

I. Introduction

1. Review of Postulates and Formalism

Postulate 1.

The state of a quantum system can be described by a wavefunction in a Hilbert space.

We denote the elements of the Hilbert space as $|\psi\rangle$, and the complex conjugate by $\langle\psi|$.

Postulate 2.

Every observable/measurable quantity is described by an operator \hat{A} on a Hilbert space.

Postulate 3.

The result of measuring an observable is one of its eigenvalues.

Postulate 4. Born's Rule

For an observable \hat{A} and its eigenvalue a corresponding to $|a\rangle$, the probability of measuring a is

$$\mathbb{P}(a) = |\langle a|\psi\rangle|^2,$$

where $|\psi\rangle$ is the quantum state before the measurement.

Postulate 5.

For an observable \hat{A} , if an eigenvalue a is measured, then the quantum state after the measurement is $|a\rangle$.

Postulate 6. Schrodinger Equation

The time evolution of a quantum state $|\psi\rangle$ satisfies

$$i\hbar \frac{\partial}{\partial t} |\psi\rangle = H |\psi\rangle,$$

where H is the Hamiltonian operator.

2. Time Evolution Operator

Consider the time dependent Schrodinger equation

$$i\hbar \frac{\partial}{\partial t} |\psi\rangle = H |\psi\rangle.$$

Then the state $|\psi\rangle$ evolves over time according to the *time evolution operator* $U(t, t_0)$ by

$$|\psi(t)\rangle = U(t, t_0) |\psi(t_0)\rangle$$

with the initial condition $U(t_0, t_0) = I$, the identity operator. Note that U has to be unitary, since we want to preserve the norm. Therefore, the differential equation for U is given by

$$i\hbar \frac{\partial}{\partial t} U(t, t_0) |\psi(t_0)\rangle = H U(t, t_0) |\psi(t_0)\rangle.$$

Rewriting in terms of U ,

$$\frac{\partial}{\partial t} U(t, t_0) = -\frac{i}{\hbar} H U(t, t_0).$$

In case H is independent of the time,

$$U = Ae^{-\frac{i}{\hbar}Ht},$$

where A is a constant depending on the initial condition $U(t_0, t_0) = I$. That is,

$$I = U(t_0, t_0) = Ae^{-\frac{i}{\hbar}Ht_0} \implies A = e^{\frac{i}{\hbar}Ht_0}.$$

This solution is useful when paired with the *time independent Schrodinger equation*:

$$H|E_n\rangle = E_n|E_n\rangle.$$

In this case, for any analytic function f ,

$$f(H)|E_n\rangle = f(E_n)|E_n\rangle,$$

so in particular,

$$U(t, t_0)|E_n\rangle = e^{-\frac{i}{\hbar}E_n(t-t_0)}|E_n\rangle.$$

For a general state $|\psi(t_0)\rangle$, we write it down as a linear combination of energy eigenstates,

$$|\psi(t_0)\rangle = \left(\sum_n |E_n\rangle \langle E_n| \right) |\psi(t_0)\rangle = \sum_n c_n |E_n\rangle,$$

where $c_n = \langle E_n | \psi(t_0) \rangle$. Then,

$$|\psi(t)\rangle = U(t, t_0)|\psi(t_0)\rangle = e^{-\frac{i}{\hbar}H(t-t_0)} \sum_n c_n |E_n\rangle = \sum_n c_n e^{-\frac{i}{\hbar}E_n(t-t_0)} |E_n\rangle.$$

Thus

$$U(t, t_0) = \sum_n e^{-\frac{i}{\hbar}E_n(t-t_0)} |E_n\rangle \langle E_n|.$$

Example 1.1. Time Evolution of Spin- $\frac{1}{2}$

Let

$$H = \hbar\Omega\sigma_x = \hbar\Omega(|\uparrow\rangle\langle\downarrow| + |\downarrow\rangle\langle\uparrow|) = \hbar\Omega \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix},$$

where $|\uparrow\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$, $|\downarrow\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$. Note that the energy eigenvectors are

$$\begin{aligned} |E_1\rangle &= \frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle) \text{ corresponding to } \hbar\Omega = E_1 \\ |E_2\rangle &= \frac{1}{\sqrt{2}}(|\uparrow\rangle - |\downarrow\rangle) \text{ corresponding to } -\hbar\Omega = E_2 \end{aligned}.$$

Consider

$$|\psi(0)\rangle = |\downarrow\rangle.$$

Then the coefficients with respect to the basis $(|E_1\rangle, |E_2\rangle)$ are

$$\begin{aligned} c_1 &= \langle E_1 | \downarrow \rangle = \frac{1}{\sqrt{2}}(\langle\uparrow| + \langle\downarrow|) |\downarrow\rangle = \frac{1}{\sqrt{2}} \\ c_2 &= \langle E_2 | \downarrow \rangle = \frac{1}{\sqrt{2}}(\langle\uparrow| - \langle\downarrow|) |\downarrow\rangle = -\frac{1}{\sqrt{2}} \end{aligned},$$

which means

$$|\psi(0)\rangle = \frac{1}{\sqrt{2}}|E_1\rangle - \frac{1}{\sqrt{2}}|E_2\rangle.$$

It follows that

$$\begin{aligned}
|\psi(t)\rangle &= U(t, 0) |\psi(0)\rangle = \left(\sum_n e^{-\frac{i}{\hbar} E_n t} |E_n\rangle \langle E_n| \right) |\psi(0)\rangle = (e^{-i\Omega t} |E_1\rangle \langle E_1| + e^{i\Omega t} |E_2\rangle \langle E_2|) \frac{1}{\sqrt{2}} (|E_1\rangle - |E_2\rangle) \\
&= \frac{1}{\sqrt{2}} e^{-i\Omega t} |E_1\rangle - \frac{1}{\sqrt{2}} e^{i\Omega t} |E_2\rangle = \frac{1}{2} e^{-i\Omega t} (|\uparrow\rangle + |\downarrow\rangle) - \frac{1}{2} e^{i\Omega t} (|\uparrow\rangle - |\downarrow\rangle) = \frac{1}{2} (e^{-i\Omega t} - e^{i\Omega t}) |\uparrow\rangle + \frac{1}{2} (e^{-i\Omega t} + e^{i\Omega t}) |\downarrow\rangle \\
&= i \sin(\Omega t) |\uparrow\rangle + \cos(\Omega t) |\downarrow\rangle.
\end{aligned}$$

3. Harmonic Oscillator

Consider the Hamiltonian operator

$$H = \frac{p^2}{2m} = \frac{1}{2} m \omega^2 x^2. \quad [1.1]$$

Suppose $H|\psi\rangle = E|\psi\rangle$, where E is an eigenvalue of H . How do we calculate $E, |\psi\rangle$?

First approach: substitute

$$p = -i\hbar \frac{\partial}{\partial x} \quad [1.2]$$

into [1.1]. We won't use this approach, as it does not give much intuition to the problem.

Second approach: rewrite Hamiltonian in terms of *ladder operators*. Let

$$a = \frac{1}{\sqrt{2\hbar m \omega}} (ip + m\omega x),$$

so that

$$a^\dagger = \frac{1}{\sqrt{2\hbar m \omega}} (-ip + m\omega x).$$

Then, using the commutator formula $[x, p] = i\hbar$,

$$\begin{aligned}
a^\dagger a &= \frac{1}{2\hbar m \omega} (-ip + m\omega x) (ip + m\omega x) = \frac{1}{2\hbar m \omega} (p^2 + im\omega (xp - px) + m^2 \omega^2 x^2) \\
&= \frac{1}{2\hbar m \omega} (p^2 + im\omega [x, p] + m^2 \omega^2 x^2) = \frac{1}{2\hbar m \omega} (p^2 + im\omega i\hbar + m^2 \omega^2 x^2) \\
&= \frac{1}{2\hbar m \omega} (p^2 + m^2 \omega^2 x^2 - \hbar m \omega) = \frac{1}{\hbar \omega} \left(\frac{p^2}{2m} + \frac{1}{2} m \omega^2 x^2 \right) - \frac{1}{2} = \frac{1}{\hbar \omega} H - \frac{1}{2}.
\end{aligned}$$

Thus we conclude

$$H = \hbar \omega \left(a^\dagger a + \frac{1}{2} \right). \quad [1.3]$$

Observe that [1.3] tells us that the eigenvectors of H are precisely the eigenvectors of $a^\dagger a$;

$$a^\dagger a |E_n\rangle = n |E_n\rangle \implies H |E_n\rangle = \hbar \omega \left(n + \frac{1}{2} \right) |E_n\rangle.$$

We can find n using commutators. First

$$\begin{aligned}
[a, a^\dagger] &= \frac{1}{2\hbar m \omega} [ip + m\omega x, -ip + m\omega x] = \frac{1}{2\hbar m \omega} ([ip, -ip] + [ip, m\omega x] + [m\omega x, -ip] + [m\omega x, m\omega x]) \\
&= \frac{1}{2\hbar m \omega} (im\omega [p, x] - im\omega [x, p]) = \frac{i}{2\hbar} (-i\hbar - i\hbar) = 1.
\end{aligned}$$

Now, observe that $a |E_n\rangle$ is an eigenstate of $a^\dagger a$ corresponding to $n - 1$: since $[a, a^\dagger] = 1$,

$$a^\dagger a (a |E_n\rangle) = (aa^\dagger - 1) a |E_n\rangle = a (a^\dagger a) |E_n\rangle - a |E_n\rangle = an |E_n\rangle - a |E_n\rangle = (n - 1) a |E_n\rangle .$$

Hence

$$a |E_n\rangle = c_n |E_{n-1}\rangle .$$

Similarly,

$$a^\dagger |E_n\rangle = b_n |E_{n+1}\rangle .$$

Let us find what c_n, b_n are. Observe

$$n = \langle E_n | n | E_n \rangle = \langle E_n | a^\dagger a | E_n \rangle = \langle E_{n-1} | c_n^* c_n | E_{n-1} \rangle = |c_n|^2 .$$

Therefore n is nonnegative and

$$c_n = \sqrt{n}$$

or

$$a |E_n\rangle = \sqrt{n} |E_{n-1}\rangle .$$

In a similar fashion, we find out

$$b_n = \sqrt{n+1},$$

so that

$$a^\dagger |E_n\rangle = \sqrt{n+1} |E_{n+1}\rangle .$$

Note that we have to have n to be an integer, so that

$$a^n |E_n\rangle = 0.$$

Since we may write x, p in terms of the ladder operators as

$$x = \sqrt{\frac{\hbar}{2m\omega}} (a + a^\dagger)$$

and

$$p = i\sqrt{\frac{\hbar m\omega}{2}} (a^\dagger - a) ,$$

we have

$$\langle x^2 \rangle = \langle E_n | x^2 | E_n \rangle = \frac{\hbar}{2m\omega} \langle E_n | aa + aa^\dagger + a^\dagger a + a^\dagger a^\dagger | E_n \rangle = \frac{\hbar}{2m\omega} \langle E_n | aa + 2a^\dagger a + 1 + a^\dagger a^\dagger | E_n \rangle .$$

But, using orthonormality of $\{|E_n\rangle\}_{n=0}^\infty$, we obtain

$$\langle E_n | aa | E_n \rangle = \langle E_n | a^\dagger a^\dagger | E_n \rangle = 0,$$

so that

$$\langle x^2 \rangle = \frac{\hbar}{2m\omega} \langle E_n | 2a^\dagger a + 1 | E_n \rangle = \frac{\hbar}{2m\omega} (2n + 1) \langle E_n | E_n \rangle = \frac{\hbar}{2m\omega} (2n + 1) .$$

Summary 1.1. Harmonic Oscillator, Ladder Operators

Given Hamiltonian

$$H = \frac{1}{2} m \omega^2 x^2 ,$$

we have that

$$H = \hbar \omega \left(a^\dagger a + \frac{1}{2} \right) ,$$

where

$$a = \frac{1}{\sqrt{2\hbar m\omega}} (ip + m\omega x)$$

is the *ladder operator*. a, a^\dagger acts on the energy eigenstates by

$$a |E_n\rangle = \sqrt{n} |E_{n-1}\rangle$$

and

$$a^\dagger |E_n\rangle = \sqrt{n+1} |E_{n+1}\rangle.$$

With respect to the ladder operators, x, p can be written as

$$x = \sqrt{\frac{\hbar}{2m\omega}} (a + a^\dagger)$$

and

$$p = i\sqrt{\frac{\hbar m\omega}{2}} (a^\dagger - a),$$

Example 1.2.

Consider the harmonic oscillator states $|0\rangle = |E_0\rangle, \dots$ and suppose $|\varphi(0)\rangle = \frac{1}{\sqrt{2}}(|n\rangle + |n+1\rangle)$. What is $\langle x(t) \rangle$?

Answer. Observe that

$$|\varphi(t)\rangle = \frac{1}{\sqrt{2}} \left(e^{-\frac{i}{\hbar} E_n t} |n\rangle + e^{-\frac{i}{\hbar} E_{n+1} t} |n+1\rangle \right) = \frac{1}{\sqrt{2}} \left(e^{-i\omega(n+\frac{1}{2})t} |n\rangle + e^{-i\omega(n+\frac{3}{2})t} |n+1\rangle \right),$$

so that

$$\begin{aligned} \langle x(t) \rangle &= \langle \psi(t) | x | \psi(t) \rangle = \sqrt{\frac{\hbar}{2m\omega}} \langle \psi(t) | a + a^\dagger | \psi(t) \rangle \\ &= \sqrt{\frac{\hbar}{2m\omega}} \frac{1}{2} \left(\langle n | e^{i\omega(n+\frac{1}{2})t} + \langle n+1 | e^{i\omega(n+\frac{3}{2})t} \right) (a + a^\dagger) \sqrt{\frac{\hbar}{2m\omega}} \frac{1}{2} \left(e^{-i\omega(n+\frac{1}{2})t} |n\rangle + e^{-i\omega(n+\frac{3}{2})t} |n+1\rangle \right) \\ &= \frac{1}{2} \sqrt{\frac{\hbar}{2m\omega}} \left(e^{i\omega(n+\frac{3}{2})t} e^{-i\omega(n+\frac{1}{2})t} \langle n+1 | a^\dagger | n \rangle + e^{i\omega(n+\frac{1}{2})t} e^{-i\omega(n+\frac{3}{2})t} \langle n | a | n+1 \rangle \right) \\ &= \frac{1}{2} \sqrt{\frac{\hbar}{2m\omega}} (e^{i\omega t} \sqrt{n+1} + e^{-i\omega t} \sqrt{n+1}) = \sqrt{\frac{\hbar(n+1)}{2m\omega}} \cos(\omega t). \end{aligned}$$

Thus

$$\langle x(t) \rangle = \sqrt{\frac{\hbar(n+1)}{2m\omega}} \cos(\omega t).$$

QED

4. Angular Momentum Commutators

We start with classical *orbital angular momentum* (OAM):

$$\vec{L} = \vec{r} \times \vec{p}.$$

By definition,

$$\vec{L} = \begin{bmatrix} yp_z - zp_y \\ zp_x - xp_z \\ xp_y - yp_x \end{bmatrix}.$$

We are going to use *canonical commutation relations*

$$\begin{aligned} [r_i, r_j] &= 0 \\ [p_i, p_j] &= 0 \\ [r_i, p_j] &= i\hbar\delta_{ij} \end{aligned} ,$$

where r_1, r_2, r_3 are position components (say x, y, z for instance) and p_1, p_2, p_3 are the momentum components, to figure out $[L_i, L_j]$. For instance,

$$[L_x, L_y] = [yp_z - zp_y, zp_x - xp_z] = [yp_z, zp_x] - [zp_y, zp_x] - [yp_z, xp_z] + [zp_y, xp_z] .$$

But note that z commutes with itself and p_y, p_z commutes, so that $[zp_y, zp_x] = 0$. Similarly, x, y commutes so that $[yp_z, xp_z] = 0$. Hence,

$$[L_x, L_y] = [yp_z, zp_x] + [zp_y, xp_z] = y[p_z, zp_x] + [y, zp_x]p_z + [zp_y, xp_z] .$$

Since y commutes with z, p_x , it follows $[y, zp_x] = 0$. This means

$$[L_x, L_y] = y[p_z, zp_x] + [zp_y, xp_z] = yz \underbrace{[p_z, p_x]}_{=0} + y[p_z, z]p_x + xz \underbrace{[p_y, p_z]}_{=0} + x[z, p_z]p_y = i\hbar(xp_y - yp_x) = i\hbar L_z .$$

Similarly, we have

$$[L_y, L_z] = i\hbar L_x, [L_z, L_x] = i\hbar L_y .$$

Summary 1.2. Orbital Angular Momentum Commutation Relation

Let $L = (L_x, L_y, L_z)$ be the orbital angular momentum operator. Then

$$[L_x, L_y] = i\hbar L_z, [L_y, L_z] = i\hbar L_x, [L_z, L_x] = i\hbar L_y .$$

We are going to *define* angular momentum operator J as $J = (J_x, J_y, J_z)$ satisfying the above relations. That is,

$$[J_i, J_j] = i\hbar J_k \epsilon_{ijk}, \quad \forall i, j, k.$$

ϵ_{ijk} is the *Levi-Civita symbol*.

Along with

$$J^2 = J_x^2 + J_y^2 + J_z^2,$$

we can find quantization restrictions on amount of angular momentums.

Claim 1. $[J^2, J_z] = 0$.

Observe that

$$\begin{aligned} [J^2, J_z] &= [J_x^2 + J_y^2 + J_z^2, J_z] = [J_x^2, J_z] + [J_y^2, J_z] + \underbrace{[J_z^2, J_z]}_{=0} \\ &= J_x \underbrace{[J_x, J_z]}_{=-i\hbar J_y} + [J_x, J_z]J_x + J_y \underbrace{[J_y, J_z]}_{=i\hbar J_x} + [J_y, J_z]J_y = -i\hbar J_x J_y - i\hbar J_y J_x + i\hbar J_y J_x + i\hbar J_x J_y = 0. \end{aligned}$$

(End of Claim 1)

In a similar manner, we obtain that

$$[J^2, J_x] = [J^2, J_y] = [J^2, J_z] = 0.$$

Hence we can find a common eigenbasis for J^2, J_i for all i .

We are also going to introduce *ladder operators* for angular momentum (these operators are not the same as in quantum harmonic oscillators):

$$J_{\pm} = J_x \pm iJ_y.$$

Observe that

$$[J^2, J_{\pm}] = 0,$$

since J_{\pm} is a linear combination of J_x, J_y which commute with J^2 . Also,

$$[J_z, J_{\pm}] = [J_z, J_x] \pm i [J_z, J_y] = i\hbar J_y \pm i(-i\hbar J_x) = i\hbar J_y \pm \hbar J_x = \pm \hbar (J_x \pm iJ_y) = \pm \hbar J_{\pm}.$$

Let us find the common eigenbasis for J^2, J_z first. Consider the system of eigenvalue equations

$$\begin{aligned} J^2 |a, b\rangle &= a |a, b\rangle \\ J_z |a, b\rangle &= b |a, b\rangle \end{aligned}$$

Similar to how we did to harmonic oscillators, apply the raising operator J_+ to $|a, b\rangle$. Observe that

$$J_z (J_+ |a, b\rangle) = J_z J_+ |a, b\rangle = (J_+ J_z + \hbar J_+) |a, b\rangle = J_+ b |a, b\rangle + \hbar J_+ |a, b\rangle = (b + \hbar) J_+ |a, b\rangle.$$

That is, $J_+ |a, b\rangle$ is an eigenvector of J_z corresponding to $b + \hbar$, so we may write

$$J_+ |a, b\rangle = c |a', b + \hbar\rangle$$

for some a' . In a similar manner, we have

$$J^2 J_+ = a J_+ |a, b\rangle,$$

so that $J_+ |a, b\rangle$ is an eigenvector of J^2 corresponding to a , which means

$$J_+ |a, b\rangle = c |a, b + \hbar\rangle. \quad [1.4]$$

We can also get:

$$J_- |a, b\rangle = c' |a, b - \hbar\rangle. \quad [1.5]$$

Let us utilize [1.4], [1.5] to find which values of a, b are allowed.

Claim 2. $\langle J^2 - J_z^2 \rangle_{|a, b\rangle} \geq 0$.

Since $|a, b\rangle$ is an eigenvector of J^2, J_z corresponding to a, b , respectively,

$$\langle J^2 - J_z^2 \rangle_{|a, b\rangle} = a - b^2.$$

We also have

$$J^2 - J_z^2 = J_x^2 + J_y^2 + J_z^2 - J_z^2 = J_x^2 + J_y^2 = \frac{1}{2} (J_+ J_- + J_- J_+),$$

so that

$$\langle J^2 - J_z^2 \rangle = \left\langle \frac{1}{2} (J_+ J_- + J_- J_+) \right\rangle = \frac{1}{2} \langle J_+ J_- + J_- J_+ \rangle.$$

Since $J_{\pm} = J_x \pm iJ_y$ where J_x, J_y are Hermitian, it follows that $J_{\pm}^\dagger = J_{\mp}$. Therefore, $J_+ J_-, J_- J_+$ are Hermitian. This means

$$\langle J_+ J_- + J_- J_+ \rangle = \langle J_+ J_+^\dagger + J_+^\dagger J_+ \rangle = \langle J_+ J_+^\dagger \rangle + \langle J_+^\dagger J_+ \rangle = \|J_+^\dagger |a, b\rangle\|^2 + \|J_+ |a, b\rangle\|^2 \geq 0.$$

(End of Claim 2)

Consequently,

$$a - b^2 \geq 0 \implies a \geq b^2.$$

Because of this define b_+ be the smallest value such that

$$(b_+ + \hbar)^2 > a.$$

Using the properties of raising and lowering operators, we can write the value of b_+ in terms of a . For this b_+ , we have

$$J_+ |a, b_+\rangle = 0.$$

Similarly, let b_- be the largest value such that $(b_- - \hbar)^2 > a$, so that

$$J_- |a, b_-\rangle = 0.$$

Then

$$J_- J_+ |a, b_+\rangle = 0,$$

where

$$J_- J_+ = (J_x - iJ_y)(J_x + iJ_y) = \underbrace{J_x^2 + J_y^2}_{=J^2 - J_z^2} + i \underbrace{(J_x J_y - J_y J_x)}_{=[J_x, J_y] = i\hbar J_z} = J^2 - J_z^2 - \hbar J_z.$$

This means

$$0 = J_- J_+ |a, b_+\rangle = (J^2 - J_z^2 - \hbar J_z) |a, b_+\rangle = (a - b_+^2 - \hbar b_+) |a, b_+\rangle,$$

solving which gives

$$a = b_+ (b_+ + \hbar). \quad [1.6]$$

In a similar manner, we obtain

$$a = b_- (b_- - \hbar). \quad [1.7]$$

Note [1.6], [1.7] are satisfied if $b_- = -b_+$.

Assuming that we can obtain b_+ by applying J_+ $n \in \mathbb{N}$ times on b_- , we gain

$$b_+ = b_- + n\hbar = -b_+ + n\hbar \implies b_+ = \frac{n\hbar}{2}.$$

It follows that

$$a = \frac{n\hbar}{2} \left(\frac{n\hbar}{2} + \hbar \right) = \hbar^2 \frac{n}{2} \left(\frac{n}{2} + 1 \right). \quad [1.8]$$

Since the expression $\hbar^2 \frac{n}{2} \left(\frac{n}{2} + 1 \right)$ in [1.8] is ugly, we substitute $j = \frac{n}{2}, m = \frac{b}{\hbar}$ so that

$$\begin{aligned} J^2 |j, m\rangle &= \hbar^2 j(j+1) |j, m\rangle \\ J_z |j, m\rangle &= \hbar m |j, m\rangle \end{aligned}, \quad [1.9]$$

where j is a half-integer and m satisfy $m \in \{-j, -j+1, \dots, j-1, j\}$.

[1.9] is the usual convention for angular momentum operators.

Summary 1.3. Angular Momentum Operators

We define angular momentum operators $J = (J_x, J_y, J_z)$ as operators satisfying

$$[J_i, J_j] = i\hbar J_k \epsilon_{ijk}, \quad \forall i, j, k.$$

We define $J^2 = J_x^2 + J_y^2 + J_z^2$, which commutes with J_x, J_y, J_z :

$$[J^2, J_x] = [J^2, J_y] = [J^2, J_z] = 0.$$

The ladder operators are

$$J_+ = J_x + iJ_y, J_- = J_x - iJ_y,$$

which are also called the raising and lowering operators. Then

$$[J_z, J_{\pm}] = \pm \hbar J_{\pm}.$$

The eigenvalues of J^2, J_z are

$$\begin{aligned} J^2 |j, m\rangle &= \hbar^2 j(j+1) |j, m\rangle \\ J_z |j, m\rangle &= \hbar m |j, m\rangle \end{aligned},$$

where j is a half-integer and $m \in \{-j, -j+1, \dots, j\}$.

Notationally, we write $J = L$ and $j = l$ for orbital angular momentum and $J = S$ and $j = s$ for spin angular momentum.

In case $J = L$, an orbital angular momentum, the only allowed values of $j = l$ are integers. But in case $J = S$, a spin angular momentum, any half integer $j = s$ is allowed.

Let us find the matrix representation of the operators. Since

$$J_{\pm} |j, m\rangle = c_{\pm} |j, m \pm 1\rangle$$

for some constants c_{\pm} ,

$$\langle j, m | J_- J_+ |j, m\rangle = |c_+|^2 \langle j, m | j, m\rangle = |c_+|^2.$$

But we also know that

$$J_- J_+ = \dots = J^2 - J_z^2 - \hbar J_z,$$

so that

$$|c_+|^2 = \langle j, m | J_- J_+ |j, m\rangle = \hbar^2 j(j+1) - (\hbar m)^2 - \hbar^2 m = \hbar^2 (j(j+1) - m(m+1)).$$

Ignoring global phase, it follows

$$c_+ = \hbar \sqrt{j(j+1) - m(m+1)},$$

so that

$$J_+ |j, m\rangle = \hbar \sqrt{j(j+1) - m(m+1)}.$$

In a similar manner, we find

$$J_- |j, m\rangle = \hbar \sqrt{j(j+1) - m(m-1)}.$$

We can use this to find matrix representations.

Example 1.3.

Suppose $j = \frac{1}{2}$, so that we have two eigenstates

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

Then $J_z |1\rangle = \frac{\hbar}{2} |1\rangle, J_z |0\rangle = -\frac{\hbar}{2} |0\rangle$, so that

$$J_z = \frac{\hbar}{2} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

is the matrix representation of J_z .

For J_x , recall

$$J_x = \frac{1}{2} (J_+ - J_-).$$

The matrix representation of J_+ is

$$J_+ = \begin{bmatrix} 0 & \hbar \\ 0 & 0 \end{bmatrix}.$$

On the other hand,

$$J_- = \begin{bmatrix} 0 & 0 \\ \hbar & 0 \end{bmatrix},$$

so that

$$J_x = \frac{\hbar}{2} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}.$$

In a similar manner,

$$J_y = -\frac{i}{2} (J_+ - J_-) = \frac{\hbar}{2} \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$$

Squaring each J_x, J_y, J_z , we obtain

$$J^2 = \frac{3}{4} \hbar^2 \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}.$$

5. Spherical Harmonics

Consider $\vec{L} = \vec{r} \times \vec{p}$. We expect to see

$$\begin{aligned} J^2 |j, m\rangle &= \hbar^2 j(j+1) |j, m\rangle \\ J_z |j, m\rangle &= \hbar m |j, m\rangle \end{aligned}.$$

Moreover, we want an explicit form of $|l, m\rangle$ in 3D coordinates. To do so, we can use

$$L_z = -i\hbar x \partial_y + i\hbar y \partial_x$$

or use *spherical coordinates*. That is

$$\vec{L} = \vec{r} \times \vec{p} = -i\hbar \vec{r} \times \vec{\nabla},$$

where

$$\vec{\nabla} = \hat{r} \partial_r + \frac{1}{r} \hat{\theta} \partial_\theta + \frac{1}{r \sin(\theta)} \hat{\phi} \partial_\phi.$$

Then

$$\begin{aligned} L^2 &= -\hbar^2 \left(\frac{\partial^2}{\partial \theta^2} + \cot(\theta) \frac{\partial}{\partial \theta} + \frac{1}{\sin^2(\theta)} \frac{\partial^2}{\partial \phi^2} \right) \\ L_x &= -i\hbar \left(-\sin(\phi) \partial_\theta - \cot(\theta) \cos(\phi) \partial_\phi \right) \\ L_y &= -i\hbar \left(\cos(\phi) \partial_\theta - \cot(\theta) \sin(\phi) \partial_\phi \right) \\ L_z &= -i\hbar \partial_\phi \end{aligned}.$$

Observe that L^2, L_x, L_y, L_z does not depend on the radial coordinate r . Hence an eigenfunction of L^2, L_z depends only on θ, ϕ , say

$$\begin{aligned} L^2 Y(\theta, \phi) &= \hbar^2 l(l+1) Y(\theta, \phi) \\ L_z Y(\theta, \phi) &= \hbar m Y(\theta, \phi) \end{aligned}.$$

As an *ansatz*, suppose

$$Y(\theta, \phi) = \Theta(\theta) \Phi(\phi).$$

In this case,

$$L_z Y(\theta, \phi) = \hbar m Y(\theta, \phi)$$

becomes a differential equation

$$-i\hbar\partial_\varphi\Theta\Phi = \hbar m\Theta\Phi.$$

But Θ only depends on θ , so that

$$-i\hbar\partial_\varphi\Phi = \hbar m\Phi \implies \Phi(\theta) = e^{im\varphi}.$$

By the 2π periodicity of $e^{i\theta}$, we have

$$e^{im\varphi} = e^{im\varphi} e^{2\pi mi}. \quad [1.10]$$

Observe that [1.10] is satisfied if and only if m is an integer. This is why for orbital angular momentums integer values of m are only permitted values.

Now that we know how Φ looks like, we have

$$L^2 Y(\theta, \varphi) = L^2 e^{im\varphi} \Theta(\theta) = \hbar^2 l(l+1) e^{im\varphi} \Theta(\theta)$$

Recall that

$$L^2 = -\hbar^2 \left(\partial_\theta^2 + \cot(\theta) \partial_\theta + \frac{1}{\sin^2(\theta)} \partial_\varphi^2 \right),$$

so that we have

$$-\hbar^2 \left(\partial_\theta^2 + \cot(\theta) \partial_\theta + \frac{1}{\sin^2(\theta)} \partial_\varphi^2 \right) e^{im\varphi} \Theta(\theta) = \hbar^2 l(l+1) \Phi(\theta).$$

Cancelling out $\hbar^2, e^{im\varphi}$,

$$-\partial_\theta^2 \Theta - \cot(\theta) \partial_\theta \Theta - \frac{1}{\sin^2(\theta)} \partial_\varphi^2 (-m^2) \Theta = l(l+1) \Theta,$$

or

$$\left(-\partial_\theta^2 - \cot(\theta) \partial_\theta + \frac{m^2}{\sin^2(\theta)} \partial_\varphi^2 - l(l+1) \right) \Theta = 0, \quad [1.11]$$

which is of the form of the *general Legendre equation*. A general solution to [1.11] is

$$\Theta = P_l^m(\cos(\theta)),$$

where the *Legendre polynomial* P_l^m is

$$P_l^m = (1-x^2)^{\frac{|m|}{2}} \left(\frac{d}{dx} \right)^{|m|} P_l$$

and

$$P_l = \frac{1}{2^l l!} \left(\frac{d}{dx} \right)^l (x^2 - 1)^l. \quad [1.12]$$

Since [1.12] is *usually* defined for nonnegative integer l only, it puts additional restriction on l : $l \in \mathbb{N} \cup \{0\}$.

In conclusion, the spherical harmonics $Y_l^m(\theta, \varphi)$ have the form

$$Y_l^m = A P_l^m(\cos(\theta)) e^{im\varphi},$$

where A is a normalization constant. $Y_l^m(\theta, \varphi)$ are the eigenstates of L^2, L_z with eigenvalues $\hbar^2 l(l+1), \hbar m$. The collection $\{Y_l^m\}$ is an orthonormal basis for the space of functions of θ, φ .

Recall that symmetric 2D/3D systems feature degeneracy (i.e. there are different states with same energy). Hence we need another observable to *unambiguously* label eigenstates. That is, we are going to pick an observable A with

$$[A, H] = 0$$

and use eigenvalues of A as a second *label*.

We are going to consider *complete set of commuting operators*, CSCO: all operators commute with each other and eigenvalues of all operators are sufficient to fully distinguish basis states. Recall that

$$H = \frac{p_x^2 + p_y^2}{2m} + \frac{m\omega^2}{2} (x^2 + y^2) = \hbar\omega \left(a_x^\dagger a_x + a_y^\dagger a_y + 1 \right)$$

with energy eigenvalues $E_n = \hbar\omega (n + 1)$ where $n = n_x + n_y$. To uniquely label eigenstates, we could use $|n, n_x\rangle$ or use L_z ,

$$[L_z, H] = 0,$$

as done previously. That is, we can find basis with fixed energy and angular momentum for each eigenstate.

The states $|n_x\rangle |n_y\rangle$ are not eigenstates of L_z :

$$L_z |n_x\rangle |n_y\rangle = (xp_y - yp_x) |n_x\rangle |n_y\rangle,$$

where

$$xp_y - yp_x = i\hbar (a_x a_y^\dagger - a_x^\dagger a_y).$$

Observe

$$a_x |n_x\rangle |n_y\rangle = \sqrt{n_x} |n_x - 1\rangle |n_y\rangle, a_x^\dagger = \sqrt{n_x + 1} |n_x + 1\rangle |n_y\rangle$$

and

$$a_y |n_x\rangle |n_y\rangle = \sqrt{n_y} |n_x\rangle |n_y - 1\rangle, a_y^\dagger = \sqrt{n_y + 1} |n_x\rangle |n_y + 1\rangle.$$

Therefore,

$$L_z |n_x\rangle |n_y\rangle = i\hbar (\sqrt{n_x} \sqrt{n_y + 1} |n_x - 1\rangle |n_y + 1\rangle - \sqrt{n_x + 1} \sqrt{n_y} |n_x + 1\rangle |n_y - 1\rangle).$$

Observe that $|n_x - 1\rangle |n_y + 1\rangle, |n_x + 1\rangle |n_y - 1\rangle$ are orthonormal to $|n_x\rangle |n_y\rangle$, so $|n_x\rangle |n_y\rangle$ is not an eigenstate of L_z .

To make things work out, we'd like to use different ladder operators a_1, a_2 such that

$$H = \hbar\omega (a_1^\dagger a_1 + a_2^\dagger a_2 + 1)$$

and

$$L_z = \alpha a_1^\dagger a_1 + \beta a_2^\dagger a_2.$$

If we can find such ladder operators, then $\hbar\omega (n_1 + n_2 + 1)$ and $\alpha n_1 + \beta n_2$ are the eigenvalue of H, L_z , respectively, corresponding to $|n_1\rangle |n_2\rangle$. Of course, a_1, a_2 should satisfy *obvious* commutation relations for ladder operators,

$$[a_1, a_1^\dagger] = 1 [a_2, a_2^\dagger]$$

and

$$[a_1, a_2] = [a_1, a_2^\dagger] = [a_1^\dagger, a_2] = [a_1^\dagger, a_2^\dagger] = 0.$$

Define

$$a_1 = \frac{1}{\sqrt{2}} (a_x - ia_y), a_2 = \frac{1}{\sqrt{2}} (a_x + ia_y).$$

Then

$$\left[a_1, a_1^\dagger \right] = \left[\frac{1}{\sqrt{2}} (a_x - ia_y), \frac{1}{\sqrt{2}} (a_x^\dagger + ia_y^\dagger) \right] = \frac{1}{2} \left(\left[a_x, a_x^\dagger \right] - i \left[a_y, a_x^\dagger \right] + i \left[a_x, a_y^\dagger \right] + \left[a_y, a_y^\dagger \right] \right) = 1.$$

In a similar manner, a_1, a_2 satisfy other commutation relations.

Moreover, observe that

$$\begin{aligned} a_1^\dagger a_1 &= \frac{1}{2} (a_x^\dagger + ia_y^\dagger) (a_x - ia_y) = \frac{1}{2} (a_x^\dagger a_x + a_y^\dagger a_y + ia_y^\dagger a_x - ia_x^\dagger a_y), \\ a_2^\dagger a_2 &= \frac{1}{2} (a_x^\dagger - ia_y^\dagger) (a_x + ia_y) = \frac{1}{2} (a_x^\dagger a_x + a_y^\dagger a_y - ia_y^\dagger a_x + ia_x^\dagger a_y). \end{aligned}$$

This means

$$\begin{aligned} a_1^\dagger a_1 + a_2^\dagger a_2 &= a_x^\dagger a_x + a_y^\dagger a_y, \\ a_1^\dagger a_1 - a_2^\dagger a_2 &= ia_x^\dagger a_x - ia_y^\dagger a_y. \end{aligned}$$

It follows

$$\begin{aligned} L_z &= \hbar (a_1^\dagger a_1 - a_2^\dagger a_2), \\ H &= \hbar \omega (a_1^\dagger a_1 + a_2^\dagger a_2 + 1). \end{aligned}$$

This means the eigenvalues of L_z, H corresponding to $|n_1\rangle |n_2\rangle$ are $\hbar (n_1 - n_2), \hbar \omega (n_1 + n_2 + 1)$.

Consider spherically symmetric Hamiltonian

$$H = \frac{p^2}{2m} + V(r) = -\frac{\hbar^2}{2m} \nabla^2 + V(r).$$

Also recall

$$\nabla^2 = \frac{1}{r^2} \partial_r (r^2 \partial_r) + \frac{1}{r^2 \sin(\theta)} \partial_\theta (\sin(\theta) \partial_\theta) + \frac{1}{r^2 \sin(\theta)^2} \partial_\varphi^2 \quad [1.13]$$

with respect to the spherical coordinates. Let's compare [1.13] with

$$L^2 = -\hbar^2 \left(\partial_\theta^2 + \cot \theta \partial_\theta + \frac{1}{\sin(\theta)^2} \partial_\varphi^2 \right).$$

Observe that

$$\frac{1}{\sin(\theta)} \partial_\theta (\sin(\theta) \partial_\theta) = \dots = \cot(\theta) \partial_\theta + \partial_\theta^2.$$

Consequently,

$$\nabla^2 = \frac{1}{r^2} \partial_r (r^2 \partial_r) - \frac{1}{\hbar^2 r^2} L^2.$$

Hence

$$H = \underbrace{-\frac{\hbar^2}{2mr^2} \partial_r (r^2 \partial_r)}_{\text{radial kinetic energy}} + \underbrace{\frac{1}{2mr^2} L^2}_{\text{rotational energy}} + V(r).$$

To find eigenfunctions ψ of H , we use an ansatz

$$\psi(r, \theta, \varphi) = R(r) Y_l^m(\theta, \varphi).$$

Then

$$L^2 Y_l^m(\theta, \varphi) = \hbar^2 l(l+1) Y_l^m(\theta, \varphi).$$

Observe that the equation

$$H\psi = E_n \psi$$

becomes

$$-\frac{\hbar^2}{2mr^2} \partial_r (r^2 \partial_r) R Y_l^m + \underbrace{\frac{1}{2mr^2} L^2 R Y_l^m}_{=\frac{\hbar^2 l(l+1)}{2mr^2} R Y_l^m} + V R Y_l^m = E_n R Y_l^m.$$

But we are dealing with a spherically symmetrical system, so that we may cancel out Y_l^m and obtain

$$-\frac{\hbar^2}{2mr^2} \partial_r (r^2 \partial_r) R + \frac{\hbar^2 l(l+1)}{2mr^2} R + V R = E_n R. \quad [1.14]$$

Hence the radial wavefunction R depends on E_n and l , so we are going to index R with n, l .

Using change of variables $u = rR$,

$$\frac{dR}{dr} = \frac{d}{dr} \left(\frac{u}{r} \right) = \frac{1}{r} \frac{du}{dr} - \frac{u}{r^2} = \frac{1}{r^2} \left(r \frac{du}{dr} - u \right).$$

Hence

$$\frac{d}{dr} \left(r^2 \frac{dR}{dr} \right) = \frac{d}{dr} \left(r \frac{du}{dr} - \frac{u}{r} \right) = \frac{du}{dr} + r \frac{d^2 u}{dr^2} - \frac{du}{dr} = r \frac{d^2 u}{dr^2}.$$

Using this, [1.14] can be written as

$$-\frac{\hbar^2}{2m} \frac{d^2 u}{dr^2} + \left(V + \frac{\hbar^2}{2mr^2} l(l+1) \right) u = E_n u. \quad [1.15]$$

[1.15] looks like energy eigenvalue equation for 1-dimensional Hamiltonian with *effective* potential energy

$$V + \underbrace{\frac{\hbar^2}{2mr^2} l(l+1)}_{\text{centrifugal term}}.$$

We call [1.15] the *radial equation for central potential*.

Summary 1.4. Eigenfunctions for Central Potential

The eigenfunctions for central potential has the form

$$\psi_{nlm}(r, \theta, \varphi) = R_{nl}(r) Y_l^m(\theta, \varphi),$$

where n is the energy state, l is the quantum number in L^2 eigenvalue $\hbar l(l+1)$ and m is the quantum number in L_z eigenvalue $\hbar m$. Assuming a spherically symmetrical system, we have a differential equation called *radial equation*

$$-\frac{\hbar^2}{2m} \frac{d^2 u}{dr^2} + \left(V + \frac{\hbar^2}{2mr^2} l(l+1) \right) u = E_n u.$$

Example 1.4. Hydrogen Atom

Hydrogen atom has potential

$$V(r) = -\frac{e^2}{4\pi\epsilon_0} \frac{1}{r},$$

where r is the distance between proton and electron.

The radial equation becomes

$$-\frac{\hbar^2}{2m} \frac{d^2 u}{dr^2} + \left(-\frac{e^2}{4\pi\epsilon_0} \frac{1}{r} + \frac{\hbar^2}{2mr^2} l(l+1) \right) u = E_n u.$$

Rearranging,

$$\frac{d^2 u}{dr^2} + \left(\frac{2me^2}{4\pi\epsilon_0 \hbar^2} \frac{1}{r} - \frac{1}{r^2} l(l+1) \right) u = \frac{-2mE_n}{\hbar^2} u.$$

Let

$$k = \sqrt{\frac{-2mE_n}{\hbar^2}}$$

so that

$$E_n = \frac{-\hbar^2 k^2}{2m}.$$

Observe that $\hbar k$ is momentum and

$$k = \frac{2\pi}{\lambda},$$

where λ is the *de Broglie wavelength*. Also, recall the *Bohr radius*

$$a_0 = \frac{4\pi\epsilon_0\hbar^2}{me^2}.$$

Using the introduced constants and variables, the radial equation can be written as

$$\frac{d^2 u}{dr^2} + \left(\frac{2}{a_0 r} - \frac{l(l+1)}{r^2} \right) u = k^2 u. \quad [1.16]$$

We are going to attack [1.16] by

- (a) finding dimensionless variables;
- (b) looking at asymptotic behavior; and
- (c) hypothesizing power series and finding relation between coefficients.

First, we introduce the *dimensionless* version of r ,

$$\rho = kr,$$

to turn [1.16] into

$$\frac{d^2 u}{d\rho^2} = u \left(1 - \frac{\rho_0}{\rho} + \frac{l(l+1)}{\rho^2} \right). \quad [1.17]$$

When we express u as a power series in ρ , it does not play well with limits $\rho \rightarrow 0$ or $\rho \rightarrow \infty$. We hence look at the asymptotic behaviors of the solutions.

In limit $\rho \rightarrow \infty$, [1.17] becomes

$$\frac{d^2 u}{d\rho^2} = u \implies u = Ae^{-\rho} + Be^{\rho}.$$

But e^{ρ} blows up to ∞ as $\rho \rightarrow \infty$, so we conclude $u \rightarrow Ae^{-\rho}$ as $\rho \rightarrow \infty$.

In the limit $\rho \rightarrow 0$,

$$\frac{d^2 u}{d\rho^2} = \frac{l(l+1)}{\rho^2} u \implies u = C\rho^{l+1} + D\rho^{-l}.$$

But $\rho^{-l} \rightarrow \infty$ as $\rho \rightarrow 0$, it follows $u \rightarrow C\rho^{l+1}$ as $\rho \rightarrow 0$.

Hence consider the ansatz

$$u(\rho) = \rho^{l+1} e^{-\rho} v(\rho)$$

for some power series $v(\rho)$ in ρ .

Observe that

$$\frac{du}{d\rho} = \rho^l e^{-\rho} \left(v(\rho) (l+1-\rho) + \rho \frac{dv}{d\rho} \right)$$

and

$$\frac{d^2 u}{d\rho^2} = \rho^l e^{-\rho} \left(v(\rho) \left(\frac{l(l+1)}{\rho} - 2l - 2 + \rho \right) + \frac{dv}{d\rho} (2(l+1-\rho)) + \frac{d^2 v}{d\rho^2} \rho \right). \quad [1.18]$$

Plugging [1.18] into [1.17] gives

$$\rho \frac{d^2 v}{d\rho^2} + 2(l+1-\rho) \frac{dv}{d\rho} + (\rho_0 - 2l - 2) = 0. \quad [1.19]$$

Write v explicitly:

$$v(\rho) = \sum_{j=0}^{\infty} c_j \rho^j$$

to find out the recurrence relation between the coefficients. Then

$$\frac{dv}{d\rho} = \sum_{j=1}^{\infty} c_j j \rho^{j-1} = \sum_{j=0}^{\infty} (j+1) c_{j+1} \rho^j$$

and

$$\frac{d^2 v}{d\rho^2} = \sum_{j=0}^{\infty} j(j+1) c_{j+1} \rho^{j-1}.$$

Using this, [1.19] becomes

$$\sum_{j=0}^{\infty} (j(j+1) c_{j+1} + 2(l+1)(j+1) c_{j+1} - 2j c_j + (\rho_0 - 2l - 2) c_j) \rho^j = 0. \quad [1.20]$$

This means

$$(j(j+1) + 2(l+1)(j+1)) c_{j+1} + (\rho_0 - 2l - 2 - 2j) c_j = 0, \quad \forall j \geq 0 \quad [1.21]$$

or

$$c_{j+1} = \frac{2j + 2l + 2 - \rho_0}{(j+1)(j+2l+2)} c_j, \quad \forall j \geq 0$$

is the recurrence relation.

As $j \rightarrow \infty$,

$$c_{j+1} \rightarrow \frac{2j}{(j+1)j} c_j = \frac{2}{(j+1)} c_j,$$

so that

$$c_{j+1} \rightarrow \frac{2^{j+1}}{(j+1)!} c_0.$$

This means

$$v(\rho) \approx e^{2\rho} \implies u(\rho) = \rho^{l+1} e^{-\rho} C e^{2\rho} = C \rho^{l+1} e^{\rho}.$$

But this $v(\rho)$ is not normalizable, so there is j_{\max} for which $c_{j_{\max}+1} = 0$. Then

$$0 = c_{j_{\max}+1} = \frac{2j_{\max} + 2l + 2 - \rho_0}{(j_{\max} + 1)(j_{\max} + 2l + 2)} c_{j_{\max}} \implies 2j_{\max} + 2l + 2 - \rho_0 = 0.$$

It follows that

$$\rho_0 = 2(j_{\max} + l + 1) \implies n = j_{\max} + l + 1.$$

Recalling

$$\rho_0 = \frac{me^2}{2\pi\epsilon_0 \hbar^2 k}, k = \frac{\sqrt{-2mE}}{\hbar},$$

we get

$$E_n = \frac{-\hbar^2 k^2}{2m} = -\frac{\hbar^2}{2m} \left(\frac{me^2}{2\pi\epsilon_0 \hbar^2 \rho_0} \right)^2 = -\frac{\hbar^2}{2m} \left(\frac{me^2}{2\pi\epsilon_0 \hbar^2} \right) \frac{1}{(2n)^2} = -\frac{R_0}{n^2},$$

where

$$R_0 = \frac{m}{2\hbar^2} \left(\frac{e^2}{4\pi\epsilon_0} \right)^2 \approx 13.6\text{eV}$$

is the *Rydberg energy*, the energy required to *unbind* the electron from a ground state hydrogen atom.

Here is a summary of the relations for the allowed quantum numbers n, l, m_l , which index the eigenvalues $E_n, \hbar^2 l(l+1), \hbar m_l$ of H, L^2, L_z :

$$n \text{ is a positive integer, } n = j_{\max} + l + 1, n \geq l + 1, -l \leq m_l \leq l.$$

Moreover,

$$R_{nl}(r) = a_0 + a_1 r + a_2 r^2 + \cdots + a_{j_{\max}} r^{j_{\max}}.$$

Example 1.5. Degeneracy

For a hydrogen atom, when $n = 3$, what are the number of degeneracies?

Answer. Since $n = 3$, the allowed values of l are 2, 1, 0. For $l = 2$, there are 5 allowed values for m_l ; for $l = 1$, there are 3 allowed values for m_l ; and for $l = 0$ there is only one allowed value for m_l .

Thus there are 9 degeneracies for $n = 3$.

QED

6. Continuous Wavefunctions

Suppose that a $|\psi\rangle$ in an infinite-dimensional Hilbert space \mathcal{H} and a position operator \hat{x} are given. Then for any position eigenvalue x of \hat{x} , we define

$$\psi(x) = \langle x | \psi \rangle.$$

In other words, the function $\psi(\cdot)$ is a representation of $|\psi\rangle$ in an infinite-dimensional space with a fixed ONB.

The orthonormality condition and completeness relation are modified to

$$\langle n | m \rangle = \delta_{n,m} \rightarrow \langle x | x' \rangle = \delta(x - x') \quad \text{orthonormality}$$

and

$$\sum_n |n\rangle \langle n| = I \rightarrow \int_{-\infty}^{\infty} |x\rangle \langle x| dx = I, \quad \text{completeness relation}$$

where $\delta(\cdot)$ is the *Dirac delta distribution*.

Using completeness relation, we can expand $|\psi\rangle$ in $\{|x\rangle\}_x$ basis:

$$|\psi\rangle = \int_{-\infty}^{\infty} |x\rangle \langle x | \psi \rangle dx = \int_{-\infty}^{\infty} \psi(x) |x\rangle dx$$

analogous to the finite-dimensional case.

Similar to how we use coefficients c_n 's of $|\psi\rangle$ in an ONB to find out useful quantities about $|\psi\rangle$, we can use $\psi(\cdot)$ to find calculate inner products, probabilities, expectation values, and so on. For instance,

$$\langle \varphi | \psi \rangle = \int_{-\infty}^{\infty} \varphi(x)^* \psi(x) dx. \quad \text{inner product}$$

When we stick in an operator in between,

$$\langle \varphi | A | \psi \rangle = \langle \varphi | I A I | \psi \rangle = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \langle \varphi | x \rangle \langle x | A | y \rangle \langle y | \psi \rangle dx dy.$$

For simplicity, consider the case where $A = \hat{x}$, the position operator. Then

$$\langle \varphi | \hat{x} | \psi \rangle = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \langle \varphi | x \rangle \langle x | \hat{x} | y \rangle \langle y | \psi \rangle dx dy = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \varphi(x)^* y \delta(x - y) \psi(x) dx dy = \int_{-\infty}^{\infty} \varphi(x)^* x \psi(x) dx.$$

More generally,

$$\langle \varphi | \hat{A} | \psi \rangle = \int_{-\infty}^{\infty} \varphi(x)^* A(x) \psi(x) dx.$$

We interpret ψ as the *probability density* (or to be more precisely, $|\varphi|^2$ is a pdf). That is,

$$\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1.$$

7. Addition of Angular Momentum

Suppose \vec{J}_1, \vec{J}_2 are angular momenta. Consider $\vec{J} = \vec{J}_1 + \vec{J}_2$.¹ Then \vec{J} obeys the same commutation relation

$$[J^i, J^j] = i\hbar J_k \epsilon_{ijk}, \quad \forall i, j, k.$$

What basis states should we use?

An *obvious* choice is uncoupled basis. That is, the common eigenbasis of $J_1^2, J_2^2, J_{1,z}, J_{2,z}$, with

$$\begin{aligned} J_1^2 |j_1, j_2, m_1, m_2\rangle &= \hbar^2 j_1(j_1 + 1) |j_1, j_2, m_1, m_2\rangle, \\ J_2^2 |j_1, j_2, m_1, m_2\rangle &= \hbar^2 j_2(j_2 + 1) |j_1, j_2, m_1, m_2\rangle, \\ J_{1,z} |j_1, j_2, m_1, m_2\rangle &= \hbar m_1 |j_1, j_2, m_1, m_2\rangle, \\ J_{2,z} |j_1, j_2, m_1, m_2\rangle &= \hbar m_2 |j_1, j_2, m_1, m_2\rangle, \end{aligned}$$

where

$$|j_1, j_2, m_1, m_2\rangle = |j_1, m_1\rangle |j_2, m_2\rangle.$$

Another choice is better if J_1, J_2 interact: common eigenbasis of J_1^2, J_2^2, J^2, J_z^2 .

$$\begin{aligned} J_1^2 |j_1, j_2, j, m\rangle &= \hbar^2 j_1(j_1 + 1) |j_1, j_2, j, m\rangle, \\ J_2^2 |j_1, j_2, j, m\rangle &= \hbar^2 j_2(j_2 + 1) |j_1, j_2, j, m\rangle, \\ J^2 |j_1, j_2, j, m\rangle &= \hbar^2 j(j + 1) |j_1, j_2, j, m\rangle, \\ J_z^2 |j_1, j_2, j, m\rangle &= \hbar m |j_1, j_2, j, m\rangle. \end{aligned}$$

Often we write

$$\begin{aligned} |m_1, m_2\rangle &= |j_1, j_2, m_1, m_2\rangle \\ |j, m\rangle &= |j_1, j_2, j, m\rangle \end{aligned}$$

provided we know j_1, j_2 .

Then we know

$$|j, m\rangle = \sum_{m_1, m_2} \langle m_1, m_2 | j, m \rangle |m_1, m_2\rangle.$$

The coefficients $\langle m_1, m_2 | j, m \rangle$ are called the *Clebsch-Gordan coefficient* of $|j, m\rangle$.

The following selection rules tell us when the coefficients are nonzero.

Fact 1.1. Selection Rule I

$m = m_1 + m_2$ or $\langle m_1, m_2 | j, m \rangle = 0$.

¹Since \vec{J}_1, \vec{J}_2 are angular momenta, they belong to *different systems*, so more precisely $\vec{J} = \vec{J}_1 \otimes I_2 + I_1 \otimes \vec{J}_2$.

Example 1.6.

Consider $j_1 = 2, j_2 = 1$. Then there are $(2j_1 + 1)(2j_2 + 1) = 15$ total basis states.

The allowed values of m are $-3, \dots, 3$ and we know $-j \leq m \leq j$. This means $j = 3, 2, 1$ must be allowed, and we have

$$j = 3 \implies 7 \text{ total states}$$

$$j = 2 \implies 5 \text{ total states}$$

$$j = 1 \implies 3 \text{ total states}$$

Hence here is an upgraded version of the selection rule

Fact 1.2. Selection Rule II

$m = m_1 + m_2$, $|j_1 - j_2| \leq j \leq j_1 + j_2$ or $\langle m_1, m_2 | j, m \rangle = 0$.

Consider writing

$$|j, m\rangle = \sum_{m_1, m_2} \langle m_1, m_2 | j, m \rangle |m_1, m_2\rangle.$$

To find the coefficients, start with the state that has maximum projection along z :

$$|m_1 = j_1, m_2 = j_2\rangle = |j = j_1 + j_2, m = j_1 + j_2\rangle,$$

which is unique in both bases.

Start with

$$|j = 1, m = 1\rangle = \left| m_1 = \frac{1}{2}, m_2 = \frac{1}{2} \right\rangle.$$

Using

$$J_- = J_{1,-} + J_{2,-}, J_{\alpha,-} |j_{\alpha}, m_{\alpha}\rangle = \hbar \sqrt{j_{\alpha}(j_{\alpha} + 1) - m_{\alpha}(m_{\alpha} - 1)} |j_{\alpha}, m_{\alpha} - 1\rangle,$$

we get

$$\begin{aligned} J_- &= J_{1,-} \left| m_1 = \frac{1}{2}, m_2 = \frac{1}{2} \right\rangle + J_{2,-} \left| m_1 = \frac{1}{2}, m_2 = \frac{1}{2} \right\rangle \\ &= \hbar \sqrt{\frac{1}{2} \left(\frac{1}{2} + 1 \right) - \frac{1}{2} \left(\frac{1}{2} - 1 \right)} \left(\left| m_1 = -\frac{1}{2}, m_2 = \frac{1}{2} \right\rangle + \left| m_1 = \frac{1}{2}, m_2 = -\frac{1}{2} \right\rangle \right). \end{aligned}$$

It follows

$$|j = 1, m = 0\rangle = \frac{1}{\sqrt{2}} \left(\left| m_1 = -\frac{1}{2}, m_2 = \frac{1}{2} \right\rangle + \left| m_1 = \frac{1}{2}, m_2 = -\frac{1}{2} \right\rangle \right).$$