(17) Angular Momentum

1 Last Time

- Schrödinger Equation in 3D
- Separation of variables

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2 Where we are going

- Angular Momentum Eigenstates
- Central Potentials
- Hydrogen!

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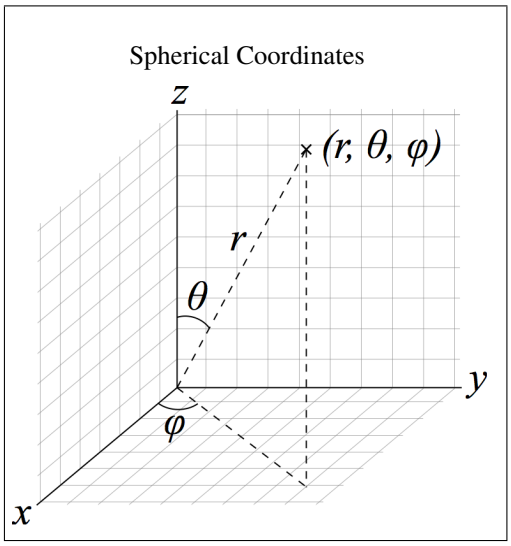
3 Quantum Angular Momentum

Last time we generalized to 3D and made use of separation of variable in rectangular coordinates $\{x, y, z\}$. What do we do if we have a potential that depends only on r in spherical coordinates?

Recall: Laplacian in Spherical Coordinates (r, θ, ϕ)

$$\begin{aligned} x &= r\sin\theta\ \cos\phi \\ y &= r\sin\theta\ \sin\phi \\ z &= r\cos\theta \\ \nabla^2 &= \partial_r^2 + \frac{2}{r}\partial_r + \frac{1}{r^2}\left(\partial_\theta^2 + \cot\theta\ \partial_\theta + \frac{1}{\sin^2\theta}\partial_\phi^2\right) \\ &= \frac{1}{r}\partial_r^2\, r + \frac{1}{r^2}\left[\frac{1}{\sin\theta}\partial_\theta\left(\sin\theta\ \partial_\theta\right) + \frac{1}{\sin^2\theta}\partial_\phi^2\right] \end{aligned}$$



Central Potential

$$V(\vec{r}) \;=\; V(|\vec{r}|) = V(r)$$

This is a potential that depends only on distance from the origin, such as a gravitational force, or electric force. As you learned in Classical Mechanics, the special thing about such forces is that they exert no torques. That is, the force vector is always parallel to $\vec{r}$, such that their cross-product is always zero. No torque means that angular momentum is conserved.

But what is angular momentum in Quantum Mechanics?

Let's start with the classical notion of angular momentum that we all know and love.

Angular Momentum

$$\vec{L} = \vec{r} \times \vec{p} \;\rightarrow\; \hat{\vec{L}} = \hat{\vec{r}} \times \hat{\vec{p}}$$

We can unpack those vector operators and then compute the cross-product one component at a time.

$$\hat{r}_x = \hat{x}, \;\; \hat{r}_y = \hat{y}, \;\; \hat{r}_z = \hat{z}$$
$$\hat{p}_y = -i\hbar\,\partial_x, \;\; \hat{p}_y = -i\hbar\,\partial_y, \;\; \hat{p}_z = -i\hbar\,\partial_z$$
$$\Rightarrow [\hat{x}, \hat{p}_y] = 0, \quad \cdots$$

Writing out the cross-product gives

Angular Momentum Operator

$$\hat{\vec{L}} = \begin{bmatrix} \hat{L}_x \\ \hat{L}_y \\ \hat{L}_z \end{bmatrix} = \begin{bmatrix} \hat{y}\,\hat{p}_z - \hat{z}\,\hat{p}_y \\ \hat{z}\,\hat{p}_x - \hat{x}\,\hat{p}_z \\ \hat{x}\,\hat{p}_y - \hat{y}\,\hat{p}_x \end{bmatrix}$$

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4 Angular Momentum Operators

Imagine that we want to make energy eigenstates of our central potential. In the 3D example potentials we saw in the last lecture, where separation of variables in an x, y, z basis worked, we had 3 commuting momentum operators. Recall that these are just partial derivatives, so

$$[\hat{p}_x, \hat{p}_y] = 0, \quad [\hat{p}_z, \hat{p}_x] = 0, \quad [\hat{p}_y, \hat{p}_z] = 0$$

and you could rightly claim that this is *why* separation of variables works.

In spherical coordinates, thing are more complicated. The momentum in the radial direction $\hat{p}_r$ separates nicely from the angular components, but the angular momentum operators we derived above do not commute. You will show that

Angular Momentum Commutators

$$\begin{aligned} \left[\hat{L}_x, \hat{L}_y\right] &= i\hbar\hat{L}_z \\ \left[\hat{L}_z, \hat{L}_x\right] &= i\hbar\hat{L}_y \\ \left[\hat{L}_y, \hat{L}_z\right] &= i\hbar\hat{L}_x \end{aligned}$$

Just like the fact that $[\hat{x}, \hat{p}_x] \neq 0$ means that we cannot have eigenstates which are eigenfunctions of both $\hat{x}$ and $\hat{p}_x$, this means that we cannot have simultaneous eigenstates of the components of angular momentum.

(The exception is the state with zero angular momentum.)

Fortunately, we have an out: total angular momentum.

Total Angular Momentum

$$\begin{aligned} \left|\hat{\vec{L}}\right| = \hat{L}^2 &= \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2 \\ &= \text{ something messy in x,y,z ...} \\ &= -\hbar^2 \left[\frac{1}{\sin\theta} \partial_\theta \left(\sin\theta \, \partial_\theta \right) + \frac{1}{\sin^2\theta} \partial_\phi^2 \right] \end{aligned}$$

In spherical coordinates $\hat{L}_x$ and $\hat{L}_y$ are messy (see Griffiths equation 4.127 and 4.128), but $\hat{L}_z$ is simple, thanks to it being the axis around which ϕ rotates, and from which θ decends.

$$\hat{L}_z = -i\hbar\partial_\phi, \quad \text{note} \quad \left[\hat{L}^2, \hat{L}_z\right] = 0$$

Physically there is nothing special about L_z relative to L_x and L_y, it is just a choice of coordinates which singles out z.

This looks promising since

Momentum in Spherical Coordinates

$$\begin{aligned} \hat{p}^2 &= -\hbar^2\nabla^2 = \frac{-\hbar^2}{r}\partial_r^2 \, r + \frac{1}{r^2}\hat{L}^2 \\ &= \hat{p}_r^2 + \frac{1}{r^2}\hat{L}^2, \quad \text{where } \hat{p}_r = -i\hbar\frac{1}{r}\,\partial_r \, r \end{aligned}$$

which leads to a reasonable expression for energy in a central potential

Energy in a Central Potential

$$\begin{aligned} \hat{E} &= \frac{1}{2m}\hat{p}^2 + V(r) \\ &= \frac{\hat{p}_r^2}{2m} + \frac{1}{2m\,r^2}\hat{L}^2 + V(r) \\ \text{and} \quad & \left[\hat{p}_r, \hat{L}^2\right] = 0, \quad \left[\hat{p}_r, \hat{L}_z\right] = 0 \end{aligned}$$

We will get back to the radial part of this in the next lecture. For now, we focus on the angular momentum part.

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5 Angular Momentum Eigenfunctions

We will start our exploration of angular momentum with the simplest of our angular momentum operators, $\hat{L}_z$. The eigenfunctions of $\hat{L}_z$ are easy to find.

Eigenfunctions of $\hat{L}_z$

$$\begin{gathered} \hat{L}_z\psi_\phi(\phi) = L_z\psi_\phi(\phi) = -i\hbar\,\partial_\phi\,\psi_\phi(\phi) \\ \Rightarrow \psi_\phi(\phi) = e^{im\phi}, \;\; \text{where} \;\; m = L_z/\hbar \neq \text{mass!} \\ \hat{L}_z\psi_\phi = -i\hbar\,\partial_\phi\,\psi_\phi = (-i\hbar)(im)\psi_\phi = L_z\psi_\phi \end{gathered}$$

So the eigenfunction of $\hat{L}_z$ turn out to be complex phases, but note the curious implication of our coordinate system: $\phi \to \phi + 2\pi$ should not change anything. That is, if you turn some object all the way around, it should be the same as what you started with, right?

$$\begin{aligned} \psi_\phi(\phi) = \psi_\phi(\phi + 2\pi) \;\; &\Rightarrow e^{im\phi} = e^{im(\phi+2\pi)} = e^{im\phi+2i\pi m} \\ \Rightarrow e^{2i\pi m} = 1 \;\; &\Rightarrow m \in \{\ldots, -2, -1, 0, 1, 2, \ldots\} \\ L_z = \hbar m \;\; &\Rightarrow \text{ that } L_z \text{ is quantized in units of } \hbar\text{!!} \end{aligned}$$

Once again, the physics behind our solution to the differential equation has limited the meaningful solutions to a discrete subset. In this case, it has told us that the eigenfunctions of $\hat{L}_z$, which we will use to make energy eigenstates of central potentials (like Hydrogen), have angular momentum quantized in units of $\hbar$. This is why Bhor's shot in the dark payed off, even though he knew nothing of the Schrödinger Equation at the time.

With the eigenfunction of $\hat{L}_z$ in hand, we are ready to move on the $\hat{L}^2$.

Eigenfunctions of $\hat{L}^2$

$$\begin{aligned} L^2\,\psi_\theta\,\psi_\phi &= \hat{L}^2\,\psi_\theta\,\psi_\phi \\ &= -\hbar^2\left[\frac{1}{\sin\theta}\partial_\theta\left(\sin\theta\,\partial_\theta\right)+\frac{1}{\sin^2\theta}\partial_\phi^2\right]\psi_\theta\psi_\phi \end{aligned}$$

We can put in $\psi_\phi = e^{im\phi}$ since we know that we will need that to have our WF be an eigenfunction of $\hat{L}_z$,

$$\begin{aligned} L^2\,\psi_\theta\,\psi_\phi &= -\hbar^2\psi_\phi\left[\frac{1}{\sin\theta}\partial_\theta\left(\sin\theta\,\partial_\theta\right)-\frac{m^2}{\sin^2\theta}\right]\psi_\theta \\ \Rightarrow L^2\,\psi_\theta &= -\hbar^2\left[\frac{1}{\sin\theta}\partial_\theta\left(\sin\theta\,\partial_\theta\right)-\frac{m^2}{\sin^2\theta}\right]\psi_\theta \\ &= \text{ack!!! The solution is terrible...} \end{aligned}$$

Fortunately the solutions are known, and they are called the "spherical harmonics", and written as $Y_{lm}(\theta,\phi)$.

$$\begin{aligned} \psi_\theta(\theta)\,\psi_\phi(\phi) &= Y_{lm}(\theta,\phi) \quad \text{defined such that} \\ L^2\,Y_{lm} &= \hbar^2 l(l+1)\,Y_{lm} \\ L_z\,Y_{lm} &= \hbar m\,Y_{lm} \quad \text{as above} \end{aligned}$$

The Y_{lm} are kind of messy functions, but here are a few to give you an idea of how they work.

Spherical Harmonics

$$\begin{aligned} Y_{00} &= \sqrt{\frac{1}{4\pi}} \\ Y_{10} &= \sqrt{\frac{3}{4\pi}}\cos\theta \\ Y_{1\pm1} &= \mp\sqrt{\frac{3}{8\pi}}\sin\theta e^{\pm i\phi} \end{aligned}$$

Two things to note:
(1) all of them have $e^{im\phi}$ for their ϕ dependence, as required to be an eigenfunction of $\hat{L}_z$.
(2) the θ dependence changes with l ***and*** *m.*

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6 Angular Momentum Ladder Operators

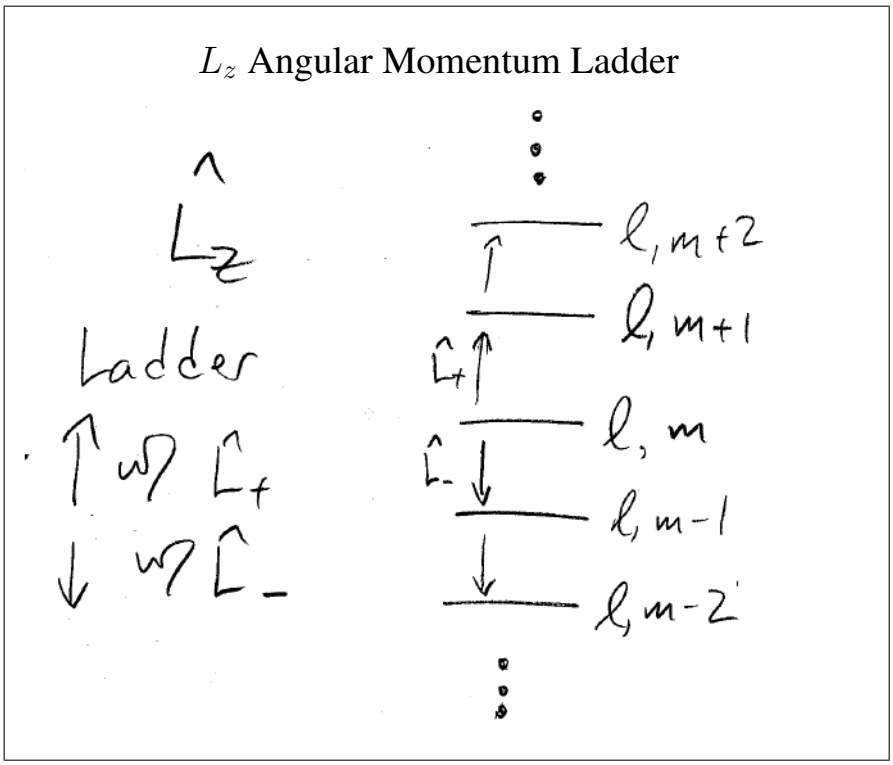
Before we call it a day, let's look a little harder at our angular momentum eigenfunctions and the corresponding operators. We'll start by noting that we can make raising and lowering operators for L_z much like we did for energy in the Quantum Harmonic Oscillator.

Raising and Lowering Operators for $\hat{L}_z$

$$\begin{aligned} \hat{L}_+ &= \hat{L}_x + i\hat{L}_y \\ \hat{L}_- &= \hat{L}_+^\dagger = \hat{L}_x - i\hat{L}_y \\ \left[\hat{L}_z, \hat{L}_\pm\right] &= \left[\hat{L}_z, \hat{L}_x\right] \pm i\left[\hat{L}_z, \hat{L}_y\right] \\ &= i\hbar\left(\hat{L}_y \mp i\hat{L}_x\right) \\ &= \pm\hbar\left(\hat{L}_x \pm i\hat{L}_y\right) \\ &= \pm\hbar\hat{L}_\pm \end{aligned}$$

We have seen this kind of commutator before! For energy in the QHO, we had $\left[\hat{E}, \hat{a}^\dagger\right] = \hbar\omega\hat{a}^\dagger$, indicating that $\hat{a}^\dagger$ changes an energy eigenstate to make it the next higher state, with $\hbar\omega$ more energy.

$\hat{L}_+$ increases L_z by $\hbar$, which means $m \to m+1$. $\hat{L}_-$ does the opposite.



Note, however, that while $\hat{L}_\pm$ change the z-axis angular momentum, they do not change the total angular momentum. You can think of them as moving angular momentum from L_x and L_y into L_z.

$$\begin{aligned}
\left[\hat{L}^2, \hat{L}_\pm\right] &= 0 \\
\Rightarrow \hat{L}^2\ \hat{L}_\pm\ Y_{lm} &= \hat{L}_\pm\ \hat{L}^2\ Y_{lm} \\
&= \hat{L}_\pm\ \hbar^2 l(l+1)\ Y_{lm} \\
\hat{L}^2\ \left(\hat{L}_\pm\ Y_{lm}\right) &= \hbar^2 l(l+1)\ \left(\hat{L}_\pm\ Y_{lm}\right)
\end{aligned}$$

from which you can see that the raising and lowering operators do not change L^2.

Like the QHO we have a ladder of states, and like the QHO there is no obvious reason from the "solution to a differential equation" point of view why this ladder should not be infinite. However, physics has certain requirements, and in this case we require that L_z^2 not be greater than the total angular momentum.

Limiting L_z

$$\begin{aligned} L^2 &= L_x^2 + L_y^2 + L_z^2 \geq L_z^2 \\ \Rightarrow & \quad \hbar^2\, l(l+1) \geq \hbar^2 m^2 \\ \Rightarrow & \quad \text{there exists } \hat{L}_+ Y_{lm_+} = 0 \\ & \quad \text{for some maximal value of } m_+ \end{aligned}$$

Let's see if we can figure this out without doing any integrals of nasty functions...

What is m_+??

$$\begin{aligned} 0 &= \hat{L}_+ Y_{lm_+} \\ \Rightarrow\ 0 &= \langle \hat{L}_+ Y_{lm_+} | \hat{L}_+ Y_{lm_+} \rangle \\ &= \langle Y_{lm_+} | \hat{L}_+^\dagger \hat{L}_+ | Y_{lm_+} \rangle \\ &= \langle Y_{lm_+} | \hat{L}_- \hat{L}_+ | Y_{lm_+} \rangle \end{aligned}$$

That's not obvious progress, but what is $\hat{L}_-\hat{L}_+$??

$$\begin{aligned} \hat{L}_-\hat{L}_+ &= \left(\hat{L}_x - i\hat{L}_y\right)\left(\hat{L}_x + i\hat{L}_y\right) \\ &= \hat{L}_x^2 + \hat{L}_y^2 + i\left(\hat{L}_x\hat{L}_y - \hat{L}_y\hat{L}_x\right) \\ &= \hat{L}^2 - \hat{L}_z^2 - \hbar\hat{L}_z \end{aligned}$$

Did you see that? We just went from the L_z ladder operators, to the x and y operators, and back to L_z. As a matter of strategy, you should never get stuck in

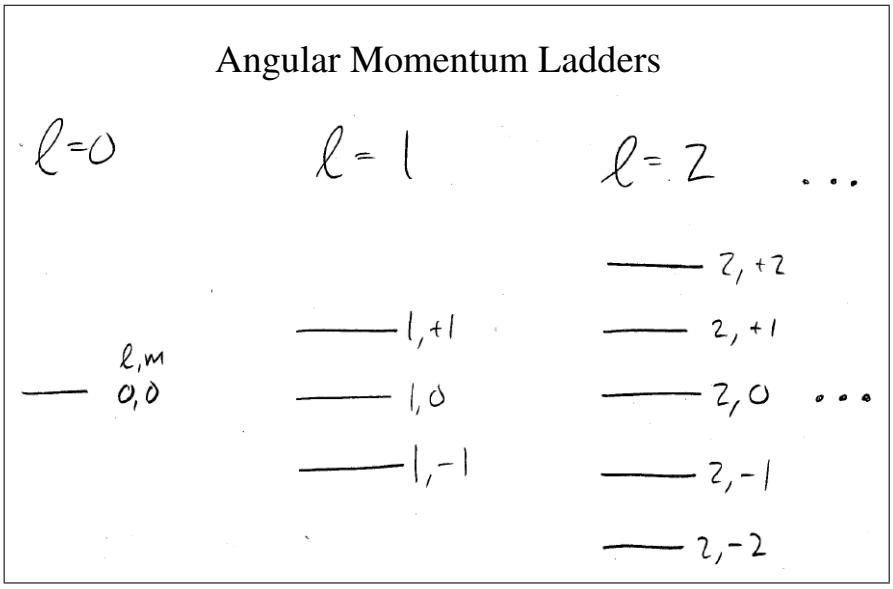
x, y land when working on angular momentum, but a quick run through it can be useful.

So, we now have something we can work with.

$$\begin{aligned} 0 &= \langle Y_{lm_+}|\hat{L}_-\hat{L}_+|Y_{lm_+}\rangle \\ &= \langle Y_{lm_+}|\hat{L}^2 - \hat{L}_z^2 - \hbar\hat{L}_z|Y_{lm_+}\rangle \\ &= \hbar^2 l(l+1) - \hbar^2 m_+^2 - \hbar^2 m_+ \\ &= \hbar^2\left[l(l+1) - m_+(m_+ + 1)\right] \\ \Rightarrow l(l+1) &= m_+(m_+ + 1) \\ \Rightarrow m_+ &= l \text{ so } m \text{ cannot be larger than } l \end{aligned}$$

And now you know why L^2 has $l(l+1)$ in it. Following the same path, but starting with $\hat{L}_- Y_{lm_-} = 0$ leads to the minimum value $m_- = -l$.

$L_z = \hbar m$ is limited by $-l < m < l$.



And that's it! Now we know how to deal with θ and ϕ for energy eigenfunctions of **any** central potential, $V(\vec{r}) = V(r)$.

Energy Eigenfunctions when $V(\vec{r}) = V(r)$

$$\begin{aligned} \phi(\vec{r}) &= \phi_r(r)\, Y_{lm}(\theta, \phi) \\ \hat{E}\, \phi_r\, Y_{lm} &= \left(\frac{\hat{p}_r^2}{2m} + \frac{1}{2m\, r^2} \hat{L}^2 + V(r) \right) \phi_r\, Y_{lm} \\ \hat{E}\, \phi_r &= \left(\frac{\hat{p}_r^2}{2m} + \frac{\hbar^2 l(l+1)}{2m\, r^2} + V(r) \right) \phi_r \end{aligned}$$

Note that ϕ_r does not depend on the L_z quantum number m! That is, the radial function cares about total angular momentum, but not the details of which way it points.

This could reasonably make you wonder why Bhor's ansatz (read "wild guess") worked. L_z is quantized, as he guessed, but that quantum number does not play a role in the energy of the eigenstates. The total angular momentum quantum number l, on the other hand, impacts the energy eigenstates, and will be a source of discrete energy levels.

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7 Next Time

- Finding Energy Eigenfunctions in Central Potentials: the Radial Part