

PHYS 3803: Quantum Mechanics I, Spring 2021

Lecture 18, April 01, 2021 (Thursday)

- Reading:
Harmonic Oscillator: My Notes and Griffiths 2.3
Angular Momentum: Griffiths 4.1 and 4.3
- Assignments: Problem Set 8 due April 07 (Wednesday).
Submit your homework assignments to Canvas.

Topics for Today: Harmonic Oscillator [Griffiths 2.3]

4.3 The Harmonic Oscillator in the Coordinate Basis

4.4 Oscillator in Higher Dimensions

5.1 Rotations in Two Dimensions

Topics for Next Lecture: Angular Momentum

5.2 Rotations and Angular Momentum

5.3 Schrödinger equation for spherically symmetric potentials

4.3 The Harmonic Oscillator in the Coordinate Basis

In the x basis, the Hamiltonian for the Harmonic Oscillator is give by

$$H = \frac{P^2}{2m} + \frac{1}{2}m\omega^2 X^2 = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2.$$

Since the Hamiltonian has no time dependence, we have stationary solutions. We know that the wave function for stationary solutions are

$$\Psi(x, t) = \psi_E(x)e^{-iEt/\hbar}$$

and the time independent Schrödinger Equation

$$H\psi_n(x) = E_n\psi_n(x) \quad \text{becomes}$$
$$\left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2 \right) \psi_n(x) = E_n\psi_n(x)$$

where $\psi_n(x)$ is the eigenfunction of the Hamiltonian with energy E_n .

We have found that the normalized eigenfunctions for the oscillator are

$$\begin{aligned}\psi_n(x) &= A_n H_n \left[\left(\frac{m\omega}{\hbar} \right)^{1/2} x \right] e^{-\frac{1}{2} \frac{m\omega}{\hbar} x^2} \\ &= \left(\frac{m\omega}{\pi\hbar} \right)^{1/4} \frac{1}{(2^n \cdot n!)^{1/2}} H_n \left(\sqrt{\frac{m\omega}{\hbar}} x \right) e^{-\frac{1}{2} \frac{m\omega}{\hbar} x^2} .\end{aligned}$$

And the wave function becomes

$$\Psi_n(x, t) = \left(\frac{m\omega}{\pi\hbar} \right)^{1/4} \frac{1}{(2^n \cdot n!)^{1/2}} H_n \left(\sqrt{\frac{m\omega}{\hbar}} x \right) e^{-\frac{1}{2} \frac{m\omega}{\hbar} x^2} e^{-iE_n t/\hbar}$$

with

$$E_n = \left(n + \frac{1}{2} \right) \hbar\omega .$$

That is the same energy derived from the matrix operator formalism.

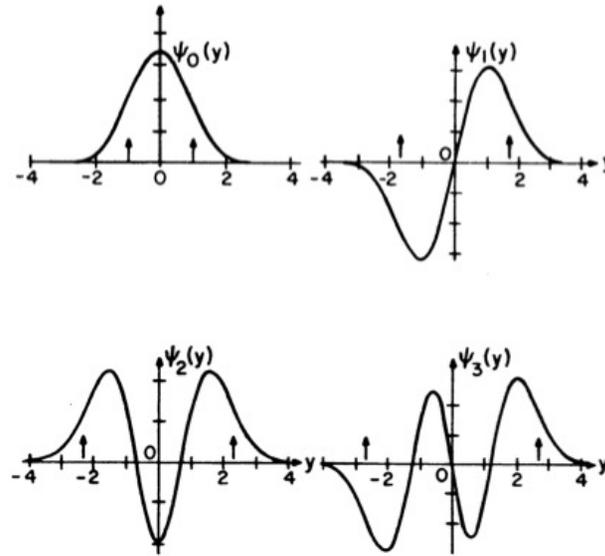


Figure 1: Normalized eigenfunctions versus $y = \xi = (m\omega/\hbar)^{1/2}x$.

If we plot the probability density for the oscillator in the ground state its maximum probability is around the point of equilibrium ($x = 0$) and tails off at large distances. This is the opposite of classical prediction.

However, if we plot the probability for large values of the quantum number (n) the behavior is as follows:

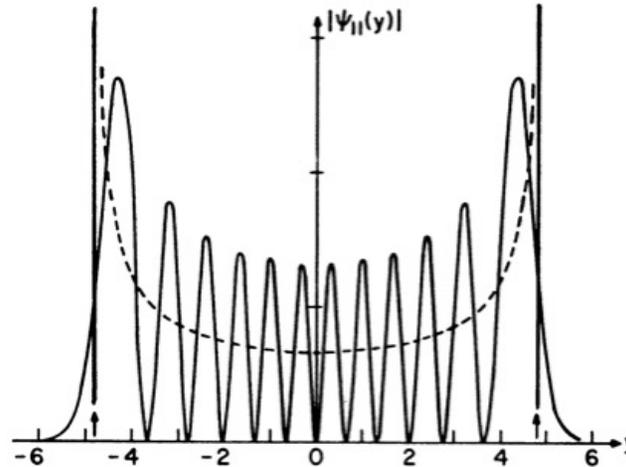


Figure 2: Probability density for $n = 11$ versus $y = \xi = (m\omega/\hbar)^{1/2}x$.

Thus as $n \rightarrow \infty$ the average of these plots behave like the classical oscillator. This is what the correspondence principle says, namely, when the energy becomes large the system must behave like a macroscopic system.

The energy of a quantum harmonic oscillator is quantized.

- The energy levels of the oscillator are spaced uniformly without any dependence on any parameter of the theory like the mass.
- The levels differ from the adjacent ones by $\hbar\omega$.
- Thus we can consider that an oscillator of frequency ω are associated with fictitious particles called quanta with energy $\hbar\omega$.
- In crystal physics these quanta are known as phonons whereas the interaction matter with radiation is described in terms of quanta known as photons.

The matrix elements of an operator represent the expectation values and the transition amplitudes.

- The diagonal values of an operator represent expectation values of that operator. In a stationary state these are time independent

$$\Omega_{nn} = \int \Psi_n^*(x, t) [\Omega \Psi_n(x, t)] dx .$$

- The off-diagonal elements of an operator become

$$\Omega_{mn} = \int \Psi_m^*(x, t) [\Omega \Psi_n(x, t)] dx .$$

Such elements can be thought of as transition amplitudes between states n and m .

- Just as in Hydrogen atom, the electron can drop down from an excited level to a lower level with the emission of a photon, here also any transition amplitude is accompanied by an emission or absorption of quanta.
- Furthermore, since

$$\Psi_n(x, t) \sim e^{-\left(\frac{i}{\hbar}\right) E_n t}$$

therefore, the transition amplitudes

$$\Omega_{mn} \sim e^{-\left(\frac{i}{\hbar}\right) (E_n - E_m) t}$$

and varies with time for $n \neq m$.

4.4 Oscillator in Higher Dimensions

Let us consider an oscillator in D dimensions. Thus

$$H = \sum_{i=1}^D H_i, \text{ and}$$
$$H_i = \frac{P_i^2}{2m} + \frac{1}{2}m\omega^2 X_i^2.$$

Such an oscillator whose frequency is the same in every direction is known as the isotropic oscillator. We know the basic commutation relations

$$[X_i, X_j] = 0$$

$$[P_i, P_j] = 0$$

$$[X_i, P_j] = i\hbar\delta_{ij}.$$

To solve this problem we can think of them as a set of decoupled harmonic oscillators. Each oscillator can be solved independently. The Hilbert space of states \mathcal{E} , therefore, separates now into product spaces. Thus we can consider

$$\mathcal{E} = \mathcal{E}_1 \otimes \mathcal{E}_1 \otimes \dots \otimes \mathcal{E}_D$$

where H_i acts only on $|E_i\rangle$. We can also define operators

$$a_i = \sqrt{\frac{m\omega}{2\hbar}} \left(X_i + \frac{i}{m\omega} P_i \right), \text{ and}$$
$$a_i^\dagger = \sqrt{\frac{m\omega}{2\hbar}} \left(X_i - \frac{i}{m\omega} P_i \right)$$

and

$$N_i = a_i^\dagger a_i$$

which are only on $|E_i\rangle$. The eigenvectors of N_i which are denoted by $|n_i\rangle$ define the vector space \mathcal{E}_i

$$\begin{aligned} N_i |n_i\rangle &= n_i |n_i\rangle \\ H_i |n_i\rangle &= E_{n_i} |n_i\rangle = \left(n_i + \frac{1}{2}\right) \hbar \omega |n_i\rangle \end{aligned}$$

with $n_i = 0, 1, 2, \dots, \infty$. Thus $\mathcal{E} = \mathcal{E}_1 \otimes \mathcal{E}_1 \otimes \dots \otimes \mathcal{E}_D$. We can define the states in \mathcal{E} by the quantum numbers of the product spaces. Thus for example

$$|n_1, n_2, \dots, n_D\rangle = |n_1\rangle \otimes |n_2\rangle \otimes \dots \otimes |n_D\rangle$$

where $n_1, n_2, \dots, n_D = 0, 1, 2, \dots, \infty$. We can show that

$$[a_i, a_j] = [a_i^\dagger, a_j^\dagger] = 0$$

$$[a_i, a_j^\dagger] = \delta_{ij}.$$

Furthermore we can define an operator

$$N = \sum_i N_i = \sum_i a_i^\dagger a_i$$

and

$$\begin{aligned} N|n_1, n_2, \dots, n_D\rangle &= \left(\sum_i N_i\right)|n_1\rangle \otimes |n_2\rangle \otimes \dots \otimes |n_D\rangle \\ &= N_1|n_1\rangle \otimes |n_2\rangle \otimes \dots \otimes |n_D\rangle \\ &\quad + |n_1\rangle \otimes N_2|n_2\rangle \otimes \dots \otimes |n_D\rangle \\ &\quad + \dots + |n_1\rangle \otimes |n_2\rangle \otimes \dots \otimes N_D|n_D\rangle \\ &= (n_1 + n_2 + \dots + n_D)|n_1\rangle \otimes |n_2\rangle \otimes \dots \otimes |n_D\rangle \\ &= (n_1 + n_2 + \dots + n_D)|n_1, n_2, \dots, n_D\rangle \\ &= n|n_1, n_2, \dots, n_D\rangle \end{aligned}$$

where $n = n_1 + n_2 + \dots + n_D$.

Similarly

$$H = \sum H_i = \hbar\omega \sum_i^D (N_i + \frac{1}{2})$$

and

$$\begin{aligned} H|n_1, n_2, \dots, n_D\rangle &= \hbar\omega \sum_i^D (N_i + \frac{1}{2})|n_1, n_2, \dots, n_D\rangle \\ &= \hbar\omega(n_1 + \frac{1}{2} + n_2 + \frac{1}{2} + \dots + n_D + \frac{1}{2})|n_1, n_2, \dots, n_D\rangle \\ &= \hbar\omega(n + \frac{D}{2})|n_1, n_2, \dots, n_D\rangle \end{aligned}$$

Thus the energy levels of the oscillator are

$$E_n = \hbar\omega(n + \frac{D}{2})$$

where $n = 0, 1, \dots, \infty$.

Furthermore, the ground state which is denoted by

$$|0, 0, \dots, 0\rangle = |0\rangle \otimes |0\rangle \otimes \dots \otimes |0\rangle$$

satisfies

$$a_i |0, 0, \dots, 0\rangle = 0$$

for all i , and has an energy

$$E_0 = \frac{D}{2} \hbar \omega$$

This corresponds to an uncertainty of energy $\hbar \omega / 2$ for every direction.

Furthermore, any higher state can be written as

$$|n_1, n_2, \dots, n_p\rangle = (n_1! n_2! \dots n_D!)^{-1/2} (a_1^\dagger)^{n_1} (a_2^\dagger)^{n_2} \dots (a_D^\dagger)^{n_D} |0, 0, \dots, 0\rangle$$

It is clear now that in higher dimensions there is degeneracy of states.

- (a) The state with energy $E_1 = (1 + D/2)\hbar\omega$ is D -fold degenerate. This is easily seen by noting that a state of the form $|1, 0, 0, \dots, 0\rangle$ has energy E_1 . But so does $|0, 1, 0, \dots, 0\rangle$, $|0, 0, 1, \dots, 0\rangle$, and so on. And there are D such states.
- (b) A state with energy $E_2 = (2 + D/2)\hbar\omega$ has $(1/2)(D + 1)D$ fold degeneracy. This can be seen by noting that a state of the form $|1, 1, 0, \dots, 0\rangle$ has energy E_2 . There are $(1/2)D(D - 1)$ such states. But also a state of the form $|2, 0, 0, \dots, 0\rangle$ has energy E_2 . There are D such states. Thus the total number of states with energy E_2 is $\frac{1}{2}D(D - 1) + D = \frac{1}{2}D(D + 1)$.
- (c) In general, we can show that in D dimensions, a state with energy $E_n = (n + \frac{D}{2})\hbar\omega$ has a C_n^{n+D-1} fold degeneracy.

5 Rotations and Angular Momentum

5.1 Rotations in Two Dimensions

In classical mechanics, if we rotate a position vector (\vec{r}) by an angle ϕ about the z -axis, then the coordinates of the particle change as

$$x \rightarrow x' = x \cos \phi - y \sin \phi$$

$$y \rightarrow y' = x \sin \phi + y \cos \phi$$

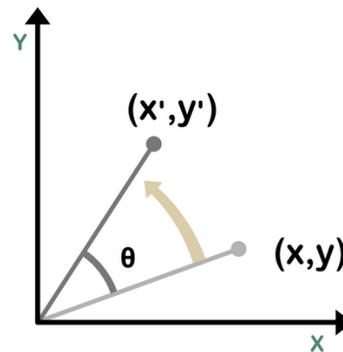


Figure 3: Rotation in the two dimensional (x,y) plane with $\theta \rightarrow \phi$.

Similarly

$$p_x \rightarrow p'_x = p_x \cos \phi - p_y \sin \phi$$

$$p_y \rightarrow p'_y = p_x \sin \phi + p_y \cos \phi$$

We can also write it in the matrix form as

$$\begin{pmatrix} x \\ y \end{pmatrix} \rightarrow \begin{pmatrix} x' \\ y' \end{pmatrix} = \begin{pmatrix} \cos \phi & -\sin \phi \\ \sin \phi & \cos \phi \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}$$

and

$$\begin{pmatrix} p_x \\ p_y \end{pmatrix} \rightarrow \begin{pmatrix} p'_x \\ p'_y \end{pmatrix} = \begin{pmatrix} \cos \phi & -\sin \phi \\ \sin \phi & \cos \phi \end{pmatrix} \begin{pmatrix} p_x \\ p_y \end{pmatrix} .$$

Let us denote by $R(\phi)$ the matrix that rotates these vectors and $U_R(\phi)$ the operator which acts on the Hilbert space of states corresponding to the rotation $R(\phi)$. Then in the active picture

$$|\psi\rangle \rightarrow |\psi_R\rangle = U_R|\psi\rangle.$$

To find out the effect of rotation on an arbitrary state, let us examine the effect of rotation on the coordinate basis

$$U_R(\phi)|x, y\rangle = |x \cos \phi - y \sin \phi, x \sin \phi + y \cos \phi\rangle$$

From this again we can show that rotation operator is unitary

$$U_R^\dagger(\phi)U_R(\phi) = I.$$

Let us write the generator for infinitesimal rotation about the z -axis as

$$U_R(\epsilon) = I - \frac{i\epsilon}{\hbar} G.$$

The generators of infinitesimal rotation are Hermitian because the rotation operators are unitary

$$U_R^\dagger(\phi)U_R(\phi) = I \implies U_R^\dagger(\phi) = U_R^{-1}(\phi) \quad \text{and} \quad G^\dagger = G.$$

Under infinitesimal rotations with small angle approximation, we have

$$\cos \epsilon \simeq 1 \quad \text{and} \quad \sin \epsilon \simeq \epsilon$$

$$U_R(\epsilon)|x, y\rangle = |x - \epsilon y, \epsilon x + y\rangle \quad \text{and} \quad U_R^{-1}(\epsilon)|x, y\rangle = |x + \epsilon y, -\epsilon x + y\rangle$$

such that $|\psi_R\rangle = U_R(\epsilon)|\psi\rangle$ and

$$\begin{aligned} \psi_R(x, y) &\equiv \langle x, y | \psi_R \rangle \\ &= \langle x, y | U_R(\epsilon) | \psi \rangle \\ &= \langle x + \epsilon y, -\epsilon x + y | \psi \rangle \\ &= \psi(x + \epsilon y, -\epsilon x + y). \end{aligned}$$

We have applied

$$\begin{aligned}\langle x, y|U_R &= [U_R^\dagger|x, y\rangle]^\dagger = [U_R^{-1}|x, y\rangle]^\dagger \\ &= [|x + \epsilon y, -\epsilon x + y\rangle]^\dagger \\ &= \langle x + \epsilon y, -\epsilon x + y|.\end{aligned}$$

Thus

$$\psi_R(x, y) = \langle x, y|U_R(\epsilon)|\psi\rangle = \langle x + \epsilon y, -\epsilon x + y|\psi\rangle \equiv \psi(x + \epsilon y, -\epsilon x + y)$$

or

$$\psi_R(x, y) = \langle x, y|I - \frac{i\epsilon}{\hbar}G|\psi\rangle = \psi(x, y) + \epsilon y \frac{\partial}{\partial x} \psi(x, y) - \epsilon x \frac{\partial}{\partial y} \psi(x, y)$$

Therefore

$$G = XP_y - YP_x = L_z$$

Therefore the angular momentum operator is the generator of infinitesimal rotations.

Furthermore, the theory is invariant if

$$U^\dagger(R)HU(R) = H$$

Putting in the infinitesimal structure of $U_R(\epsilon)$, we have

$$\frac{i\epsilon}{\hbar}[L_z, H] = 0 \quad \text{with} \quad U_R(\epsilon) = I - \frac{i}{\hbar}\epsilon L_z$$

or

$$[L_z, H] = 0$$

We can construct a finite rotation about the z -axis by taking successive infinitesimal rotations such that $\epsilon = \phi/N$, $N \rightarrow \infty$. Thus we have

$$\begin{aligned} U_R(\phi) &= \lim_{N \rightarrow \infty} \left(1 - \frac{i\epsilon}{\hbar} L_z\right)^N \\ &= \lim_{N \rightarrow \infty} \left(1 - \frac{i\phi}{N\hbar} L_z\right)^N \\ &= e^{-\frac{i\phi}{\hbar} L_z} \end{aligned}$$

Since $[L_z, L_z] = 0$, it is clear that

$$U_R(\phi_1)U_R(\phi_2) = U_R(\phi_1 + \phi_2).$$

That is, rotations about the same axis are additive.

The two dimensional vectors (x, y) can equivalently be described by the circular coordinates (r, ϕ) .

- A rotation does not change the radial vector.
- It changes the angle(s).
- Thus in this basis

$$U_R(\Delta\phi)|r, \phi\rangle = |r, \phi + \Delta\phi\rangle$$

Furthermore, note that since $0 \leq \phi \leq 2\pi$, the parameter of rotation is also bounded $0 \leq \phi \leq 2\pi$.

In this basis with polar coordinates (r, ϕ) ,

$$\begin{aligned} |\psi_R\rangle &= U_R |\psi\rangle \\ &= \int r dr d\phi U_R(\Delta\phi) |r, \phi\rangle \psi(r, \phi) \\ &= \int r dr d\phi |r, \phi + \phi\rangle \psi(r, \phi) \\ &= \int r dr d\phi |r, \phi\rangle \psi(r, \phi - \Delta\phi) \end{aligned}$$

Thus

$$\langle r, \phi | \psi_R \rangle = \psi(r, \phi - \Delta\phi)$$

or

$$\psi_R(r, \phi) = \psi(r, \phi - \Delta\phi)$$

Furthermore,

$$\psi_R(r, \phi) = \langle r, \phi | U(R) | \psi \rangle = \psi(r, \phi - \Delta\phi)$$

For an infinitesimal rotation $\Delta\phi = \epsilon \rightarrow 0+$,

$$\begin{aligned}\psi_R(r, \phi) &= \langle r, \phi | I - \frac{i\epsilon}{\hbar} L_z | \psi \rangle \\ &= \left(1 - \frac{i\epsilon}{\hbar} L_z \right) \psi(r, \phi) \\ &= \psi(r, \phi - \epsilon) = \psi(r, \phi) - \epsilon \frac{\partial}{\partial \phi} \psi(r, \phi).\end{aligned}$$

Thus in the (r, ϕ) basis

$$L_z \rightarrow -i\hbar \frac{\partial}{\partial \phi}$$

Furthermore, we can show that rotations form a group. This is a Lie group with transformation operators

$$U_R(\theta) = e^{-\left(\frac{i}{\hbar}\right)\theta_i L_i} \quad i = 1, 2, 3$$

where L_i are generators and θ_i are group parameters.

5.2 Rotations and Angular Momentum

Let us generalize the results of two dimensions to three dimensions. There are three generators of infinitesimal rotations in the 3-dimensional space. Let us denote them by

$$\begin{aligned}L_x &= YP_z - ZP_y \\L_y &= ZP_x - XP_z \\L_z &= XP_y - YP_x.\end{aligned}$$

Let us find various commutators

$$[L_x, X] = [YP_z - ZP_y, X] = 0$$

$$[L_y, X] = [ZP_x - XP_z, X] = Z[P_x, X] = -i\hbar Z$$

$$[L_z, X] = [XP_y - YP_x, X] = -Y[P_x, X] = i\hbar Y.$$

To use a more compact notation, let us define

$$\begin{aligned}x &= x_1, \quad y = x_2, \quad z = x_3, \quad \text{and} \\p_x &= p_1, \quad p_y = p_2, \quad p_z = p_3. \\X &= X_1, \quad Y = X_2, \quad Z = X_3, \quad \text{and} \\P_x &= P_1, \quad P_y = P_2, \quad P_z = P_3.\end{aligned}$$

Thus we can define the angular momentum operator as

$$\begin{aligned}L_i &= \epsilon_{ijk} X_j P_k, \quad i, j, k = 1, 2, 3 \quad \text{and} \\ \epsilon_{123} &= 1, \quad \epsilon_{213} = -1, \quad \epsilon_{iik} = 0.\end{aligned}$$

where ϵ_{ijk} is the anti-symmetric Levi-Civita symbol.

Clearly, then

$$\begin{aligned}[L_i, X_j] &= [\epsilon_{ikl} X_k P_l, X_j] \\ &= \epsilon_{ikl} X_k (-i\hbar \delta_{lj}) \\ &= (-i\hbar) \epsilon_{ikj} X_k\end{aligned}$$

$$= i\hbar\epsilon_{ijk}X_k$$

Similary we can show that

$$\begin{aligned} [L_i, P_j] &= [\epsilon_{ikl}X_kP_l, P_j] \\ &= \epsilon_{ikl}(i\hbar\delta_{kj})P_l \\ &= (i\hbar)\epsilon_{ijl}P_l \\ &= (i\hbar)\epsilon_{ijk}P_k \end{aligned}$$

Furthermore, the commutation relation of two angular momentum operators is now

$$\begin{aligned} [L_i, L_j] &= [\epsilon_{ikl}X_kP_l, \epsilon_{jmn}X_mP_n] \\ &= \epsilon_{ikl}\epsilon_{jmn}[X_kP_l, X_mP_n] \\ &= \epsilon_{ikl}\epsilon_{jmn}(X_m[X_k, P_n]P_l + X_k[P_l, X_m]P_n) \\ &= \epsilon_{ikl}\epsilon_{jmn}(X_m(i\hbar\delta_{kn})P_l + X_k(-i\hbar\delta_{lm})P_n) \\ &= i\hbar\epsilon_{ikl}\epsilon_{jmk}X_mP_l - i\hbar\epsilon_{ikl}\epsilon_{jln}X_kP_n \end{aligned}$$

$$\begin{aligned}
&= -i\hbar(\delta_{ij}\delta_{lm} - \delta_{im}\delta_{lj})X_mP_l + i\hbar(\delta_{ij}\delta_{kn} - \delta_{in}\delta_{kj})X_kP_n) \\
&= i\hbar(-\delta_{ij}X_lP_l + X_iP_j + \delta_{ij}X_kP_k - X_jP_i) \\
&= i\hbar(X_iP_j - X_jP_i) \\
&= i\hbar\epsilon_{ijk}L_k
\end{aligned}$$

N.B. (i) $\epsilon_{ijk}\epsilon_{lmk} = \delta_{il}\delta_{jm} - \delta_{im}\delta_{jl}$. (ii) ϵ_{ijk} is anti-symmetric. (iii) Repeated indices are summed.

Thus

$$[L_i, L_j] = i\hbar\epsilon_{ijk}L_k$$

This shows that generators of angular momentum along different directions do not commute. However

$$[L_i, L_i] = 0, ; \text{ for any } i.$$

Defining another operator

$$L^2 = \sum_i L_i L_i$$

we have

$$\begin{aligned} [L_i, L^2] &= [L_i, L_j L_j] \\ &= L_j [L_i, L_j] + [L_i, L_j] L_j \\ &= L_j (i\hbar \epsilon_{ijk} L_k) + (i\hbar \epsilon_{ijk} L_k) L_j \\ &= i\hbar \epsilon_{ijk} (L_j L_k + L_k L_j) \\ &= 0 \end{aligned}$$

Thus the operator L^2 commutes with all generators of infinitesimal rotation.

Furthermore, a theory is rotationally invariant if the generators commute with the Hamiltonian. This implies

$$[L_i, H] = 0$$

for rotational symmetry for all i , and

$$[L^2, H] = 0$$

for symmetric Hamiltonians.

However, since different components of the angular momentum operator do not commute among themselves, it is clear that H, L^2 and one component of the angular momentum can be simultaneously diagonalized for a rotationally invariant theory. A simple example of rotationally invariant theory is

$$H = \frac{P^2}{2\mu} + V(r) = \frac{P^2}{2\mu} + V(X^2 + Y^2 + Z^2)$$

where the potential only depends on the radial component. Higher dimensional isotropic Harmonic Oscillator is a simple example.

In such a problem, we can always choose to diagonalize H, L^2 , and L_3 simultaneously. That means they can have common eigenvectors.

To study the eigenvalue spectrum of these operators, we further define

$$L_+ \equiv L_1 + iL_2$$

$$L_- \equiv L_1 - iL_2$$

$$L_- = (L_+)^\dagger$$

and we have

$$[L_+, L^2] = [L_1 + iL_2, L^2] = 0$$

Since L^2 commutes with any component L_i .

Similarity

$$[L_-, L^2] = [L_1 - iL_2, L^2] = 0$$

On the other hand,

$$\begin{aligned} [L_+, L_3] &= [L_1 + iL_2, L_3] \\ &= -i\hbar L_2 + i(i\hbar)L_1 \end{aligned}$$

$$\begin{aligned}
&= -\hbar(L_1 + iL_2) \\
&= -\hbar L_+
\end{aligned}$$

and

$$\begin{aligned}
[L_-, L_3] &= [L_1 - iL_2, L_3] \\
&= -i\hbar L_2 - i(i\hbar)L_1 \\
&= \hbar(L_1 + iL_2) \\
&= \hbar L_-
\end{aligned}$$

Furthermore

$$\begin{aligned}
[L_+, L_-] &= [L_1 + iL_2, L_1 - iL_2] \\
&= [L_1 - iL_2] + [iL_2, L_1] \\
&= (-i)(i\hbar L_3) + i(-i\hbar L_3) \\
&= 2\hbar L_3
\end{aligned}$$

We know that for a rotationally invariant theory the Hamiltonian

commutes with all components of the angular momentum operator.
Thus

$$[L_+, H] = [L_-, H] = 0$$

Let $|\lambda, \mu\rangle$ represent the simultaneous eigenstates of the operators L^2 and L_3 such that

$$\begin{aligned}L_3|\lambda, \mu\rangle &= \mu|\lambda, \mu\rangle \text{ and} \\L^2|\lambda, \mu\rangle &= \Lambda|\lambda, \mu\rangle\end{aligned}$$

Let us now examine the effect of the operator L_+ on a given state,

$$\begin{aligned}L_3L_+|\lambda, \mu\rangle &= ([L_3, L_+] + L_+L_3)|\lambda, \mu\rangle \\&= (\hbar L_+ + L_+L_3)|\lambda, \mu\rangle \\&= (\mu + \hbar)L_+|\lambda, \mu\rangle\end{aligned}$$

Similarly

$$L^2L_+|\lambda, \mu\rangle = ([L^2, L_+] + L_+L^2)|\lambda, \mu\rangle$$

$$\begin{aligned}
&= L_+ L^2 |\lambda, \mu\rangle \\
&= \Lambda L_+ |\lambda, \mu\rangle
\end{aligned}$$

Thus we see that the effect of L_+ acting on a given state is to raise its eigenvalue μ by a unit of \hbar while leaving the eigenvalue of L^2 unchanged. Thus we must have

$$L_+ |\lambda, \mu\rangle = d_m |\lambda, \mu + \hbar\rangle$$

where d_m are constants depending on λ and m .

We can also show that

$$\begin{aligned}
L_3 L_- |\lambda, \mu\rangle &= ([L_3, L_-] + L_- L_3) |\lambda, \mu\rangle \\
&= (-\hbar L_- + L_- L_3) |\lambda, \mu\rangle \\
&= (\mu - \hbar) L_- |\lambda, \mu\rangle
\end{aligned}$$

Similarly

$$L^2 L_- |\lambda, \mu\rangle = ([L^2, L_-] + L_- L^2) |\lambda, \mu\rangle$$

$$\begin{aligned}
&= L_- L^2 |\lambda, \mu\rangle \\
&= \Lambda L_- |\lambda, \mu\rangle
\end{aligned}$$

Here we notice that the operator L_- decrease the eigenvalue of L_3 by a unit of \hbar while leaving the eigenvalue of L^2 unchanged. Thus we expect

$$L_- |\lambda, \mu\rangle = c_m |\lambda, \mu - \hbar\rangle$$

where c_m are constants depending on λ and m .

Since the operators L_+ and L_- raise and lower the eigenvalue of L_3 , they are also known as the raising and lowering operators. Furthermore, it follows that given a state $|\lambda, \mu\rangle$ we can construct a sequence of states $|\lambda, \mu + \hbar\rangle, |\lambda, \mu + 2\hbar\rangle, \dots$, and $|\lambda, \mu - \hbar\rangle, |\lambda, \mu - 2\hbar\rangle, \dots$, respectively by applying the raising and lowering operators. However, physically this sequence cannot go on without termination. For the operator

$$L^2 = L_1^2 + L_2^2 + L_3^2$$

Thus

$$L^2 - L_3^2 = L_1^2 + L_2^2 \geq 0.$$

This is a positive semidefinite operator. Thus the eigenvalues must satisfy

$$\Lambda - \mu^2 \geq 0$$

or

$$\Lambda \geq \mu^2.$$

This implies that there must exist states with a maximum m such that

$$\begin{aligned} L_+ |\lambda, \mu_{\max}\rangle &= 0 \\ \langle \lambda, \mu_{\max} | L_- L_+ | \lambda, \mu_{\max}\rangle &= 0 \\ \langle \lambda, \mu_{\max} | (L^2 - L_3^2 - \hbar L_3) | \lambda, \mu_{\max}\rangle &= 0 \\ (\lambda - \mu_{\max}^2 - \hbar m_{\max}) \langle \lambda, \mu_{\max} | \lambda, \mu_{\max}\rangle &= 0 \\ \lambda - \mu_{\max}(m_{\max} + \hbar) &= 0. \end{aligned}$$

One can similarly show that there must also exist a state with a maximum m such that

$$\begin{aligned}
 L_- |\lambda, \mu_{\min}\rangle &= 0 \\
 \langle \lambda, \mu_{\min} | L_+ L_- | \lambda, \mu_{\min}\rangle &= 0 \\
 \langle \lambda, \mu_{\min} | (L^2 - L_3^2 + \hbar L_3) | \lambda, \mu_{\min}\rangle &= 0 \\
 (\Lambda - \mu_{\min}^2 + \hbar m_{\min}) \langle \lambda, \mu_{\min} | \lambda, \mu_{\min}\rangle &= 0 \\
 \Lambda - \mu_{\min}(m_{\min} - \hbar) &= 0.
 \end{aligned}$$

Comparing the two relations we obtain

$$\mu_{\min} = -\mu_{\max}$$

N.B. The other solution has $\mu_{\max} = \mu_{\min} - \hbar$ that is not meaningful.

Furthermore, let us assume that we can go from the state $|\lambda, \mu_{\min}\rangle$ to $|\lambda, \mu_{\max}\rangle$ by applying the operator L_+ k times. Thus

$$\mu_{\max} - \mu_{\min} = \hbar k$$

$$2\mu_{\max} = \hbar k$$

$$\mu_{\max} = \frac{\hbar}{2}k = -\mu_{\min}.$$

Then

$$\begin{aligned} \Lambda &= \mu_{\max}(\mu_{\max} + \hbar) \\ &= \frac{\hbar}{2}k\left(\frac{\hbar}{2}k + \hbar\right) \\ &= \hbar^2\left[\frac{k}{2}\left(\frac{k}{2} + 1\right)\right] \end{aligned}$$

We may define $\ell = \frac{k}{2}$ which takes only multiples of half integral values. Thus we have

$$\Lambda = \hbar^2 \ell(\ell + 1)$$

and

$$-\hbar\ell \leq \hbar m \leq \hbar\ell$$

where m takes $2\ell + 1$ values and ℓ takes values

$$\ell = 0, \frac{1}{2}, 1, \frac{3}{2}, \dots$$

that has positive multiple of half integers.

Let us define m to be a number $-\ell \leq m \leq \ell$ and we can determine the normalized states

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

$$L_3|\ell, m\rangle = -\hbar m|\ell, m\rangle$$

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

Thus

$$\langle \ell, m | L_- L_+ | \ell, m \rangle = |d_m|^2$$

$$\langle \ell, m | L^2 - L_3^2 - \hbar L_3 | \ell, m \rangle = |d_m|^2$$

$$\hbar^2[\ell(\ell + 1) - m(m + 1)] = |d_m|^2$$

Choosing d_m to be real, we have

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

Hence

$$\begin{aligned} L_+|\ell, m\rangle &= \hbar[\ell(\ell + 1) - m(m + 1)]^{1/2}|\ell, m + 1\rangle \\ |\ell, m + 1\rangle &= \frac{1}{\hbar[\ell(\ell + 1) - m(m + 1)]^{1/2}}L_+|\ell, m\rangle. \end{aligned}$$

Similarly, we can also show that

$$\begin{aligned} L_-|\ell, m\rangle &= \hbar[\ell(\ell + 1) - m(m - 1)]^{1/2}|\ell, m - 1\rangle \\ |\ell, m - 1\rangle &= \frac{1}{\hbar[\ell(\ell + 1) - m(m - 1)]^{1/2}}L_-|\ell, m\rangle. \end{aligned}$$

This, therefore, defines all the eigenstates for a particular value of ℓ . They define a Hilbert space \mathcal{E}^ℓ which 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

- (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 $m = \pm\frac{1}{2}$. Let the states be

$$\left|\frac{1}{2}, \frac{1}{2}\right\rangle \quad \text{and} \quad \left|\frac{1}{2}, -\frac{1}{2}\right\rangle.$$

We have

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

This implies

$$\begin{aligned} \left\langle \frac{1}{2}, \frac{1}{2} \left| L_3 \right| \frac{1}{2}, \frac{1}{2} \right\rangle &= \frac{\hbar}{2} = \left\langle \frac{1}{2}, -\frac{1}{2} \left| L_3 \right| \frac{1}{2}, -\frac{1}{2} \right\rangle \\ \left\langle \frac{1}{2}, \frac{1}{2} \left| L_3 \right| \frac{1}{2}, -\frac{1}{2} \right\rangle &= 0 = \left\langle \frac{1}{2}, -\frac{1}{2} \left| L_3 \right| \frac{1}{2}, \frac{1}{2} \right\rangle. \end{aligned}$$

Thus

$$L_3 = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Similarly

$$\begin{aligned} \langle \ell, m' | L^2 | \ell, m \rangle &= \hbar^2 \ell(\ell + 1) \langle \ell, m' | \ell, m \rangle \\ &= \hbar^2 \ell(\ell + 1) \delta_{mm'} \end{aligned}$$

$$\begin{aligned} \langle \ell, m' | L_+ | \ell, m \rangle &= d_m \langle \ell, m' | \ell, m + 1 \rangle \\ &= d_m \delta_{m', m+1} \\ &= \hbar[\ell(\ell + 1) - m(m + 1)]^{1/2} \delta_{m', m+1} \end{aligned}$$

$$\begin{aligned} \langle \ell, m' | L_- | \ell, m \rangle &= c_m \langle \ell, m' | \ell, m - 1 \rangle \\ &= c_m \delta_{m', m-1} \\ &= \hbar[\ell(\ell + 1) - m(m - 1)]^{1/2} \delta_{m', m-1}. \end{aligned}$$

Thus

$$L^2 = \hbar^2 \frac{1}{2} \left(\frac{1}{2} + 1 \right) \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \frac{3}{4} \hbar^2 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

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

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

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

$$L_1 = L_x = i\hbar \left(\sin \phi \frac{\partial}{\partial \theta} + \cos \phi \cot \theta \frac{\partial}{\partial \phi} \right)$$

$$L_2 = L_y = i\hbar \left(-\cos \phi \frac{\partial}{\partial \theta} + \sin \phi \cot \theta \frac{\partial}{\partial \phi} \right)$$

$$L_3 = L_z = -i\hbar \frac{\partial}{\partial \phi}$$

Thus

$$\begin{aligned} L_{\pm} &= L_1 \pm iL_2 \\ &= i\hbar \left[(\sin \phi \mp i \cos \phi) \frac{\partial}{\partial \theta} + (\cos \phi \pm i \sin \phi) \cot \theta \frac{\partial}{\partial \phi} \right] \\ &= \pm \hbar e^{\pm i\phi} \left(\frac{\partial}{\partial \theta} \pm i \cot \theta \frac{\partial}{\partial \phi} \right) \end{aligned}$$

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

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

In the spherical coordinate basis, this becomes

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

Thus

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

Let us separate variables and rewrite

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

Putting this back into the equation we have

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

$$\left[\frac{d}{d\theta} + i\cot\theta(i\ell)\right]\Theta_{\ell,\ell}(\theta) = 0 \text{ or}$$

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

Thus

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

and

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

Furthermore, note that rotation only affects the angular parts. The

radial component, therefore, should not depend on any angular momentum quantum numbers. In fact, it should be the same for all wavefunctions of different angular momentum quantum numbers and is determined by the dynamics of the system. Thus

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

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

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

where we have used

$$\begin{aligned} \left(\frac{\partial}{\partial \theta} + i \cot \theta \frac{\partial}{\partial \phi}\right) U_{\ell, \ell}(r, \theta, \phi) &= 0 \text{ and} \\ +i \cot \theta \frac{\partial}{\partial \phi} U_{\ell, \ell}(r, \theta, \phi) &= -\frac{\partial}{\partial \theta} U_{\ell, \ell}(r, \theta, \phi). \end{aligned}$$

Thus

$$\begin{aligned} U_{\ell, \ell-1}(r, \theta, \phi) &= \frac{(-1)}{(2\ell)^{1/2}} \cdot 2e^{-i\phi} R(r) e^{i\ell\phi} \frac{d}{d\theta} (\sin \theta)^\ell \\ &= \frac{(-1)}{(2\ell)^{1/2}} \cdot 2R(r) e^{-i(\ell-1)\phi} \cdot \ell (\sin \theta)^{\ell-1} \cos \theta \\ &= (-1)(2\ell)^{1/2} R(r) e^{-i(\ell-1)\phi} (\sin \theta)^{\ell-1} \cos \theta \end{aligned}$$

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 conclusion of this operator method is that the angular momentum operator L^2 has eigenvalues of the form

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

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 is denoted by

$$E_{\theta} = \frac{L^2}{2I}$$

The separations of energy levels in molecules were observed to be in proportions

$$1 : 2 : 3 : 4 : \dots$$

We can convince ourselves that this is true if

$$L^2 = \hbar^2 \ell(\ell + 1), \quad \ell = 0, 1, 2, \dots$$

This says that 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.