Week 5

Three-Dimensional Systems

5.1 Three-Dimensional Problems

1/29:

- 3D problems still solve the Schrödinger equation, just in 3D.

$$\hat{H}\psi = i\hbar\frac{\partial\psi}{\partial t}$$
$$-\frac{\hbar^2}{2m}\vec{\nabla}^2\psi + V(\vec{r},t)\psi = i\hbar\frac{\partial\psi}{\partial t}$$

  - Slightly more complicated here, but not too much.
- Focus: Time-independent potentials for now, that is

$$V(\vec{r},t) = V(\vec{r})$$

  - 3D time-independent potentials still allow us to split the wave function as on the left below, and we also still seek energy eigenvalues of the system on the right below.

$$\psi(\vec{r},t) = \psi(\vec{r})\cdot\phi(t) \qquad\qquad -\frac{\hbar^2}{2m}\vec{\nabla}^2\psi(\vec{r}) + V(\vec{r})\psi(\vec{r}) = E\psi(\vec{r})$$

  - These two facts still imply that the solution will be of the form

$$\psi(\vec{r},t) = \psi(\vec{r})\mathrm{e}^{-iEt/\hbar}$$

    - No difference between 1D and 3D!
- So 1D and 3D are remarkably similar. But where do they differ?
- Example: In 3D, there will be 3 components of the momentum, given as follows.

$$\hat{p}_x = -i\hbar\frac{\partial}{\partial x} \qquad \hat{p}_y = -i\hbar\frac{\partial}{\partial y} \qquad \hat{p}_z = -i\hbar\frac{\partial}{\partial z}$$

  - Note that these three momenta commute as follows.

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

- Example: 3 components of the position, also commutative.

$$[\hat{x},\hat{y}] = [f(\hat{x}),f(\hat{y})] = [f(\hat{x}),g(\hat{x})] = [f(\hat{x}),g(\hat{z})] = 0$$

  - As in PSet 4, f,g are arbitrary real functions of the operator.

- The only commutators that are not zero are those we obtained before, e.g.,

$$[\hat{p}_x, \hat{x}] = -i\hbar \qquad\qquad [\hat{\vec{p}}, V(\vec{r})] = -i\hbar\vec{\nabla}V(\vec{r})$$

  - Recall that we still have

$$[\hat{p}_x, \hat{y}] = [\hat{p}_x, \hat{z}] = 0 \qquad\qquad [V(\vec{r}), \hat{\vec{r}}] = 0$$

- In the presence of $V(\vec{r})$, neither of $\hat{\vec{p}}, \hat{x}$ are conserved quantities. We know this because

$$[\hat{H}, \vec{p}] = [\hat{H}, \vec{r}] \neq 0$$

- In an atom...
  - Potential is only a function of the *magnitude* of distance from the nucleus. Mathematically,

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

  - Likewise, angular momentum $\vec{L} = \vec{r} \times \vec{p}$ is conserved. Here's why:
    - Recall that

$$\begin{aligned}\frac{\mathrm{d}\vec{L}}{\mathrm{d}t} &= \frac{\mathrm{d}\vec{r}}{\mathrm{d}t} \times \vec{p} + \vec{r} \times \frac{\mathrm{d}\vec{p}}{\mathrm{d}t}\\ &= \frac{1}{m}\underbrace{\vec{p} \times \vec{p}}_{0} + \vec{r} \times \underbrace{\frac{\mathrm{d}\vec{p}}{\mathrm{d}t}}_{-\vec{\nabla}V(r)}\end{aligned}$$

    - Working with the second term a bit more, we have that

$$\begin{aligned}\vec{\nabla}V(r) &= \vec{x}\frac{\partial V}{\partial x} + \vec{y}\frac{\partial V}{\partial y} + \vec{z}\frac{\partial V}{\partial z}\\ &= \vec{x}\left(\frac{\partial V}{\partial r}\frac{\partial r}{\partial x}\right) + \vec{y}\left(\frac{\partial V}{\partial r}\frac{\partial r}{\partial y}\right) + \vec{z}\left(\frac{\partial V}{\partial r}\frac{\partial r}{\partial z}\right)\\ &= \frac{\partial V}{\partial r}\left(\vec{x}\frac{\partial r}{\partial x} + \vec{y}\frac{\partial r}{\partial y} + \vec{z}\frac{\partial r}{\partial z}\right)\end{aligned}$$

      - Taking the cross product of the above (evaluated at $r = \sqrt{x^2 + y^2 + z^2}$) with $\vec{r}$ yields zero.
      - Alternatively, we may observe that like each $\partial V/\partial x \propto x$, we have $\vec{\nabla}V \propto \vec{r}$ for a central potential (just picture it), and therefore the cross product of $\vec{r}$ and a vector proportional to $\vec{r}$ will be zero.
    - Therefore,

$$\frac{\mathrm{d}\vec{L}}{\mathrm{d}t} = \frac{1}{m}\underbrace{\vec{p} \times \vec{p}}_{0} + \underbrace{\vec{r} \times c\vec{r}}_{0} = 0$$

    so angular momentum is conserved, as desired.

- What does it mean that these two quantities are conserved?
  - It means that when we take the classical Hamiltonian

$$\hat{H} = \frac{\vec{p}^{\,2}}{2m} + V(r)$$

  we can separate it into a radial and a perpendicular component so that

$$\begin{aligned}\hat{H} &= \frac{\hat{p}_r^2}{2m} + \frac{\hat{p}_\perp^2}{2m} + V(r)\\ &= \frac{\hat{p}_r^2}{2m} + \underbrace{\frac{\vec{L}^2}{2mr^2} + V(r)}_{V_{\text{eff}}(r)}\end{aligned}$$

- Here's why we can make the above algebraic manipulations.
  - To begin, we can always split the momentum operator into radial and perpendicular components.
  - We also know, since $\vec{p}_\perp$ and $\vec{r}$ are perpendicular, that

$$\vec{L}^2 = (\vec{p}_\perp \times \vec{r})^2 = [p_\perp r \sin(90^\circ)]^2 = p_\perp^2 r^2 = \hat{p}_\perp^2 r^2$$

  - However, it is the conservation of angular momentum, in particular, which implies that $\vec{L}^2$ is a constant, and hence that making the substitution $\hat{p}_\perp^2 = \vec{L}^2/r^2$ will allow the sum of the second two terms to be *purely* a function of r (as opposed to, per se, a function of r and $\vec{L}$).
- What is the implication of this effective potential?

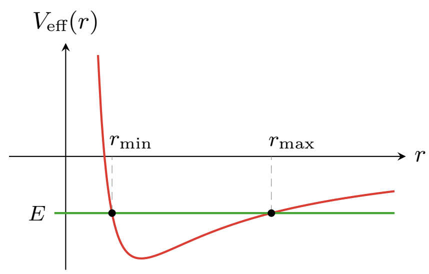

Figure 5.1: Effective potential.

  - Consider the classical case of planetary motion with

$$V_{\text{eff}}(r) = -\frac{GM_0 m}{r} + \frac{\vec{L}^2}{2mr^2}$$

  - Given a total energy E for the system, the planets dance between an r_{min} and r_{max}.
  - This gives the elliptical planetary motion.
  - Of course, we will not deal with planetary motion in this course, but we will deal with something very similar called the **hydrogen atom**.
- We now investigate some analogies and differences between classical and quantum mechanics.
- Before we begin, a quick aside on some commutator rules will be useful.
  1. $[\hat{A}^2, \hat{B}] = \hat{A}[\hat{A}, \hat{B}] + [\hat{A}, \hat{B}]\hat{A}$.

     Proof.

$$\begin{aligned}
[\hat{A}^2, \hat{B}] &= \hat{A}^2\hat{B} - \hat{B}\hat{A}^2\\
&= \hat{A}(\hat{A}\hat{B} - \hat{B}\hat{A}) + (\hat{A}\hat{B} - \hat{B}\hat{A})\hat{A}\\
&= \hat{A}[\hat{A}, \hat{B}] + [\hat{A}, \hat{B}]\hat{A}
\end{aligned}$$

$\square$

  2. $[\hat{A}\hat{B}, \hat{C}] = \hat{A}[\hat{B}, \hat{C}] + [\hat{A}, \hat{C}]\hat{B}$.
  3. $[\hat{A}, \hat{B}\hat{C}] = \hat{B}[\hat{A}, \hat{C}] + [\hat{A}, \hat{B}]\hat{C}$.
  4. Bilinearity, i.e.,

$$\begin{aligned}
[\hat{A} + \hat{B}, \hat{C}] &= [\hat{A}, \hat{C}] + [\hat{B}, \hat{C}] & [c\hat{A}, \hat{B}] &= c[\hat{A}, \hat{B}]\\
[\hat{A}, \hat{B} + \hat{C}] &= [\hat{A}, \hat{B}] + [\hat{A}, \hat{C}] & [\hat{A}, c\hat{B}] &= c[\hat{A}, \hat{B}]
\end{aligned}$$

- None of these rules is trivial, but they can all be demonstrated by expanding as with the first rule.

- So getting back to it, the analogies and differences we will prove are...
  1. The quantum angular momentum is conserved directionally and overall;
  2. The square of the quantum angular momentum is conserved;
  3. The quantum angular momentum *cannot* be determined to infinite precision in more than one direction simultaneously;
  4. The square of the quantum angular momentum and the quantum angular momentum can be determined to infinite precision simultaneously.
- Task 1: To prove that the quantum angular momentum is conserved directionally, we will show that the angular momentum in different directions commutes with the Hamiltonian. To prove that it is conserved overall, we will add the previous three results. Let's begin.
  - Mathematically, we want to determine
    $$[\hat{H},\hat{L}_i] \stackrel{?}{=} 0$$
    since if $[\hat{H},\hat{L}_i]=0$, then
    $$\frac{\mathrm{d}}{\mathrm{d}t}\Big(\langle\psi|\hat{L}_i|\psi\rangle\Big) = \frac{i}{\hbar}\langle\psi|\underbrace{[\hat{H},\hat{L}_i]}_{0}|\psi\rangle = 0$$
  - Let's start with $\hat{L}_x$.
  - Since
    $$\vec{L} = \vec{r}\times\vec{p} = \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ x & y & z \\ p_x & p_y & p_z \end{vmatrix} = \hat{x}(yp_z - p_yz) + \hat{y}(p_xz - p_zx) + \hat{z}(xp_y - p_xy)$$
    we know that
    $$\hat{L}_x = yp_z - p_yz$$
  - Additionally, recall that
    $$\hat{H} = \frac{\hat{p}_x^2+\hat{p}_y^2+\hat{p}_z^2}{2m} + V(r)$$
  - Thus, we have that
    $$\begin{aligned}[\hat{H},\hat{L}_x] &= \left[\frac{\hat{p}_x^2+\hat{p}_y^2+\hat{p}_z^2}{2m} + V(r), \hat{y}\hat{p}_z - \hat{z}\hat{p}_y\right] \\ &= \left[\frac{\hat{p}_x^2}{2m},\hat{y}\hat{p}_z\right] + \left[\frac{\hat{p}_y^2}{2m},\hat{y}\hat{p}_z\right] + \left[\frac{\hat{p}_z^2}{2m},\hat{y}\hat{p}_z\right] \\ &\quad + \left[\frac{\hat{p}_x^2}{2m},-\hat{z}\hat{p}_y\right] + \left[\frac{\hat{p}_y^2}{2m},-\hat{z}\hat{p}_y\right] + \left[\frac{\hat{p}_z^2}{2m},-\hat{z}\hat{p}_y\right] \\ &\quad + [V(r),\hat{y}\hat{p}_z] + [V(r),-\hat{z}\hat{p}_y] \\ &= \left[\frac{\hat{p}_y^2}{2m},\hat{y}\hat{p}_z\right] + \left[\frac{\hat{p}_z^2}{2m},-\hat{z}\hat{p}_y\right] + i\hbar\left(\hat{y}\frac{\partial V}{\partial z} - \hat{z}\frac{\partial V}{\partial y}\right) \\ &= -\frac{i\hbar\hat{p}_y\hat{p}_z}{m} + \frac{i\hbar\hat{p}_y\hat{p}_z}{m} + i\hbar\frac{\partial V}{\partial r}\left(\hat{y}\frac{\partial r}{\partial z} - \hat{z}\frac{\partial r}{\partial y}\right) \\ &= 0\end{aligned}$$
  - Now let's investigate some of the above substitutions a bit more closely.
  - From line 1 to line 2, we split the commutator into $4\cdot 2 = 8$ terms using its bilinearity.

- From line 2 to line 3, we eliminated all commutators that go to zero among the first six, and evaluated the last two commutators using a combination of Rule 3 and properties mentioned at the beginning of the lecture.
  - Notice that the only two of the first six commutators that did *not* go to zero were those for which the variable in the squared momentum operator matched the position operator, i.e., in

$$\left[\frac{\hat{p}_y^2}{2m},\hat{y}\hat{p}_z\right]$$

    we may observe that $\hat{p}_y^2$ and $\hat{y}$ both concern y.
  - Example evaluation:

$$\begin{aligned}
\left[\frac{\hat{p}_x^2}{2m},\hat{y}\hat{p}_z\right] &= \frac{1}{2m}[\hat{p}_x^2,\hat{y}\hat{p}_z] && \text{Rule 4}\\
&= \frac{1}{2m}(\hat{p}_x[\hat{p}_x,\hat{y}\hat{p}_z]+[\hat{p}_x,\hat{y}\hat{p}_z]\hat{p}_x) && \text{Rule 1}\\
&= \frac{1}{2m}(\hat{p}_x(\hat{y}\underbrace{[\hat{p}_x,\hat{p}_z]}_{0}+\underbrace{[\hat{p}_x,\hat{y}]}_{0}\hat{p}_z)+(\hat{y}\underbrace{[\hat{p}_x,\hat{p}_z]}_{0}+\underbrace{[\hat{p}_x,\hat{y}]}_{0}\hat{p}_z)\hat{p}_x) && \text{Rule 3}\\
&= 0
\end{aligned}$$

  - Example evaluation:

$$\begin{aligned}
\left[\frac{\hat{p}_y^2}{2m},\hat{y}\hat{p}_z\right] &= \frac{1}{2m}[\hat{p}_y^2,\hat{y}\hat{p}_z] && \text{Rule 4}\\
&= \frac{1}{2m}(\hat{p}_y[\hat{p}_y,\hat{y}\hat{p}_z]+[\hat{p}_y,\hat{y}\hat{p}_z]\hat{p}_y) && \text{Rule 1}\\
&= \frac{1}{2m}(\hat{p}_y(\hat{y}\underbrace{[\hat{p}_y,\hat{p}_z]}_{0}+\underbrace{[\hat{p}_y,\hat{y}]}_{-i\hbar}\hat{p}_z)+(\hat{y}\underbrace{[\hat{p}_y,\hat{p}_z]}_{0}+\underbrace{[\hat{p}_y,\hat{y}]}_{-i\hbar}\hat{p}_z)\hat{p}_y) && \text{Rule 3}\\
&= \frac{1}{2m}(\hat{p}_y(-i\hbar\hat{p}_z)+(-i\hbar\hat{p}_z)\hat{p}_y)\\
&= -\frac{i\hbar}{2m}(\hat{p}_y\hat{p}_z+\hat{p}_z\hat{p}_y)\\
&= -\frac{i\hbar}{2m}(\hat{p}_y\hat{p}_z+\hat{p}_y\hat{p}_z)\\
&= -\frac{i\hbar\hat{p}_y\hat{p}_z}{m}
\end{aligned}$$

    - Note that $\hat{p}_z\hat{p}_y=\hat{p}_y\hat{p}_z$ because $[\hat{p}_y,\hat{p}_z]=0$.
  - Example evaluation:

$$\begin{aligned}
[V(r),\hat{y}\hat{p}_z] &= \hat{y}\underbrace{[V(r),\hat{p}_z]}_{i\hbar\,\partial V/\partial z}+\underbrace{[V(r),\hat{y}]}_{0}\hat{p}_z && \text{Rule 3}\\
&= i\hbar\hat{y}\frac{\partial V}{\partial z}
\end{aligned}$$

- From line 3 to line 4, we evaluated the last two commutators and applied the chain rule.
- From line 4 to line 5, we algebraically expanded and cancelled everything (using $r=\sqrt{x^2+y^2+z^2}$ for the partial derivatives).
- Moving on, similar to the above, we obtain that

$$[\hat{H},\hat{L}_y]=[\hat{H},\hat{L}_z]=0$$

  - Thus, by bilinearity once more,

$$[\hat{H}, \hat{\vec{L}}] = [\hat{H}, \hat{L}_x + \hat{L}_y + \hat{L}_z] = 0$$

- Task 2: The fact that the Hamiltonian commutes with the constant $\hat{\vec{L}}^2$ is obvious, implying the claim.
- Task 3.
  - Here, we want to investigate if

$$[\hat{L}_x, \hat{L}_y] \stackrel{?}{=} 0$$

  - We do this via

$$\begin{aligned}
[\hat{L}_x, \hat{L}_y] &= [\hat{y}\hat{p}_z - \hat{z}p_y, p_x z - xp_z] \\
&= [yp_z, p_x z] + [\hat{z}\hat{p}_y, \hat{x}\hat{p}_z] \\
&= \hat{y}\hat{p}_x(-i\hbar) + \hat{p}_y\hat{x}(i\hbar) \\
&= i\hbar\hat{L}_z
\end{aligned}$$

  - Similarly, we can see that no $\hat{L}_i$'s commute with each other. Indeed, altogether, we have

$$[\hat{L}_x, \hat{L}_y] = i\hbar\hat{L}_z \qquad [\hat{L}_y, \hat{L}_z] = i\hbar\hat{L}_x \qquad [\hat{L}_z, \hat{L}_x] = i\hbar\hat{L}_y$$

- Task 4.
  - We have that

$$\begin{aligned}
[\hat{\vec{L}}^2, \hat{L}_x] &= [\hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2, \hat{L}_x] \\
&= 0 + [\hat{L}_y^2, \hat{L}_x] + [\hat{L}_z^2, \hat{L}_x] \\
&= \hat{L}_y[\hat{L}_y, \hat{L}_x] + [\hat{L}_y, \hat{L}_x]\hat{L}_y + \hat{L}_z[\hat{L}_z, \hat{L}_x] + [\hat{L}_z, \hat{L}_x]\hat{L}_z \\
&= \hat{L}_y(-i\hbar\hat{L}_z) + (-i\hbar\hat{L}_z)\hat{L}_y + \hat{L}_z(i\hbar\hat{L}_y) + (i\hbar\hat{L}_y)\hat{L}_z \\
&= i\hbar(-\hat{L}_y\hat{L}_z - \hat{L}_z\hat{L}_y + \hat{L}_z\hat{L}_y + \hat{L}_y\hat{L}_z) \\
&= 0
\end{aligned}$$

  - Thus, the squares commute:

$$[\hat{\vec{L}}^2, \hat{L}_x] = [\hat{\vec{L}}^2, \hat{L}_y] = [\hat{\vec{L}}^2, \hat{L}_z] = 0$$

- Conclusion.
  - $\hat{L}_i, \hat{\vec{L}}^2$ are conserved. That is,

$$[\hat{H}, \hat{L}_i] = [\hat{H}, \hat{\vec{L}}^2] = 0$$

    - This means that $\hat{H}, \hat{L}_z, \hat{\vec{L}}^2$ have compatible observables.
    - In other words, we can only define the angular momentum in one direction and the modulus of the angular momentum squared.
  - All this will characterize three-dimensional motion as we'll see.

5.2 Angular Momentum; Ladder Operators

1/31:

- Is there an operator $\hat{L}$?
  - There *is* an operator $\hat{\vec{L}}$ with components $\hat{L}_x, \hat{L}_y, \hat{L}_z$; it's just that we cannot measure it because the components are incompatible.
  - This is why we measure $\hat{\vec{L}}^2$ and one $\hat{L}_i$.
- Recap of 3D.
  - The 3D Hamiltonian is
$$\hat{H} = -\frac{\hbar^2}{2m}\vec{\nabla}^2 + V(\vec{r})$$
  - We are interested in obtaining the energy eigenvalues of such a potential, which we do via the 3D Schrödinger equation,
$$\hat{H}\psi(\vec{r},t) = E\psi(\vec{r},t)$$
  - The potentials we work with will be **central**, i.e.,
$$V(\vec{r}) = V(r)$$
  - For central potentials, we have the following compatibility relations.
$$[\hat{H},\hat{L}_z] = [\hat{H},\hat{L}_x] = [\hat{H},\hat{L}_y] = [\hat{H},\hat{\vec{L}}^2] = [\hat{\vec{L}}^2,\hat{L}_z] = 0$$
$$[\hat{L}_x,\hat{L}_y] = i\hbar\hat{L}_z$$
  - Thus, we can get good eigenstates of $\hat{H}$, $\hat{\vec{L}}^2$, and $\hat{L}_z$ all together.
    - We choose $\hat{L}_z$ instead of $\hat{L}_x, \hat{L}_y$ WLOG.
- **Central** (potential): A potential that depends only on the distance.
- Before we go any further, we need to express the Laplacian
$$\vec{\nabla}^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$
  in spherical coordinates.
  - Recall that spherical coordinates have a distance r, a polar angle θ, and an azimuthal angle ϕ.
  - Drawing out the Cartesian and polar coordinates of a point, we may rederive that
$$\begin{aligned} z &= r\cos\theta \\ x &= r\sin\theta\cos\phi \\ y &= r\sin\theta\sin\phi \end{aligned}$$
  - The Laplacian has a rather nasty form in spherical coordinates. In particular, it is given by
$$\vec{\nabla}^2\psi(r,\theta,\phi) = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2\psi}{\partial\phi^2}$$
- A nice thing about spherical coordinates is that like $\hat{p}_z = -i\hbar\,\partial/\partial z$ in Cartesian coordinates, we have in spherical coordinates that
$$\hat{L}_z = -i\hbar\frac{\partial}{\partial\phi}$$

- Eigenstates of $\hat{L}_z$.
  - We wish to solve
$$\hat{L}_z\psi = c\psi$$
    where ψ is the desired eigenstate and c the corresponding eigenvalue.
  - Expanding, we have that
$$\begin{aligned}
-i\hbar\frac{\partial\psi}{\partial\phi} &= c\psi \\
\frac{\partial\psi}{\partial\phi} &= \frac{ic}{\hbar}\psi \\
\psi(r,\theta,\phi) &= F(r,\theta)\mathrm{e}^{ic\phi/\hbar}
\end{aligned}$$
  - We now apply the boundary condition to determine c. Since
$$\begin{aligned}
\psi(r,\theta,\phi+2\pi) &= \psi(r,\theta,\phi) \\
\mathrm{e}^{2\pi ic/\hbar} &= 1
\end{aligned}$$
    we must have that $c/\hbar = m \in \mathbb{Z}$.
  - Thus, ψ as written above is an eigenstate of $\hat{L}_z$ with eigenvalue $\hbar m$.
  - Sanity check:
$$\hat{L}_z\psi = -i\hbar(im)F(r,\theta)\mathrm{e}^{im\phi} = \hbar m\psi$$
- **Ladder operator**: Either of the two operators defined as follows. *Denoted by* $\hat{\boldsymbol{L}}_\pm$. *Given by*
$$\hat{L}_\pm = \hat{L}_x \pm i\hat{L}_y$$
- Commutator of the ladder operators and the angular momentum operators.
  - We have by the the commutator relations among the $\hat{L}_i$ that
$$[\hat{L}_\pm,\hat{L}_z] = [\hat{L}_x \pm i\hat{L}_y,\hat{L}_z] = -i\hbar\hat{L}_y \pm i(i\hbar\hat{L}_x) = -i\hbar\hat{L}_y \mp \hbar\hat{L}_x = \mp\hbar(\hat{L}_x \pm i\hat{L}_y) = \mp\hbar\hat{L}_\pm$$
- Commutator of the ladder operators with each other.
  - We have that
$$\begin{aligned}
\hat{L}_+\hat{L}_- &= (\hat{L}_x + i\hat{L}_y)(\hat{L}_x - i\hat{L}_y) \\
&= \hat{L}_x^2 + \hat{L}_y^2 + i(\hat{L}_y\hat{L}_x) - i(\hat{L}_x\hat{L}_y) \\
&= \hat{L}_x^2 + \hat{L}_y^2 - i[\hat{L}_x,\hat{L}_y] \\
&= \hat{L}_x^2 + \hat{L}_y^2 + \hbar\hat{L}_z \\
&= \hat{L}_x^2 + \hat{L}_y^2 + \hbar\hat{L}_z + \hat{L}_z^2 - \hat{L}_z^2 \\
&= \hat{\vec{L}}\,^2 - \hat{L}_z^2 + \hbar\hat{L}_z
\end{aligned}$$
  - Similarly, we have that
$$\begin{aligned}
\hat{L}_-\hat{L}_+ &= (\hat{L}_x - i\hat{L}_y)(\hat{L}_x + i\hat{L}_y) \\
&= \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2 - i[\hat{L}_y,\hat{L}_x] - \hat{L}_z^2 \\
&= \hat{\vec{L}}\,^2 - \hat{L}_z^2 - \hbar\hat{L}_z
\end{aligned}$$
  - Thus, we can calculate that
$$[\hat{L}_+,\hat{L}_-] = 2\hbar\hat{L}_z$$

- The ladder operators also "raise" and "lower."
  - Let $|\ell, m\rangle$ be an eigenstate of $\hat{\vec{L}}^2, \hat{L}_z$.
  - Then we have the following, where we will withhold proof of the left equality below for now.

$$\hat{\vec{L}}^2 |\ell, m\rangle = \hbar^2 \ell(\ell+1) |\ell, m\rangle \qquad\qquad \hat{L}_z |\ell, m\rangle = \hbar m |\ell, m\rangle$$

  - Now, what happens when we apply $\hat{L}_z$ to $\hat{L}_+ |\ell, m\rangle$? As we might expect at this point,

$$\begin{aligned}\hat{L}_z(\hat{L}_+ |\ell, m\rangle) &= \left[\hat{L}_+\hat{L}_z - (\hat{L}_+\hat{L}_z - \hat{L}_z\hat{L}_+)\right] |\ell, m\rangle \\ &= \hat{L}_+\hbar m |\ell, m\rangle + \hbar\hat{L}_+ |\ell, m\rangle \\ &= \hbar(m+1)(\hat{L}_+ |\ell, m\rangle)\end{aligned}$$

  - Thus,

$$\hat{L}_+ |\ell, m\rangle \propto |\ell, m+1\rangle$$

  - We can prove in a similar fashion that

$$\hat{L}_- |\ell, m\rangle \propto |\ell, m-1\rangle$$

- Relating the numbers m, ℓ.
  - Recall that $\hat{\vec{L}}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$.
  - The eigenvalue corresponding to an eigenstate of $\hat{\vec{L}}^2$ is $\hbar^2\ell(\ell+1)$.
  - The eigenvalue corresponding to an eigenstate of $\hat{L}_z^2$ is $(\hbar m)^2$.
  - Thus, since all quantities are positive, $\hbar^2\ell(\ell+1) > \hbar^2 m^2$; it follows that $|m| < |\ell|$.
  - But since ladder operators give larger and larger values of m without changing ℓ, it appears that eventually, this rule will be violated. Therefore, there must be an m_{max} such that

$$L_+ |\ell, m_{\text{max}}\rangle = 0$$

  - Similarly, there must be an m_{min} such that

$$L_- |\ell, m_{\text{min}}\rangle = 0$$

  - Since we have $\hat{\vec{L}}^2 = \hat{L}_-\hat{L}_+ + \hbar\hat{L}_z + \hat{L}_z^2$, we have that

$$\hat{\vec{L}}^2 |\ell, m_{\text{max}}\rangle = \hat{L}_- \underbrace{\hat{L}_+ |\ell, m_{\text{max}}\rangle}_{0} + (\hbar^2 m_{\text{max}} + \hbar^2 m_{\text{max}}^2) |\ell, m_{\text{max}}\rangle$$

  - This combined with the fact that

$$\hat{\vec{L}}^2 |\ell, m_{\text{max}}\rangle = \hbar^2\ell(\ell+1) |\ell, m_{\text{max}}\rangle$$

    implies that

$$m_{\text{max}} = \ell \qquad\qquad m_{\text{min}} = -\ell$$

  - Thus, $|\ell, m\rangle$ has $2m+1$ eigenstates for $-\ell \leq m \leq \ell$. Additionally, we have that

$$\hat{\vec{L}}^2 |\ell, m\rangle = \hbar^2 \ell(\ell+1) |\ell, m\rangle \qquad\qquad \hat{L}_z |\ell, m\rangle = \hbar m |\ell, m\rangle$$

5.3 Spherical Harmonics

2/2:

- Ask Wagner in OH: Did I miss something here, especially as pertains to the spherical harmonic oscillator?? Did you cover something not in the lecture notes?
- Recall our discussion of spherical coordinates from last time, where we derived

$$\vec{\nabla}^2\psi(r,\theta,\phi) = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2\psi}{\partial\phi^2}$$

- Once we've defined the Laplacian in spherical coordinates, we can obtain the energy eigenvalues as per usual via

$$\left[-\frac{\hbar^2}{2M}\vec{\nabla}^2 + V(\vec{r})\right]\psi(\vec{r}) = E\psi(\vec{r}) \qquad\qquad \psi(\vec{r},t) = \psi(\vec{r})\mathrm{e}^{-iEt/\hbar}$$

- Now observe that $\vec{\nabla}^2$ has a clear separation of a radial differential operator and an angular one (i.e., the left term is added to the two right ones). Hence, we shall consider a solution

$$\psi(\vec{r}) = R(r)Y(\theta,\phi)$$

- Thus,

$$-\frac{\hbar^2}{2M}\left[\frac{Y}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right) + \frac{R}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right) + \frac{R}{r^2\sin^2\theta}\frac{\partial^2 Y}{\partial\phi^2}\right] + [V(r)-E]RY = 0$$

- Now divide the above by $R(r)\cdot Y(\theta,\phi)$.

$$-\frac{\hbar^2}{2M}\frac{1}{R}\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right) + V(r) - E - \frac{\hbar^2}{2M}\left[\frac{1}{Y}\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right) + \frac{1}{Y}\frac{1}{r^2\sin^2\theta}\frac{\partial^2 Y}{\partial\phi^2}\right] = 0$$

- Multiplying by $2Mr^2/\hbar^2$ yields an expression that is a sum of a function of only r with a function of only θ,ϕ. Hence, for them to vanish, they should be equal to the same constant, which we will write in a strange way to be justified later.

$$\begin{aligned}\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2 Y}{\partial\phi^2} &= -\ell(\ell+1)Y\\ \frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right) - \frac{2Mr^2}{\hbar^2}[V(r)-E] &= \ell(\ell+1)R\end{aligned}$$