PHYS 3803: Quantum Mechanics I, Spring 2021 Lecture 22, April 20, 2021 (Tuesday)

- Reading: Angular Momentum: Griffiths 4.1 and 4.3
- Assignments: Problem Set 10 due April 30 (Friday). Submit your homework assignments to Canvas.

Topics for Today: Angular Momentum [Griffiths 4.3]5.2 Rotations and Angular Momentum

Topics for Next Lecture: Angular Momentum

5.3 Schrödinger equation for spherically symmetric potentials

5 Rotations and Angular Momentum

5.2 Rotations and Angular Momentum

To study the eigenvalue spectrum of these operators, we define

$$L_+ \equiv L_1 + iL_2 , \quad L_- \equiv L_1 - iL_2 , \quad L_- = (L_+)^{\dagger}.$$

The commutation relations of angular momentum operators L_{-}, L_{+} , and L_{3} are similar to those of a, a^{\dagger} and H for the harmonic oscillator:

$$[L_+, L_3] = -\hbar L_+, \quad [L_-, L_3] = \hbar L_-, \text{ and}$$

 $[L_+, L_-] = 2\hbar L_3, \quad [L_3, L^2] = 0.$

Let us choose the normalized states $|\ell, m\rangle$ as common eigenvectors for L^2 and L_3 :

$$L^{2}|\ell,m\rangle = \ell(\ell+1)\hbar^{2}|\ell,m\rangle, \quad -\ell \leq m \leq \ell$$

$$L_{3}|\ell,m\rangle = m\hbar|\ell,m\rangle.$$

Homework:

(a) Show that

$$L_{+}|\ell,m\rangle = d_{m}|\ell,m+1\rangle = [\ell(\ell+1) - m(m+1)]^{1/2}\hbar|\ell,m+1\rangle,$$

where

$$d_m = d_m^* = \left[\ell(\ell+1) - m(m+1)\right]^{1/2} \hbar.$$

(b) Similarly, we can also show that

$$L_{-}|\ell,m\rangle = c_{m}|\ell,m-1\rangle = [\ell(\ell+1) - m(m-1)]^{1/2}\hbar|\ell,m-1\rangle,$$

where

$$c_m = c_m^* = \left[\ell(\ell+1) - m(m-1)\right]^{1/2} \hbar.$$

There are several interesting things to note.

- This set of eigenvectors $|\ell, m\rangle$ define all the eigenstates for a particular value of ℓ .
- They define a Hilbert space \mathcal{E}^{ℓ} that is a subspace of the total Hilbert space of the angular momentum operators.
- That means the operators L^2, L_3, L_+ and L_- take any vector in this space to another vector in the space.
- In other words, they leave the space \mathcal{E}^{ℓ} invariant. The dimensionality of the space is $2\ell + 1$.

Let us now look at some specific examples for $|\ell, m\rangle, -\ell \leq m \leq \ell$,

(i) $\ell = 0$, dimensionality of the representation is $2\ell + 1 = 1$, and m = 0.

(ii) $\ell = 1/2$, dimensionality of the representation is $2\ell + 1 = 2$, and $m = \pm 1/2$. Let the states be

$$|\frac{1}{2},\frac{1}{2}
angle \ \ \, {\rm and} \ \ |\frac{1}{2},-\frac{1}{2}
angle.$$

We have

$$\langle \ell, m' | L_3 | \ell, m \rangle = m \hbar \langle \ell, m' | \ell, m \rangle = m \hbar \delta_{m'm}.$$

This implies that the matrix elements are

$$\langle \frac{1}{2}, \frac{1}{2} | L_3 | \frac{1}{2}, \frac{1}{2} \rangle = \frac{\hbar}{2} = -\langle \frac{1}{2}, -\frac{1}{2} | L_3 | \frac{1}{2}, -\frac{1}{2} \rangle$$

$$\langle \frac{1}{2}, \frac{1}{2} | L_3 | \frac{1}{2}, -\frac{1}{2} \rangle = 0 = \langle \frac{1}{2}, -\frac{1}{2} | L_3 | \frac{1}{2}, \frac{1}{2} \rangle.$$

Thus

$$L_3 = \frac{\hbar}{2} \left(\begin{array}{cc} 1 & 0 \\ 0 & -1 \end{array} \right) \ .$$

Similarly

$$\langle \ell, m' | L^2 | \ell, m \rangle = \ell(\ell+1)\hbar^2 \langle \ell, m' | \ell, m \rangle$$

$$= \ell(\ell+1)\hbar^2 \delta_{m'm}$$

$$\langle \ell, m' | L_+ | \ell, m \rangle = d_m \langle \ell, m' | \ell, m+1 \rangle$$

$$= d_m \delta_{m',m+1}$$

$$= [\ell(\ell+1) - m(m+1)]^{1/2} \hbar \delta_{m',m+1}$$

$$\langle \ell, m' | L_- | \ell, m \rangle = c_m \langle \ell, m' | \ell, m-1 \rangle$$

$$= c_m \delta_{m',m-1}$$

$$= [\ell(\ell+1) - m(m-1)]^{1/2} \hbar \delta_{m',m-1} .$$

$$L^{2} = \hbar^{2} \frac{1}{2} (\frac{1}{2} + 1) \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \frac{3}{4} \hbar^{2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$
$$L_{+} = \hbar \begin{pmatrix} 0 & (\frac{3}{4} + \frac{1}{4})^{1/2} \\ 0 & 0 \end{pmatrix} = \hbar \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$$
$$L_{-} = \hbar \begin{pmatrix} 0 & 0 \\ (\frac{3}{4} + \frac{1}{4})^{1/2} & 0 \end{pmatrix} = \hbar \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}.$$

Thus the generators of angular momentum have different representations in different spaces. To find out the spatial eigenfunctions, we note that rotational symmetry is best studied in the spherical coordinates.

In spherical coordinates,

 $x = r \sin \theta \cos \phi$ $y = r \sin \theta \sin \phi$ $z = r \cos \theta$

and the angular momentum operators take the following form

$$L_{1} = L_{x} = i\hbar \left(\sin \phi \frac{\partial}{\partial \theta} + \cos \phi \cot \theta \frac{\partial}{\partial \phi} \right)$$
$$L_{2} = L_{y} = i\hbar \left(-\cos \phi \frac{\partial}{\partial \theta} + \sin \phi \cot \theta \frac{\partial}{\partial \phi} \right)$$
$$L_{3} = L_{z} = -i\hbar \frac{\partial}{\partial \phi}.$$

$$L_{\pm} = L_{1} \pm iL_{2}$$

= $i\hbar \left[(\sin\phi \mp i\cos\phi) \frac{\partial}{\partial\theta} + (\cos\phi \pm i\sin\phi) \cot\theta \frac{\partial}{\partial\phi} \right]$
= $\pm\hbar e^{\pm i\phi} \left(\frac{\partial}{\partial\theta} \pm i\cot\theta \frac{\partial}{\partial\phi} \right).$

We know that

 $L_+|\ell,\ell\rangle=0\,.$

In the spherical coordinate basis, this becomes

$$\left[\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\phi}\right]U_{\ell,\ell}(r,\theta,\phi) = 0.$$

Furthermore, we have

$$L_z|\ell,\ell\rangle = \ell\hbar|\ell,\ell\rangle.$$

In the spherical coordinate basis, $L_z|\ell, \ell\rangle = \ell\hbar |\ell, \ell\rangle$ becomes

 $-i\hbar\frac{\partial}{\partial\phi}\langle r,\theta,\phi|\ell,\ell\rangle = \ell\hbar\langle r,\theta,\phi|\ell,\ell\rangle \quad \text{or} \quad \frac{\partial}{\partial\phi}U_{\ell,\ell}(r,\theta,\phi) = i\ell U_{\ell,\ell}(r,\theta,\phi) \,.$ Thus

$$U_{\ell,\ell}(r,\theta,\phi) = \langle r,\theta,\phi | \ell,\ell \rangle = F_{\ell,\ell}(r,\theta)\Phi(\phi) = F_{\ell,\ell}(r,\theta)e^{i\ell\phi}.$$

Let us separate variables and rewrite

 $F_{\ell,\ell}(r,\theta) = R_{\ell,\ell}(r)\Theta_{\ell,\ell}(\theta).$

Putting this back into the equation we have

$$\begin{pmatrix} \frac{\partial}{\partial \theta} + i \cot \theta \frac{\partial}{\partial \phi} \end{pmatrix} U_{\ell,\ell}(r,\theta,\phi) = 0, \quad \text{or} \\ \left[\frac{d}{d\theta} + i (\cot \theta) (i\ell) \right] \Theta_{\ell,\ell}(\theta) = 0, \quad \text{or} \\ \frac{d}{d\theta} \Theta_{\ell,\ell}(\theta) - \ell \cot \theta \Theta_{\ell,\ell}(\theta) = 0.$$

The θ equation is

$$\frac{d}{d\theta}\Theta_{\ell,\ell}(\theta) - \ell \cot\theta\Theta_{\ell,\ell}(\theta) = 0.$$

That has the solution

 $\Theta_{\ell,\ell}(\theta) = A(\sin\theta)^{\ell}$

and

$$U_{\ell,\ell}(r,\theta,\phi) = R_{\ell,\ell}(r)(\sin\theta)^{\ell} e^{i\ell\phi} \,.$$

Note that rotation only affects the angular parts.

- The radial component should not depend on any angular momentum quantum numbers.
- It should be the same for all wave functions of different angular momentum quantum numbers and is determined by the dynamics of the system.

$$U_{\ell,\ell}(r,\theta,\phi) = R_{\ell,\ell}(r)(\sin\theta)^{\ell} e^{i\ell\phi} \,.$$

Any other wave function can be obtained from this by using the lowering operator. Thus

$$\begin{aligned} |\ell, \ell - 1\rangle &= \frac{1}{[\ell(\ell+1) - \ell(\ell-1)]^{1/2}\hbar} L_{-} |\ell, \ell\rangle &= \frac{1}{\sqrt{2\ell}\hbar} L_{-} |\ell, \ell\rangle \\ U_{\ell,\ell-1}(r,\theta,\phi) &= \frac{1}{\sqrt{2\ell}\hbar} (-1)\hbar e^{-i\phi} (\frac{\partial}{\partial\theta} - i\cot\theta \frac{\partial}{\partial\phi}) U_{\ell,\ell}(r,\theta,\phi) \\ &= -\frac{2}{\sqrt{2\ell}\hbar} e^{-i\phi} \cdot \frac{\partial}{\partial\theta} U_{\ell,\ell}(r,\theta,\phi) \end{aligned}$$

where we have used

$$(\frac{\partial}{\partial \theta} + i \cot \theta \frac{\partial}{\partial \phi}) U_{\ell,\ell}(r,\theta,\phi) = 0, \text{ or}$$

$$+ i \cot \theta \frac{\partial}{\partial \phi} U_{\ell,\ell}(r,\theta,\phi) = -\frac{\partial}{\partial \theta} U_{\ell,\ell}(r,\theta,\phi).$$

$$U_{\ell,\ell-1}(r,\theta,\phi) = \frac{(-1)}{\sqrt{2\ell}} \cdot 2e^{-i\phi}R(r)e^{i\ell\phi}\frac{d}{d\theta}(\sin\theta)^{\ell}$$
$$= \frac{(-1)}{\sqrt{2\ell}} \cdot 2R(r)e^{i(\ell-1)\phi} \cdot \ell(\sin\theta)^{\ell-1}\cos\theta$$
$$= -\sqrt{2\ell}R(r)e^{i(\ell-1)\phi}(\sin\theta)^{\ell-1}\cos\theta.$$

Similarly, a general wave function $U_{\ell,m}(r,\theta,\phi)$ can be obtained by applying the lowering operator $\ell - m$ times with suitable normalization. The interesting conclusions of this operator method is that the angular momentum operator L^2 has eigenvalues of the form

1. [i] $\ell(\ell+1)\hbar^2$

2. [ii] ℓ takes integer as well as half integral values.

This is certainly a triumph of quantum mechanics.

For the energy associated with rotation, the Hamiltonian is denoted by

$$H = \frac{L^2}{2I}$$

with the eigenvalue

$$H|\ell,m
angle = E_{ heta}|\ell,m
angle$$

where I is the moment of inertia of the system.

In the old quantum theory, someone suggested the eigenvalues of L^2 as

$$L^2|\ell,m\rangle = \ell^2 \hbar^2 |\ell,m\rangle$$
 and $E_{\theta} = \frac{\ell^2 \hbar^2}{2I}$ with $\ell = 0, 1, 2, \cdots$.

That leads to the separation of energy levels in molecules in the proportions

$$\Delta E_{10} : \Delta E_{21} : \Delta E_{32} : \Delta E_{43} : \dots = 1 : 3 : 5 : 7 : \dots$$

However, this was not observed.

The correct quantum mechanics predicts

$$L^2|\ell,m\rangle = \ell(\ell+1)\hbar^2|\ell,m\rangle$$
 with $\ell = 0, 1, 2, \cdots$.

The observed energy separations were in the proportions

 $\Delta E_{10} : \Delta E_{21} : \Delta E_{32} : \Delta E_{43} : \dots = 1 : 2 : 3 : 4 : \dots = 2 : 4 : 6 : 8 : \dots$

That confirms the correct quantum theory with

$$L^2|\ell,m\rangle = \ell(\ell+1)\hbar^2|\ell,m\rangle$$
 and $E_{\theta} = \frac{\ell(\ell+1)\hbar^2}{2I}$ with $\ell = 0, 1, 2, \cdots$

- The angular momentum eigenvalues take integral values and the extra term arise from the noncommutativity of different components of the angular momentum operators.
- If we solve Schrödinger equations, we would only obtain integral values for angular momentum eigenvalue.
- The operator method, on the other hand, allows half integral eigenvalues as well.