

So, evidently $L_+ \Psi$ is an eigenfunction of L_z and its eigenvalue is one h-bar greater than the eigenvalue for Ψ itself. If we were to carry out the same operations with L_- , we would find

$$L_z L_- \Psi = (m_l - 1)\hbar L_- \Psi \quad (11-16)$$

The reason for the naming of these operators should now be clear. The raising operator takes a given angular momentum eigenfunction to another one with the z component of

the angular momentum *greater* by h-bar, and the lowering operator takes it to another one with the z component of the angular momentum lower by one h-bar.

What about the eigenvalue for the total angular momentum: is it affected by the application of the raising and lowering operators? Since the raising and lowering operators are defined in terms of L_x and L_y , and since these two operators both commute with L^2 , the raising and lowering operators must also commute with L^2 . Thus

$$\begin{aligned} L^2 L_{\pm} \Psi &= L_{\pm} L^2 \Psi \\ &= L_{\pm} l(l+1) \hbar^2 \Psi \\ &= l(l+1) \hbar^2 L_{\pm} \Psi \end{aligned} \quad (11-17)$$

So the raising and lowering operators have no effect on the eigenvalue of L^2 . If we picture in our mind the quantum mechanical notion of the angular momentum vector precessing around the circular base of the cone in the above figure with a fixed value for its z component, it is as though the raising and lowering operators move the fixed component up or down one h-bars worth, while the length of the vector remains the same, so a new circle, either smaller (if we stepped so that the angular momentum vector became closer to the z axis) or larger (if we stepped the other way), is traced out by the vector, although the total angular momentum has been conserved.

Now, consider the effect of applying the raising and lowering operators one after another in succession.

$$\begin{aligned} L_+ L_- &= (L_x + iL_y)(L_x - iL_y) \\ &= L_x^2 - iL_x L_y + iL_y L_x + L_y^2 \\ &= L_x^2 + L_y^2 + (L_x^2 - L_y^2) - i[L_x, L_y] \\ &= (L_x^2 + L_y^2 + L_z^2) - L_z^2 - i(i\hbar L_z) \\ &= L^2 - L_z^2 + \hbar L_z \end{aligned} \quad (11-18)$$

In addition, note that the raising operator is the complex conjugate of the lowering operator. Thus, writing the product of the two is just another way of writing their square modulus. The expectation value of the square modulus of an operator must be non-negative, so we can write

$$\langle \Psi | L_+ L_- | \Psi \rangle = \langle \Psi | L^2 - L_z^2 + \hbar L_z | \Psi \rangle \geq 0 \quad (11-19)$$

In this case, Ψ is an eigenfunction of all of the operators on the r.h.s. of the equality in eq. 11-19, so we can quickly solve

$$\begin{aligned}\langle \Psi | L^2 - L_z^2 + \hbar L_z | \Psi \rangle &= \langle \Psi | L^2 | \Psi \rangle - \langle \Psi | L_z^2 | \Psi \rangle + \hbar \langle \Psi | L_z | \Psi \rangle \\ &= [l(l+1) - m_l^2 + m_l] \hbar^2 \geq 0\end{aligned}\quad (11-20)$$

If we carry through the same manipulations in eqs. 11-18 through 11-20 for L_-L_+ , we end up with

$$L_-L_+ = L^2 - L_z^2 - \hbar L_z \quad (11-21)$$

and

$$\begin{aligned}\langle \Psi | L^2 - L_z^2 - \hbar L_z | \Psi \rangle &= \langle \Psi | L^2 | \Psi \rangle - \langle \Psi | L_z^2 | \Psi \rangle - \hbar \langle \Psi | L_z | \Psi \rangle \\ &= [l(l+1) - m_l^2 - m_l] \hbar^2 \geq 0\end{aligned}\quad (11-22)$$

If we now add eq. 11-20 to eq. 11-22, we have

$$l(l+1) \geq m_l^2 \quad (11-23)$$

Thus, there are minimum and maximum values of the z component of the angular momentum given a finite total angular momentum (hardly surprising). Note, however, that the z component can never equal the total angular momentum. From the Heisenberg uncertainty principle, we could have guessed that it could not be the case that the z component was equal to the total (i.e., the angular momentum lay completely along the z axis) because then we would have known the x and y components had to be zero exactly, but we're not allowed to know them exactly and simultaneously.

However, there's a more interesting consequence to the limits imposed on m_l . Since the raising operator applied to any eigenfunction increases its z component angular momentum by \hbar , there will arise a paradox for the wave function whose eigenvalue is already $m_{l,\max}$ (whose square is the last to be less than or equal to $l(l+1)$). Consider the special case of eq. 11-15

$$L_z L_+ \Psi_{\max} = (m_{l,\max} + 1) \hbar L_+ \Psi_{\max} \quad (11-24)$$

The only way in which this equation can be true (and we have already proven that it must be) while at the same time the eigenvalue cannot be greater than $m_{l,\max} \hbar$ is if the raising operator *annihilates* Ψ_{\max} . In that case, the equation will indeed hold true in a trivial sort of way: L_z operating on the wave function identically equal to zero is equal to any scalar multiplying the null wave function: both result in null. The same situation holds true for the lowering operator and the wave function having the minimal value of $m_{l,\min} \hbar$; it is annihilated by L_- .

Let us return, then, to the expectation values of eq. 11-20 and 11-22, but for the special cases of Ψ_{\max} and Ψ_{\min} .

$$\begin{aligned}\langle \Psi_{\max} | L_- L_+ | \Psi_{\max} \rangle &= \langle \Psi_{\max} | L_- | \mathbf{0} \rangle \\ &= 0 \\ &= \left[l(l+1) - m_{l,\max}^2 - m_{l,\max} \right] \hbar^2\end{aligned}\tag{11-25}$$

and

$$\begin{aligned}\langle \Psi_{\min} | L_+ L_- | \Psi_{\min} \rangle &= \langle \Psi_{\min} | L_+ | \mathbf{0} \rangle \\ &= 0 \\ &= \left[l(l+1) - m_{l,\min}^2 + m_{l,\min} \right] \hbar^2\end{aligned}\tag{11-26}$$

When we subtract eq. 11-26 from 11-25, we have

$$-m_{l,\max}^2 - m_{l,\max} + m_{l,\min}^2 - m_{l,\min} = 0\tag{11-27}$$

The only physical solution to this equation is $m_{l,\min} = -m_{l,\max}$.

Finally, since the raising and lowering operators toggle through the eigenfunctions and eigenvalues in steps of \hbar , the eigenvalues of L_z must be either $m_l = 0, \pm 1\hbar, \pm 2\hbar, \dots, \pm m_{l,\max}\hbar$, or it would also be possible that they be $m_l = \pm(1/2)\hbar, \pm(3/2)\hbar, \pm(5/2)\hbar, \dots, \pm m_{l,\max}\hbar$. We will see later that only the whole integral series works for angular momentum. For now we will simply work with that series, and note that the commutation relationships allow the half-integral series, which will perhaps show up in some other operator.

From eq. 11-25 (or 11-26), we also see that the quantum number l is equal to $m_{l,\max}$ (and we see now why we chose the form for the eigenvalue of L^2 as $l(l+1)\hbar^2$).

The Big Picture

So, without knowledge of the eigenfunctions themselves, we have established that:

- 1) The total angular momentum is quantized. It takes on values of $\sqrt{l(l+1)}\hbar$ where l is an integer (a quantum number).
- 2) For a given quantum number l , the z component of the total angular momentum can also be determined precisely; it too is quantized and it is limited to values of $0, \pm\hbar, \pm 2\hbar, \dots, \pm l\hbar$ (choice of z is arbitrary, but typical; we could more generally

say "a single component" instead of "the z component"). We call the integer multiplying \hbar the quantum number m_l .

- 3) We can never know the precise direction of a non-zero angular momentum vector, as that would violate the uncertainty principle.

Homework

To be solved in class:

What are the eigenvalues of L_x^2 ? What are the eigenvalues of L_y^2 ? Finally, what are the eigenvalues of $L_x^2 + L_y^2$? All 3 operators listed do indeed have associated eigenvalues but you may want to think carefully about what you can measure at one time without violating the uncertainty principle.

To be turned in for possible grading Feb. 17:

All of the angular momentum operators that we have discussed thus far are Hermitian. For an arbitrary function Φ having finite total angular momentum, what is required for it to be true that

$$\langle \Phi | L_+ L_- | \Phi \rangle = \langle \Phi | L_- L_+ | \Phi \rangle$$

where $L_+ L_-$ is the operator defined by sequential application of the lowering operator and then the raising operator, and vice versa? Note that an "arbitrary" function means that it need *not* be an eigenfunction of L^2 . If you don't know where to start on this problem, which is certainly not trivial, take another look at eqs. 6-7 and 6-8 and their surrounding discussion and think about how you might be able to apply analogous reasoning to this problem.