Outline

I. Solving the Simple Harmonic Oscillator with the ladder operators
II. Representing an operator as a matrix
III. Heisenberg Picture and Schroedinger Picture
IV. Equations of motion for x(t) and p(t) in the Heisenberg Picture
V. The Ehrenfest Theorem

Please read Goswami Chapter 8

I. Solving the simple harmonic oscillator with the ladder operators

Recall $a|u_0\rangle = 0$

Suppose we want to find the eigenfunctions in x-space

Write out $a = f(x)$. Use $-i\hbar\frac{\partial}{\partial x}$ for p.

$$\left\{\sqrt{\frac{m\omega}{2\hbar}}x + \frac{i}{\sqrt{2m\hbar\omega}}\left(-i\hbar\frac{\partial}{\partial x}\right)\right\}u_0(x) = 0$$

Multiply by $\sqrt{2}$ and define $\xi = \sqrt{\frac{m\omega}{\hbar}}x$

$\left\{\xi + \frac{\partial}{\partial \xi}\right\}u_0 = 0.$ Integrate:

$u_0 = Ce^{-\xi^2/2}.$ Normalize:

$$1 \equiv \int_{-\infty}^{+\infty} dx|u_0(x)|^2 = |C|^2\int_{-\infty}^{+\infty} dx \exp\left(\frac{-m\omega x^2}{\hbar}\right) = |C|^2\sqrt{\frac{\hbar\pi}{m\omega}}$$

So $C = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}$

So $u_0(\xi) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\xi^2/2}$

$$u_n(\xi) \propto u_n(x) = \langle x | u_n \rangle = \langle x | \frac{\left(a^\dagger\right)^n}{\sqrt{n!}} | u_0 \rangle$$

$$= \langle x | \frac{1}{\sqrt{n!}} \left\{ \sqrt{\frac{m\omega}{2\hbar}} x - \frac{ip}{\sqrt{2m\hbar\omega}} \right\}^n | u_0 \rangle$$

$$= \frac{1}{\sqrt{2^n}} \frac{1}{\sqrt{n!}} \underbrace{\left(\xi - \frac{\partial}{\partial \xi} \right)^n e^{-\xi^2/2}}_{\downarrow}$$

$e^{-\xi^2/2} H_n(\xi)$ This is the same solution as was found with the series method.

Note, it turns out that the $|u_n\rangle$ are orthonormal, so

$$\langle u_n | u_m \rangle = \delta_{nm}$$

To find the eigenvalues, recall $\mathrm{H}|u\rangle = \hbar\omega \left[a^\dagger a + \frac{1}{2} \right] |u\rangle = E|u\rangle$

So $a^\dagger a |u\rangle = \left(\frac{E}{\hbar\omega} - \frac{1}{2} \right) |u\rangle$

Consider $|u_0\rangle$

We know that $a|u_0\rangle = 0$

So $a^\dagger a|u_0\rangle = 0$

$$\overbrace{\left[\frac{E_0}{\hbar\omega} - \frac{1}{2}\right]}^{\uparrow}|u_0\rangle = 0$$

So $\dfrac{E_0}{\hbar\omega} - \dfrac{1}{2} = 0$

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

II. Representing an operator as a matrix

Consider the mathematical operation $\langle u_m | a^\dagger | u_n \rangle$.

What this means is:

(i) Begin with an initial state $|u_n\rangle$, the nth energy level of H or N.

(ii) Operate on it with $a^\dagger$, which raises it to state $|u_{n+1}\rangle$

That is, $a^\dagger |u_n\rangle = c|u_{n+1}\rangle$ where c is a normalization constant.

(iii) Calculate the inner product of that result with $\langle u_m|$:

$$\langle u_m | c | u_{n+1} \rangle = c \underbrace{\langle u_m | u_{n+1} \rangle}_{\substack{\downarrow \\ \delta_{m,n+1}}}$$

Now consider $\langle u_m | c | u_n \rangle$. By a similar analysis this gives $c' \langle u_m | u_{n-1} \rangle = c' \delta_{m,n-1}$.

Now find the c and c'.

Start with $\left|u_{n+1}\right\rangle = \frac{1}{\sqrt{(n+1)!}}\left(a^\dagger\right)^{n+1}\left|u_0\right\rangle$

$$= \frac{1}{\sqrt{(n+1)}}\frac{1}{\sqrt{n!}}\left(a^\dagger\right)^{n+1}\left|u_0\right\rangle$$

$$= \frac{a^\dagger}{\sqrt{(n+1)}}\underbrace{\frac{1}{\sqrt{n!}}\left(a^\dagger\right)^{n}\left|u_0\right\rangle}_{\downarrow \atop \left|u_n\right\rangle}$$

So $\left|u_{n+1}\right\rangle = \frac{a^\dagger}{\sqrt{(n+1)}}\left|u_n\right\rangle$. Rewrite this as:

$\sqrt{(n+1)}\left|u_{n+1}\right\rangle = a^\dagger\left|u_n\right\rangle$. Multiply on the left with $\left\langle u_m\right|$:

$$\underbrace{\left\langle u_m\right|\sqrt{(n+1)}\left|u_{n+1}\right\rangle}_{\downarrow \atop \sqrt{(n+1)}\underbrace{\left\langle u_m | u_{n+1}\right\rangle}_{\downarrow \atop \delta_{m,n+1}}} = \left\langle u_m\right|a^\dagger\left|u_n\right\rangle$$

So $\left\langle u_m\right|a^\dagger\left|u_n\right\rangle = \sqrt{(n+1)}\,\delta_{m,n+1}$

Now consider the case for operator a:

Start with $a\left|u_n\right\rangle = a\frac{1}{\sqrt{n!}}\left(a^\dagger\right)^n\left|u_0\right\rangle$.

Recall we showed that $a\left(a^\dagger\right)^n = n\left(a^\dagger\right)^{n-1} + \left(a^\dagger\right)^n a$

So $a\left|u_n\right\rangle = \frac{n}{\sqrt{n!}}\left(a^\dagger\right)^{n-1}\left|u_0\right\rangle + \frac{1}{\sqrt{n!}}\left(a^\dagger\right)^n \underbrace{a\left|u_0\right\rangle}_{\downarrow \atop 0}$

Now multiply on the left with $\left\langle u_m\right|$:

$$\left\langle u_m\right|a\left|u_n\right\rangle = \left\langle u_m\right|\frac{n}{\sqrt{n!}}\left(a^\dagger\right)^{n-1}\left|u_0\right\rangle$$

$$= \left\langle u_m\right|\sqrt{n}\underbrace{\frac{1}{\sqrt{(n-1)!}}\left(a^\dagger\right)^{n-1}\left|u_0\right\rangle}_{\downarrow \atop \left|u_{n-1}\right\rangle}$$

$$= \left\langle u_m\right|\sqrt{n}\left|u_{n-1}\right\rangle = \sqrt{n}\underbrace{\left\langle u_m \middle| u_{n-1}\right\rangle}_{\downarrow \atop \delta_{m,n-1}}$$

So $\left\langle u_m\right|a\left|u_n\right\rangle = \sqrt{n}\,\delta_{m,n-1}$

Construct a table for operator $a^\dagger$:

$\overrightarrow{\text{INITIAL STATES}}$ n=	0	1	2	3	4.....
FINAL STATES					
m= 0	0	0	0	0	0
1	$\sqrt{1}$	0	0	0	0
2	0	$\sqrt{2}$	0	0	0
3	0	0	$\sqrt{3}$	0	....
4	....	....	....		
....					

Construct a table for operator a :

$\overrightarrow{\text{INITIAL STATES}}$ n=	0	1	2	3	4.....
FINAL STATES					
m= 0	0	$\sqrt{1}$	0	0	0
1	0	0	$\sqrt{2}$	0	0
2	0	0	0	$\sqrt{3}$	0
3	0	0	0	0	....
4	....	....	....		
....					

These "tables" are the matrix representations of the operators $a^\dagger$ and a.
Notice that because the simple harmonic oscillator has an infinite number of eigenstates, the matrices are infinite-dimensional.

The matrices encode the

-amount of overlap between states $|u_n\rangle$ and $|u_m\rangle$

$-or-$

-the $\underbrace{\text{amplitude}}_{\substack{\downarrow \\ \sqrt{\text{probability}}}}$ for $\underbrace{\text{transition}}_{\substack{\downarrow \\ \text{(caused by } a \text{ or } a^\dagger\text{)}}}$ between $|u_n\rangle$ and $|u_m\rangle$

Recall we showed that the operator that evolves Ψ in time is

$U = e^{-iH(t-t_0)/\hbar}$.

So if $t_0 = 0$,

$|\Psi(t)\rangle = e^{-iHt/\hbar}|\Psi(0)\rangle$.

Consider some operator A which is not itself a function of time. Suppose we want to find its expectation value at time t:

$\langle A\rangle_t = \langle\Psi(t)|A|\Psi(t)\rangle$

$= \langle\Psi(0)|e^{iHt/\hbar}Ae^{-iHt/\hbar}|\Psi(0)\rangle$

We have a choice about whether to group the exponential functions with the A or with the $\Psi(0)$.

2 groupings:

$$\underbrace{\langle\Psi(0)|e^{iHt/\hbar}}\, A\, \underbrace{e^{-iHt/\hbar}|\Psi(0)\rangle}$$

$$\langle\Psi(t)|A|\Psi(t)\rangle$$

Here A is not a function of t but Ψ is.

The view that "the evolution of time changes the Ψ's, not the operators" is the Schroedinger Picture of quantum mechanics.

$$\langle\Psi(0)|\underbrace{e^{iHt/\hbar}Ae^{-iHt/\hbar}}|\Psi(0)\rangle$$

$$\langle\Psi(0)|A'|\Psi(0)\rangle$$

Here A' is a function of t but Ψ is not.

The view that "the evolution of time changes the operators, not the Ψ's" is the Heisenberg Picture of quantum mechanics.

Up to now we have viewed everything from the Schroedinger perspective (that is, the Schroedinger Equation is a time-development equation for Ψ.
Now consider the Heisenberg Picture and find a time-development equation for A'.

Start with the definition:

$$A'(t) = e^{iHt/\hbar} A e^{-iHt/\hbar}$$

$$\frac{dA'(t)}{dt} = \frac{\partial\left(e^{iHt/\hbar}\right)}{\partial t} A e^{-iHt/\hbar} + e^{iHt/\hbar} \underbrace{\frac{\partial A}{\partial t}}_{\substack{\downarrow \\ 0}} e^{-iHt/\hbar} + e^{iHt/\hbar} A \frac{\partial\left(e^{iHt/\hbar}\right)}{\partial t}$$

$$= \frac{iH}{\hbar} \underbrace{e^{iHt/\hbar} A e^{-iHt/\hbar}}_{\substack{\downarrow \\ A'(t)}} + \underbrace{e^{iHt/\hbar} A e^{-iHt/\hbar}}_{\substack{\downarrow \\ A'(t)}} \left(\frac{-iH}{\hbar}\right)$$

Conclude:

$$\frac{dA'(t)}{dt} = \frac{i}{\hbar}\left[H, A'(t)\right].$$ This is the Heisenberg equivalent to the Schroedinger Equation.

What if A (not A') is explicitly time dependent? This is called the Interaction Picture and will be addressed in Chapter 22.

IV. The equations of motion for $x_{op}(t)$ and $p_{op}(t)$ in the Heisenberg Picture

What we want:

$$\mathrm{x}_{op}(t) = f_1(t, \text{ constants})$$

$$\mathrm{p}_{op}(t) = f_2(t, \text{ constants}).$$

The constants are $x(t=0)$, $p(t=0)$, m, $\hbar$, k, and so forth.

These are constants specified by the environment of the problem.

Note these are the time-independent operators in the Schroedinger Picture.

What we know:

To find x(t) we must eventually solve some form of the equation

$$\frac{dx(t)}{dt} = \frac{i}{\hbar}\left[H, x(t)\right].$$

This is hard to solve because we do not know $\left[H, x(t)\right]$.

A "trick":

We know that $x(t)$ is related to $x(0)$ by $x(t) = e^{-iHt/\hbar} x(0) e^{iHt/\hbar}$

We know that $x(0)$ is related to $a(0)$ and $a^\dagger(0)$ by $x(0) = \dfrac{a(0) + a^\dagger(0)}{\sqrt{\dfrac{2m\omega}{\hbar}}}$.

We know that $a(0)$ and $a^\dagger(0)$ are related to $a(t)$ and $a^\dagger(t)$ by

$a(t) = e^{-iHt/\hbar} a(0) e^{iHt/\hbar}$ and $a^\dagger(t) = e^{-iHt/\hbar} a^\dagger(0) e^{iHt/\hbar}$.

It turns out that we can find $\left[H, a(t)\right]$ and $\left[H, a^\dagger(t)\right]$ and work backward to get $x(t)$.

Plan:

(i) Find $\left[H, a(t)\right]$ and $\left[H, a^\dagger(t)\right]$.

(ii) Substitute these into $\dfrac{da^{(\dagger)}(t)}{dt} = \dfrac{i}{\hbar}\left[H, a^{(\dagger)}(t)\right]$ to get $a^{(\dagger)}(t) = f(t, a^{(\dagger)}(0))$.

(iii) Work backward from $a^{(\dagger)}(t) \Rightarrow a^{(\dagger)}(0) \Rightarrow x(0) \Rightarrow x(t)$.

Carry out the plan:

(i) Find $\left[H, a(t)\right]$

Recall how we found $\left[H, a(0)\right] = -\hbar\omega a(0)$: we used $\left[a(0), a^\dagger(0)\right] = 1$.

So we need to find $\left[a(t), a^\dagger(t)\right]$. To find this, begin with

$\left[a(0), a^\dagger(0)\right] = 1$. Expand it:

$a_0 a_0^\dagger - a_0^\dagger a_0 = 1.$ Multiply each term by 1:

$a_0 \cdot 1 \cdot a_0^\dagger - a_0^\dagger \cdot 1 \cdot a_0 = 1.$ Replace $1 = e^{-iHt/\hbar} e^{+iHt/\hbar}$

$a_0 e^{-iHt/\hbar} e^{+iHt/\hbar} a_0^\dagger - a_0^\dagger e^{-iHt/\hbar} e^{+iHt/\hbar} a_0 = 1.$

Operate on everything with $e^{+iHt/\hbar}$ from the left and with $e^{-iHt/\hbar}$ from the right.

$$\underbrace{e^{+iHt/\hbar} a_0 e^{-iHt/\hbar}}_{\downarrow \; a(t)} \underbrace{e^{+iHt/\hbar} a_0^\dagger e^{-iHt/\hbar}}_{\downarrow \; a^\dagger(t)} - \underbrace{e^{+iHt/\hbar} a_0^\dagger e^{-iHt/\hbar}}_{\downarrow \; a^\dagger(t)} \underbrace{e^{+iHt/\hbar} a_0 e^{-iHt/\hbar}}_{\downarrow \; a(t)} = \underbrace{e^{+iHt/\hbar} \cdot 1 \cdot e^{-iHt/\hbar}}_{\downarrow \; 1}$$

Condense this to:

$\left[a(t), a^\dagger(t)\right] = 1.$ "Eq 1"

To find $\left[H, a(t)\right]$ we also need H(t):

Recall $H = \hbar\omega\left(a_0^\dagger a_0 + \frac{1}{2}\right)$.

As above, insert $1 = e^{-iHt/\hbar} e^{+iHt/\hbar}$ between $a_0^\dagger$ and a_0 then

operate with $e^{+iHt/\hbar}$ from the left and with $e^{-iHt/\hbar}$ from the right.

We get:

$$\underbrace{e^{+iHt/\hbar}He^{-iHt/\hbar}}_{\downarrow} = \hbar\omega\left(\underbrace{e^{+iHt/\hbar}a_0^{\dagger}e^{-iHt/\hbar}}_{\downarrow}\,\underbrace{e^{+iHt/\hbar}a_0e^{-iHt/\hbar}}_{\downarrow} + \underbrace{e^{+iHt/\hbar}\frac{1}{2}e^{-iHt/\hbar}}_{\downarrow} \right)$$

H commutes with $\quad a^{\dagger}(t) \quad a(t) \quad \frac{1}{2}$

functions of H, so
reorder this as

$$\underbrace{e^{+iHt/\hbar}e^{-iHt/\hbar}}_{\downarrow}H$$

1

Conclude:

$$H = \hbar\omega\left(a^{\dagger}(t)a(t)+\frac{1}{2}\right) \qquad \text{Eq. 2}$$

Now use Eq 1 and Eq 2 to get $\left[H,a(t)\right]$:

$$\left[H,a(t)\right] = \left[\left(\hbar\omega\left(a^{\dagger}(t)a(t)+\frac{1}{2}\right)\right),a(t)\right]$$ Expand, do all the same steps as for the time-indep case:

$$= -\hbar\omega a(t)$$

Similarly, $\left[H,a^{\dagger}(t)\right] = +\hbar\omega a^{\dagger}(t)$

Continue with the plan.

(ii) Substitute these into $\dfrac{da^{(\dagger)}(t)}{dt} = \dfrac{i}{\hbar}\left[H, a^{(\dagger)}(t)\right]$.

$\left[H, a^{(\dagger)}(t)\right] = \hbar\omega a^{\dagger}(t)$

So $\dfrac{da^{(\dagger)}(t)}{dt} = i\omega a^{\dagger}(t)$. Integrate:

$a^{\dagger}(t) = e^{i\omega t} a^{\dagger}(0)$ Eq. 3

Similarly, $\dfrac{da(t)}{dt} = \dfrac{i}{\hbar}\left[H, a(t)\right] = \dfrac{i}{\hbar}\left(-\hbar\omega a(t)\right)$. Integrate:

$a(t) = e^{-i\omega t} a(0)$ Eq. 4

Continue with the plan.

(iii) Work backward to obtain $x(t)$.

Recall $a(0) = \sqrt{\dfrac{m\omega}{2\hbar}}\, x(0) + \dfrac{i}{\sqrt{2m\hbar\omega}}\, p(0)$ Eq. 5

Operate on everything from the left with $e^{iHt/\hbar}$ and on the right with $e^{-iHt/\hbar}$

$$\underbrace{e^{iHt/\hbar} a(0)\, e^{-iHt/\hbar}} = e^{iHt/\hbar}\sqrt{\frac{m\omega}{2\hbar}}\, x(0)\, e^{-iHt/\hbar} + e^{iHt/\hbar}\frac{i}{\sqrt{2m\hbar\omega}}\, p(0)\, e^{-iHt/\hbar}$$

$$= \sqrt{\frac{m\omega}{2\hbar}}\, \underbrace{e^{iHt/\hbar} x(0)\, e^{-iHt/\hbar}} + \frac{i}{\sqrt{2m\hbar\omega}}\, \underbrace{e^{iHt/\hbar} p(0)\, e^{-iHt/\hbar}}$$

$$a(t) = \sqrt{\frac{m\omega}{2\hbar}}\, x(t) + \frac{i}{\sqrt{2m\hbar\omega}}\, p(t)$$ Eq. 6

Similarly recall that $a^{\dagger}(0)=\sqrt{\frac{m\omega}{2\hbar}}x(0)-\frac{i}{\sqrt{2m\hbar\omega}}p(0)$ Eq. 7

This leads to $a^{\dagger}(t)=\sqrt{\frac{m\omega}{2\hbar}}x(t)-\frac{i}{\sqrt{2m\hbar\omega}}p(t)$ Eq. 8

Now substitute Eq. 7 and Eq. 8 into Eq. 3:

$$\sqrt{\frac{m\omega}{2\hbar}}x(t)-\frac{i}{\sqrt{2m\hbar\omega}}p(t)=e^{i\omega t}\left\{\sqrt{\frac{m\omega}{2\hbar}}x(0)-\frac{i}{\sqrt{2m\hbar\omega}}p(0)\right\} \qquad \text{Eq. 9}$$

and substitute Eq. 5 and Eq. 6 into Eq. 4:

$$\sqrt{\frac{m\omega}{2\hbar}}x(t)+\frac{i}{\sqrt{2m\hbar\omega}}p(t)=e^{-i\omega t}\left\{\sqrt{\frac{m\omega}{2\hbar}}x(0)+\frac{i}{\sqrt{2m\hbar\omega}}p(0)\right\} \qquad \text{Eq. 10}$$

Eliminate $p(t)$ from Eq. 9 and Eq. 10 by adding them, to get:

$$2\sqrt{\frac{m\omega}{2\hbar}}x(t)=\sqrt{\frac{m\omega}{2\hbar}}x(0)\left(e^{i\omega t}+e^{-i\omega t}\right)-\frac{i}{\sqrt{2m\hbar\omega}}p(0)\left(e^{i\omega t}-e^{-i\omega t}\right)$$

So $x(t)=x(0)\cos\omega t+\frac{p(0)}{m\omega}\sin\omega t$

Similarly, eliminate x(t) from Eq. 9 and Eq. 10 to get

$$p(t)=p(0)\cos\omega t+m\omega x(0)\sin\omega t$$

V. Ehrenfest Theorem

The message of this section is:
We found the following fact about expectation values of operators. (Consider an arbitrary operator Q):

$$\frac{d}{dt}\langle Q\rangle = \frac{i}{\hbar}\langle [H,Q]\rangle + \left\langle \frac{\partial Q}{\partial t}\right\rangle$$

This allows us to find relationships between $\langle Q\rangle$ and $\frac{d}{dt}\langle Q\rangle$ for various operators including x and p.
It turns out that the relationships we get when $Q = x$ or $Q = p$ have the same form as Newton's Laws.
So Newton's Laws related quantities (x, p, F, etc.) that are accurately given by quantum mechanical expectation values $\langle x\rangle$, $\langle p\rangle$, etc.
That is why classical mechanics works in a world that is in reality quantum mechanical.
So for example, when we measure Newtonian position, what we are really measuring is $\langle x\rangle$.

To show this:
begin with $\frac{d}{dt}\langle Q\rangle = \frac{i}{\hbar}\langle [H,Q]\rangle + \left\langle \frac{\partial Q}{\partial t}\right\rangle$. Let $Q = x$. Then $\frac{\partial Q}{\partial t} = \frac{\partial x}{\partial t} = 0$. Then we have

$$\frac{d}{dt}\langle x\rangle = \frac{i}{\hbar}\langle [H,x]\rangle$$

$$= \frac{i}{\hbar}\left\langle \left[\frac{p^2}{2m} + V(x), x\right]\right\rangle \qquad \text{Expand:}$$

$$\frac{d}{dt}\langle x\rangle = \frac{i}{\hbar}\left\langle \frac{1}{2m}\underbrace{\left[p^2,x\right]} + \underbrace{\left[V(x),x\right]}_{\downarrow} \right\rangle$$

0 because a function of x commutes with x.

To find this commutator, note $\left[p^2,x\right] = p^2x - xp^2 = p^2x - (xp)p$.

But $\left[x,p\right] = xp - px = i\hbar$, so $xp = i\hbar + px$.

Then $\left[p^2,x\right] = p^2x - (i\hbar + px)p$

$$= p^2x - i\hbar p - p(xp)$$

$$= p^2x - i\hbar p - p(i\hbar + px)$$

$$= p^2x - i\hbar p - pi\hbar - p^2x = -2i\hbar p.$$

$$\frac{d}{dt}\langle x\rangle = \frac{i}{\hbar}\left\langle \frac{1}{2m}(-2i\hbar p)\right\rangle$$

$$\frac{d}{dt}\langle x\rangle = \left\langle \frac{p}{m}\right\rangle \qquad \text{Ehrenfest Equation \#1}$$

Note:

(1) This is the quantum mechanical version of $v = \dfrac{p}{m}$

(2) This formula cannot be true for individual eigenvalues of x_{op} and p_{op} since that would imply simultaneous measurement of x and p.

Now consider the case where $Q = p$. Then again $\frac{\partial p}{\partial t} = 0$, so we have

$$\frac{d}{dt}\langle p\rangle = \frac{i}{\hbar}\left\langle\left[\frac{p^2}{2m} + V(x), p\right]\right\rangle$$

$$= \frac{i}{\hbar}\left\langle \frac{1}{2m}\underbrace{\left[p^2, p\right]}_{\downarrow \; 0} + \left[V(x), p\right]\right\rangle = \frac{-i}{\hbar}\left\langle\left[p, V(x)\right]\right\rangle$$

To find $\left[p, V(x)\right]$, act with it on some test ψ:

$$\left[p, V(x)\right]\psi = pV\psi - Vp\psi.$$

Substitute $p = -i\hbar\frac{d}{dx}$

$$= -i\hbar\frac{d}{dx}(V\psi) - V\left(-i\hbar\frac{d\psi}{dx}\right)$$

$$= -i\hbar\left\{\frac{d(V\psi)}{dx} - V\frac{d\psi}{dx}\right\}$$

$$= -i\hbar\left\{V\frac{d\psi}{dx} + \frac{dV}{dx}\psi - V\frac{d\psi}{dx}\right\} = -i\hbar\frac{dV}{dx}\psi$$

So $\left[p, V(x)\right] = -i\hbar\frac{dV}{dx}$.

Plug this in to get:

$$\frac{d}{dt}\langle p\rangle = \frac{-i}{\hbar}\left\langle -i\hbar\frac{dV}{dx}\right\rangle$$

So $\frac{d}{dt}\langle p\rangle = -\left\langle\frac{dV}{dx}\right\rangle = \langle F_x\rangle$ because $\vec{F} = -\vec{\nabla}V$.

This is the x-component of the vector formula

$$\frac{d}{dt}\langle\vec{p}\rangle = \langle\vec{F}\rangle$$ Ehrenfest Equation #2

This is the quantum mechanical form of

$$\frac{d\vec{p}}{dt} = \vec{F}$$

Outline

I. The WKB Approximation: Introduction
II. WKB Connection Formulas

I. The WKB Approximation: Introduction

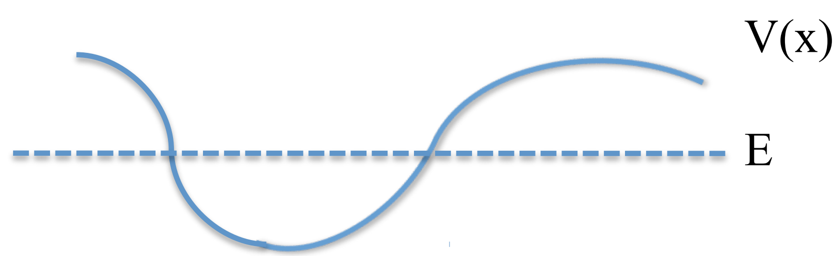
The issue: Most potentials in real applications are not simple square wells and so forth, so generally they lead to differential equations that are hard to solve.

Generally solving these requires making approximations.

There is an approximation that works well if V varies only slowly as a function of x, so if we look in a small region, we can say that V~ constant. This is the WKB Approximation.

The method:

(1) Consider a confining potential that is generally arbitrarily shaped but that does not vary rapidly:



Consider a particle trapped in the well at E.

Definition: The values of x for which V=E are called the "turning points."

(2) Write down the Schroedinger Equation, assume that because V is ~ constant in a local region, ψ is ~ a free particle in that region: that is, a plane wave. Thus assume that $\psi \sim Ae^{ikx}$.

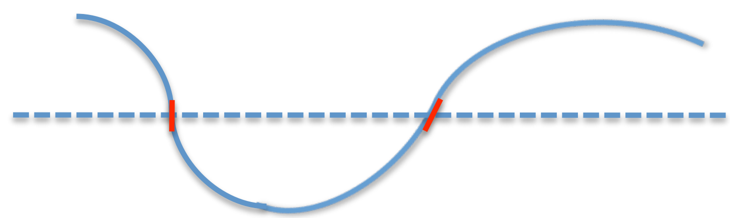
Plane waves do not change their amplitudes, so assume that $\delta^2 A/dx^2=0$.

Solve the Schroedinger Equation with this approximation.

The approximate solution is close to the exact solution everywhere except at the turning points.

(3) To repair the problem at the turning points:

in those regions only, assume V is a linear function for which the Schroedinger Equation is easily solved.



Find ψ for that V at those x's.

(4) Connect the ψ's at the turning points to the ψ's that are everywhere else.

This is the boundary condition application. This develops equations called the Connection Formulas.

(5) The formulas for ψ's that are produced by this method are general enough to be used in all problems where V is slowly varying.

Carry out the method:

(1) Consider an arbitrary smooth "slowly varying" potential which is binding a particle that has energy E. What is meant by "slowly varying"?

A potential is slowly varying if $\underbrace{\text{its change in value}}_{\left|\frac{\partial V}{\partial x}\right|}$ across $\underbrace{\text{a deBroglie wavelength}}_{\lambda}$ is much less than $\underbrace{\text{the kinetic energy of the particle}}_{E\text{ - }V}$.

Or: $\left|\frac{\partial V}{\partial x}\right| \cdot \lambda << (E - V)$

Rewrite this as:

$$\frac{1}{E-V}\left|\frac{\partial V}{\partial x}\right| \cdot \lambda << 1.$$

Where this approximation works:

Let $\psi(x) = A(x)e^{i\varphi(x)}$

The general form which can accommodate anything.

Where this approximation does not work:

Where $E = V$ (that is, at the turning points)

Continue the method:

(2) Write down the time-independent Schroedinger Equation

$$\frac{-\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}+V(x)\psi=E\psi$$

$$\frac{\partial^2\psi}{\partial x^2}=\boxed{\frac{-2m(E-V)}{\hbar^2}}\psi$$

Define $k\equiv\dfrac{\sqrt{2m(E-V)}}{\hbar}$ as usual, so

this is $k^2=\dfrac{p^2}{\hbar^2}$

Rewrite:

$$\frac{\partial^2\psi}{\partial x^2}=\frac{-p^2}{\hbar^2}\psi$$

Substitute into this $\psi=\mathrm{A(x)e}^{i\varphi(x)}$

$$\frac{\partial\psi}{\partial x}=\left(\frac{\partial A}{\partial x}+iA\frac{\partial\varphi}{\partial x}\right)e^{i\varphi}$$

$$\frac{\partial^2\psi}{\partial x^2}=\left\{\frac{\partial^2 A}{\partial x^2}+2i\frac{\partial A}{\partial x}\frac{\partial\varphi}{\partial x}+iA\frac{\partial^2\varphi}{\partial x^2}-A\left(\frac{\partial\varphi}{\partial x}\right)^2\right\}e^{i\varphi}$$

$$\frac{\partial^2 A}{\partial x^2}+2i\frac{\partial A}{\partial x}\frac{\partial\varphi}{\partial x}+iA\frac{\partial^2\varphi}{\partial x^2}-A\left(\frac{\partial\varphi}{\partial x}\right)^2=\frac{-p^2}{\hbar^2}A$$

Re Im Im Re Re

For this equation to be solved, the real and imaginary terms must be solved separately:

Imaginary terms: $2\frac{\partial A}{\partial x}\frac{\partial \varphi}{\partial x}+A\frac{\partial^2 \varphi}{\partial x^2}=0$

This is solved by $A=\frac{C}{\sqrt{\frac{\partial \varphi}{\partial x}}}$.

Real terms: $\frac{\partial^2 A}{\partial x^2}-A\left(\frac{\partial \varphi}{\partial x}\right)^2=\frac{-p^2}{\hbar^2}A$

This is not generally solvable analytically. Make the approximation $\frac{\partial^2 A}{\partial x^2} << A$.

That is, since the potential is "slowly varying," the ψ that responds to it does not radically change amplitude over short distances dx.

So ignore the $\frac{\partial^2 A}{\partial x^2}$ term. Then we have

$$-A\left(\frac{\partial \varphi}{\partial x}\right)^2=\frac{-p^2}{\hbar^2}A$$

$$\frac{\partial \varphi}{\partial x}=\pm\frac{p}{\hbar}$$

$$\varphi(x)=\pm\frac{1}{\hbar}\int p(x)\,dx$$

Combine the A and φ solutions:

$$\psi \cong \frac{C}{\sqrt{\frac{\partial\varphi}{\partial x}}} \exp\left[\pm\frac{i}{\hbar}\int p(x)\,dx\right]$$

$$= \frac{C}{\sqrt{\frac{p}{\hbar}}} \exp\left[\pm\frac{i}{\hbar}\int p(x)\,dx\right]$$

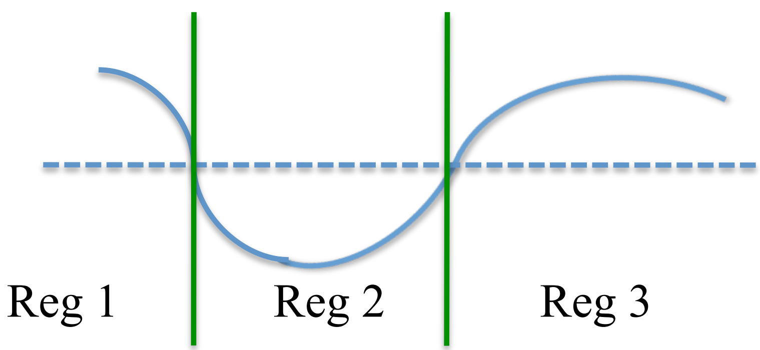
Define $C' = C\sqrt{\hbar}$

$$= \frac{C'}{\sqrt{p(x)}} \exp\left[\pm\frac{i}{\hbar}\int p(x)\,dx\right]$$

The most general ψ is a linear combination that uses both signs of the exponent:

$$\psi_{general\ \mathrm{WKB}} = \frac{C_+}{\sqrt{p(x)}} \exp\left[+\frac{i}{\hbar}\int p(x)\,dx\right] + \frac{C_-}{\sqrt{p(x)}} \exp\left[-\frac{i}{\hbar}\int p(x)\,dx\right]$$

Any potential can typically be divided into different regions based upon where the particle is classically allowed or not allowed. For example:



For each region,

(i) use the part of the $\psi_{general}$ that will properly $\to 0$ as x $\to \infty$. That is, set C_+ or $C_- = 0$ as necessary. Also:

(ii) in Regions I and III where $V > E$, $p = \sqrt{2m(E-V)}$ is intrinsically imaginary, so define $P \equiv -ip$

(This is like the definition K=-ik for the square well.)

Then in those regions, $\psi_{WKB} \sim \frac{C}{\sqrt{P(x)}} e^{\pm\frac{1}{\hbar}\int P\,dx}$ no "i", and capital P

So for a general confining potential we get

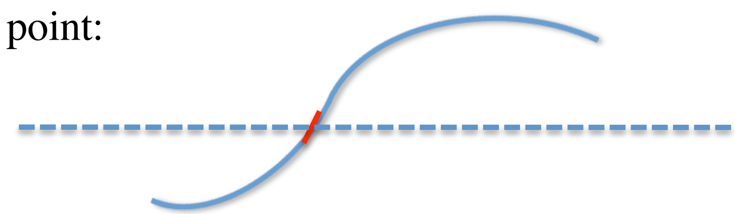
$$\psi_I \simeq \frac{A}{\sqrt{P(x)}} \exp\left(\frac{+1}{\hbar}\int P(x)\,dx\right)$$

$$\psi_{II} \simeq \frac{C}{\sqrt{p(x)}} \exp\left(\frac{+i}{\hbar}\int p(x)\,dx\right) + \frac{C}{\sqrt{p(x)}} \exp\left(\frac{-i}{\hbar}\int p(x)\,dx\right)$$

$$\psi_{III} \simeq \frac{D}{\sqrt{P(x)}} \exp\left(\frac{-1}{\hbar}\int P(x)\,dx\right)$$

Continue the method.

(3) Handle the turning points. Look closely at a turning point:



For x close to x_0, $V \sim$ a straight line. So approximate $V(x\ near\ x_0) \approx E + \left.\frac{dV}{dx}\right|_{x=x_0} \cdot x$

Substitute this V into the Time independent Schroedinger Equation to find $\psi_{\text{turning point}}$

$$\frac{-\hbar^2}{2m}\frac{\partial^2\psi_{t.p.}}{\partial x^2}+\left(E+\left.\frac{dV}{dx}\right|_{x_0}x\right)\psi_{t.p.}=E\psi_{t.p.}$$

$$\frac{\partial^2\psi_{t.p.}}{\partial x^2}=\underbrace{\frac{2m}{\hbar^2}\left.\frac{dV}{dx}\right|_{x_0}}x\psi_{t.p.}$$

Call this α^3 (that is, $\alpha=\left\{\frac{2m}{\hbar^2}\left.\frac{dV}{dx}\right|_{x_0}\right\}^{1/3}$)

$$\frac{\partial^2\psi_{t.p.}}{\partial x^2}=\alpha^3 x\psi_{t.p.}$$

Now let $z\equiv\alpha x$, so

$$\text{x}=\frac{1}{\alpha}z,$$

$$\frac{d}{dx}=\frac{dz}{dx}\frac{d}{dz}=\alpha\frac{d}{dz}$$

$$\frac{d^2}{dx^2}=\frac{d}{dx}\left(\alpha\frac{d}{dz}\right)=\frac{dz}{dx}\frac{d}{dz}\left(\alpha\frac{d}{dz}\right)=\alpha^2\frac{d^2}{dz^2}$$

$$\alpha^2\frac{d^2\psi_{t.p.}}{dz^2}=\alpha^3\frac{1}{\alpha}z\psi_{t.p.}$$

$$\frac{d^2\psi_{t.p.}}{dz^2}=z\psi_{t.p.}$$ Airy's Equation

$$\psi_{t.p.} = aAi(\alpha x) + bBi(\alpha x)$$

a, b are unspecified constants

Ai and Bi are Airy functions (like Bessel functions)

What we need to know about Airy functions:

for $z >> 0$, $Ai(z) \sim \dfrac{1}{2\sqrt{\pi}z^{1/4}} \exp\left(\dfrac{-2}{3} z^{3/2}\right)$ and $Bi(z) \sim \dfrac{1}{\sqrt{\pi}z^{1/4}} \exp\left(\dfrac{+2}{3} z^{3/2}\right)$

for $z << 0$, $Ai(z) \sim \dfrac{1}{\sqrt{\pi}(-z)^{1/4}} \sin\left(\dfrac{2}{3}(-z)^{3/2} + \dfrac{\pi}{4}\right)$ and $Bi(z) \sim \dfrac{1}{\sqrt{\pi}(-z)^{1/4}} \cos\left(\dfrac{2}{3}(-z)^{3/2} + \dfrac{\pi}{4}\right)$

II. WKB Connection Formulas

Continue the method.

(4) Connect $\psi_{\text{general WKB}}$ to $\psi_{\text{turning points}}$ at the turning points.

Technique:

(i) Write down $\psi_{\text{general WKB}}$ and $\psi_{\text{turning points}}$:

$$\psi_{general\ \text{WKB}} = \frac{C_+}{\sqrt{p(x)}}\exp\left[+\frac{i}{\hbar}\int p(x)dx\right] + \frac{C_-}{\sqrt{p(x)}}\exp\left[-\frac{i}{\hbar}\int p(x)dx\right]$$

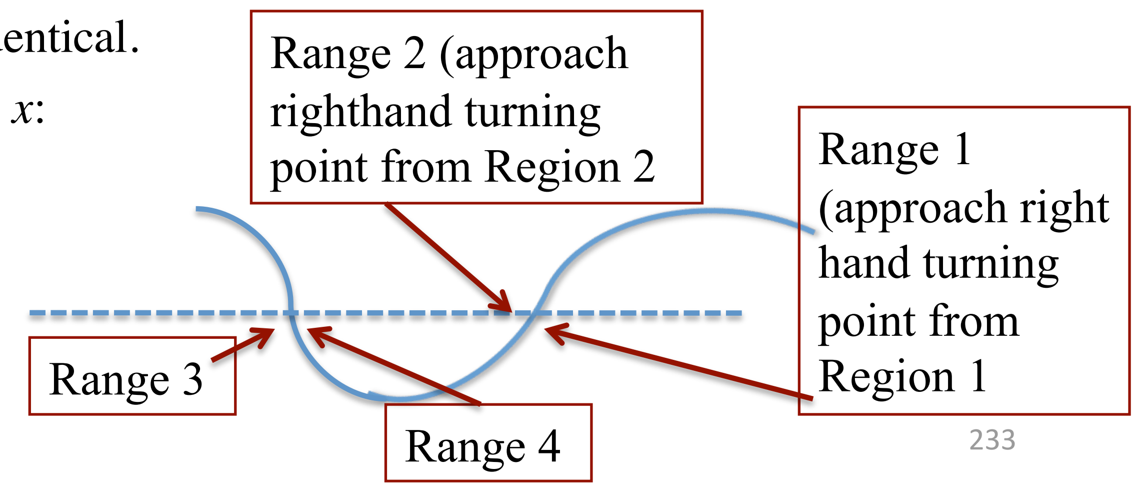
$$\psi_{t.p.} = aAi(\alpha x) + bBi(\alpha x)$$

(ii) Substitute $V \approx E + \left.\frac{dV}{dx}\right|_{x_0} \cdot x$ into $p(x) = \sqrt{2m(E-V)}$

(iii) Substitute the asymptotic form into Ai and Bi

(iv) Compare $\psi_{\text{general WKB}}$ to $\psi_{\text{turning points}}$ to see what "a" and "b" must be to make them identical.

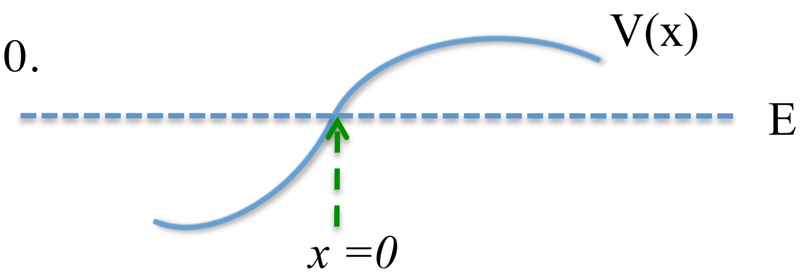
(v) Do this separately for 4 ranges in x:



(vi) To simplify the math, locate the righthand turning point at $x = 0$. Solve everything for range 1 and range 2, then move that turning point back to arbitrary x. Then get connection formulas for the lefthand turning point by symmetry arguments.

Carry this out:

Consider the righthand turning point. Call it $x = 0$.



Write the ψ's:

$$\psi_{\text{WKB, not t.p.}} = \begin{cases} \dfrac{1}{\sqrt{p(x)}} B \exp\left(\dfrac{i}{\hbar} \displaystyle\int_x^0 p(x')\,dx' \right) + \dfrac{1}{\sqrt{p(x)}} C \exp\left(\dfrac{-i}{\hbar} \displaystyle\int_x^0 p(x')\,dx' \right) & x < 0 \\ \dfrac{1}{\sqrt{P(x)}} D \exp\left(\dfrac{-1}{\hbar} \displaystyle\int_0^x P(x')\,dx' \right) & x > 0 \end{cases}$$

Notice that the limits on the integral reflect the region over which we want this ψ to be applicable.

Substitute $V = E + \left.\dfrac{\partial V}{\partial x}\right|_{x_0} x$

So $p(x) = \sqrt{2m\left(E - V(x)\right)} \rightarrow \sqrt{2m\left[E - \left(E + \left.\frac{\partial V}{\partial x}\right|_{x_0} x\right)\right]} = \sqrt{2m\left.\frac{\partial V}{\partial x}\right|_{x_0}}\sqrt{-x}$

Recall $\alpha \equiv \left\{\frac{2m}{\hbar^2}\left.\frac{\partial V}{\partial x}\right|_{x_0}\right\}^{1/3}$

$p(x) \cong \hbar\alpha^{3/2}\sqrt{-x}$

and

$P(x) = \text{-}ip(x) = \hbar\alpha^{3/2}\sqrt{x}$

Substitute this into $\psi_{\text{WKB not t.p.}}^{\text{range 1: x > 0}}$

Use the Region 3 ψ:

$$\psi = \frac{D}{\sqrt{P(x)}}\exp\left(\frac{-1}{\hbar}\int_0^x P(x)\,dx\right)$$

$$\psi_{\text{non-t.p.}}^{\text{range 1}} = \frac{D}{\sqrt{\hbar}\alpha^{3/4}x^{1/4}}\exp\left(\frac{-1}{\hbar}\int_0^x \hbar\alpha^{3/2}\sqrt{x}dx\right) = \frac{D}{\hbar^{1/2}\alpha^{3/4}x^{1/4}}\exp\left(-\alpha^{3/2}\int_0^x x^{1/2}\,dx\right)$$

$$\psi_{\text{non-t.p.}}^{\text{range 1}} = \frac{D}{\hbar^{1/2}\alpha^{3/4}x^{1/4}}\exp\left(-\frac{2}{3}(\alpha x)^{3/2}\right) \qquad \text{Eq 1}$$

Carry out the same calculation for $\psi_{\text{WKB at turning points}}$:

$$\psi_{\text{WKB at turning points}} = aAi(\alpha x) + bBi(\alpha x).$$

Substitute $Ai(\alpha x \text{ large positive}) \sim \dfrac{1}{2\sqrt{\pi}\,(\alpha x)^{1/4}} \exp\left(\dfrac{-2}{3}(\alpha x)^{3/2}\right)$ and

$$Bi(\alpha x \text{ large positive}) \sim \frac{1}{\sqrt{\pi}\,(\alpha x)^{1/4}} \exp\left(\frac{+2}{3}(\alpha x)^{3/2}\right).$$

$$\psi^{\text{range 1}}_{\text{WKB @ t.p.}} \sim \frac{a}{2\sqrt{\pi}\alpha^{1/4}x^{1/4}} \exp\left(\frac{-2}{3}(\alpha x)^{3/2}\right) + \frac{b}{\sqrt{\pi}\alpha^{1/4}x^{1/4}} \exp\left(\frac{+2}{3}(\alpha x)^{3/2}\right) \qquad \text{Eq. 2}$$

At the turning point, Eq. 1 and Eq. 2 must be equal. This will be assured if:

$$\frac{D}{\hbar^{1/2}\alpha^{3/4}} = \frac{a}{2\sqrt{\pi}\alpha^{1/4}} \qquad \text{and} \qquad b = 0$$

$$a = \sqrt{\frac{4\pi}{\hbar\alpha}}D$$

Now do Range 2 (still the righthand turning point). Rewrite, using the Region II ψ:

$$\psi_{\text{general, non-t.p.}} = \frac{1}{\sqrt{p(x)}}\exp\left(\frac{+i}{\hbar}\int_x^0 p(x')dx'\right) + \frac{C}{\sqrt{p(x)}}\exp\left(\frac{-i}{\hbar}\int_x^0 p(x')dx'\right)$$

Substitute p(x')~$\hbar\alpha^{3/2}\sqrt{-x'}$

$$\psi^{\text{range 2}}_{\text{general, non-t.p.}} = \frac{1}{\sqrt{\hbar}\alpha^{3/4}(-x)^{1/4}}\left\{B\exp\left[i\frac{2}{3}(-\alpha x)^{3/2}\right] + C\exp\left[-i\frac{2}{3}(-\alpha x)^{3/2}\right]\right\} \qquad \text{Eq. 3}$$

$$\psi^{\text{range 2}}_{@t.p.} = aAi(\alpha x) + bBi(\alpha x)$$

Since x is <0 in this range, use the Airy function forms for large negative αx:

$$Ai(\alpha x \text{ large negative}) \sim \frac{1}{\sqrt{\pi}(-\alpha x)^{1/4}}\sin\left(\frac{2}{3}(-\alpha x)^{3/2} + \frac{\pi}{4}\right) \text{ and}$$

$$Bi(\alpha x \text{ large negative}) \sim \frac{1}{\sqrt{\pi}(-\alpha x)^{1/4}}\cos\left(\frac{2}{3}(-\alpha x)^{3/2} + \frac{\pi}{4}\right)$$

Then $\psi^{\text{range 2}}_{@t.p.} = \frac{a}{\sqrt{\pi}(-\alpha x)^{1/4}}\sin\left(\frac{2}{3}(-\alpha x)^{3/2} + \frac{\pi}{4}\right) + \frac{b}{\sqrt{\pi}(-\alpha x)^{1/4}}\cos\left(\frac{2}{3}(-\alpha x)^{3/2} + \frac{\pi}{4}\right)$

Substitute what we found earlier, that $a = \sqrt{\frac{4\pi}{\hbar\alpha}}D$ and $b = 0$. Also write $\sin(\;)$ as $\frac{e^{i(\;)} - e^{-i(\;)}}{2i}$:

$$\psi^{\text{range 2}}_{@t.p.} = \sqrt{\frac{4\pi}{\hbar\alpha}}D\frac{1}{\sqrt{\pi}(-\alpha x)^{1/4}}\left\{\frac{e^{i\pi/4}e^{i\frac{2}{3}(-\alpha x)^{3/2}} - e^{-i\pi/4}e^{-i\frac{2}{3}(-\alpha x)^{3/2}}}{2i}\right\} \qquad \text{Eq. 4.}$$

Require Eq. 3 = Eq. 4. This means

$$\frac{1}{\sqrt{\hbar}\alpha^{3/4}} B = \sqrt{\frac{4}{\hbar\alpha}} \frac{De^{i\pi/4}}{2i\alpha^{1/4}} \quad \text{and} \quad \frac{1}{\sqrt{\hbar}\alpha^{3/4}} C = -\sqrt{\frac{4}{\hbar\alpha}} \frac{De^{-i\pi/4}}{2i\alpha^{1/4}}$$

$$B = -iDe^{i\pi/4} \quad \text{and} \quad C = +iDe^{-i\pi/4}$$

Recap: now we have:

$a = a(D)$

$b = 0$

$B = B(D)$

$C = C(D)$.

Summarize:

$$\psi_{WKB\text{, both @t.p. and not @ t.p.}} = \begin{cases} \frac{1}{\sqrt{p(x)}}\left(-iDe^{i\pi/4}\right)\exp\left[\frac{i}{\hbar}\int_x^0 p(x')dx'\right] + \frac{1}{\sqrt{p(x)}}\left(iDe^{-i\pi/4}\right)\exp\left[\frac{-i}{\hbar}\int_x^0 p(x')dx'\right] & \text{for } x < 0 \\ \frac{1}{\sqrt{P(x)}} D\exp\left[\frac{-1}{\hbar}\int_0^x P(x')dx'\right] & \text{for } x > 0 \end{cases}$$

Rework this:

(i) Convert $e^{i\pi/4} e^{\frac{i}{\hbar}\int p\,dx} \to e^{i\left[\frac{1}{\hbar}\int p\,dx + \frac{\pi}{4}\right]}$

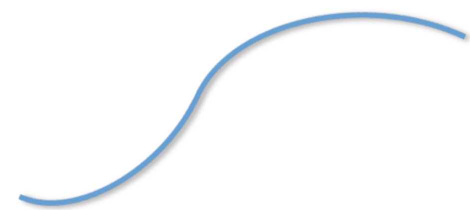
(ii) Convert $\mathrm{e}^{i\left[\int\ \right]} + \mathrm{e}^{-i\left[\int\ \right]} \to 2i\sin\left[\int\ \right]$

(iii) Convert integral limits: $0 \to \mathrm{x}_2$ (the arbitrary location of the turning point).

We get:

$$\psi_{WKB} = \begin{cases} \dfrac{1}{\sqrt{p(x)}} 2D \sin\left[\dfrac{1}{\hbar}\displaystyle\int_x^{x_2} p(x')dx' + \dfrac{\pi}{4}\right] & \text{for} \quad x < x_2 \\ \dfrac{1}{\sqrt{P(x)}} D \exp\left[\dfrac{-1}{\hbar}\displaystyle\int_{x_2}^{x} P(x')dx'\right] & \text{for} \quad x > x_2 \end{cases}$$

for the right side of the well, that is, for a potential shaped like:



We could also consider the left side of the well and develop equations around a downward sloping potential:

We would get:

$$\psi_{WKB} = \begin{cases} \dfrac{D'}{\sqrt{P(x)}} \exp\left[\dfrac{-1}{\hbar} \displaystyle\int_x^{x_1} P(x')\,dx' \right] & \text{for } x < x_1 \\ \dfrac{2D'}{\sqrt{p(x)}} \sin\left[\dfrac{1}{\hbar} \displaystyle\int_{x_1}^{x} p(x')\,dx' + \dfrac{\pi}{4} \right] & \text{for } x > x_1 \end{cases}$$

for the left side of the well.

To get D/D', require $\psi_{x>x_1} = \psi_{x<x_2}$

$$\frac{2D'}{\sqrt{p(x)}} \sin\left[\frac{1}{\hbar} \int_{x_1}^{x} p(x')\,dx' + \frac{\pi}{4} \right] = \frac{2D}{\sqrt{p(x)}} \sin\left[\frac{1}{\hbar} \int_{x}^{x_2} p(x')\,dx' + \frac{\pi}{4} \right]$$

$$\sin\left[\frac{1}{\hbar} \int_{x_1}^{x} p(x')\,dx' + \frac{\pi}{4} \right] = \frac{D}{D'} \sin\left[\frac{1}{\hbar} \int_{x}^{x_2} p(x')\,dx' + \frac{\pi}{4} \right]$$

$$\sin\left[\underbrace{\left\{ \frac{1}{\hbar} \int_{x_1}^{x_2} p\,dx \right\}} - \underbrace{\left\{ \frac{1}{\hbar} \int_{x}^{x_2} p\,dx + \frac{\pi}{4} \right\}} + \frac{\pi}{2} \right] = \frac{D}{D'} \sin \underbrace{\left[\frac{1}{\hbar} \int_{x}^{x_2} p(x')\,dx' + \frac{\pi}{4} \right]}$$

Call this "η" Call this "a" So this is also "a"

$$\sin\left(\eta - a + \frac{\pi}{2} \right) = \frac{D}{D'} \sin a$$

To solve this, use $\sin(m - n) = \sin m \cos n - \cos m \sin n$

Let $m = \eta + \dfrac{\pi}{2}$ and $n = a$

$$\sin\left(\eta+\frac{\pi}{2}\right)\cos a-\cos\left(\eta+\frac{\pi}{2}\right)\sin a=\frac{D}{D'}\sin a$$

This is solved if $\eta+\dfrac{\pi}{2}=(n+1)\pi$ for $n=0,\ 1,\ 2,\ \ldots$

We use "$n+1$" rather than "n" here to ensure that η is not negative.

Then $\dfrac{D}{D'}=(-1)^n$

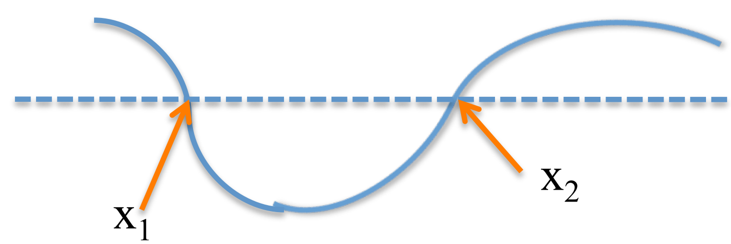
Pick $D=1$, then $D'=\dfrac{1}{(-1)^n}=(-1)^n$

The final ψ_{WKB} :

$$\frac{(-1)^n}{\sqrt{P(x)}}\exp\left[\frac{-1}{\hbar}\int_x^{x_1}P(x')dx'\right] \qquad x<x_1$$

$$\frac{(-1)^n}{\sqrt{p(x)}}2\sin\left[\frac{1}{\hbar}\int_{x_1}^{x}p(x')dx'+\frac{\pi}{4}\right] \qquad x_1<x<x_2$$

$$\frac{1}{\sqrt{P(x)}}\exp\left[\frac{-1}{\hbar}\int_{x_2}^{x}P(x')dx'\right] \qquad x>x_2$$



How to find the energy levels in the WKB approximation:

Recall we found that

$$\eta + \frac{\pi}{2} = (n+1)\pi$$

Recall $\eta \equiv \frac{1}{\hbar}\int_{x_1}^{x_2} p(x)\,dx$

$$\int_{x_1}^{x_2} p(x)\,dx = \left(n + \frac{1}{2}\right)\pi\hbar$$

But p=$\sqrt{2m\left(E - V(x)\right)}$

So plug in a specific $V(x)$, evaluate the integral, and solve for E_n.

Outline

I. Systems with 2 degrees of freedom: Introduction
II. Exchange Degeneracy
III. The Exchange Operator

Please read Goswami Chapter 9.

I. Systems with 2 degrees of freedom: Introduction

Examples of kinds of degrees of freedom:

(i) 2 particles free to move in 1 dimension

(ii) 1 particle free to move in 2 dimensions

Each of these leads to energy degeneracy.

II. Systems of 2 particles in 1 dimension have exchange degeneracy

Consider 2 particles in the same 1-dimensional infinite square well of width "a".
Both have mass m.
The particles do not interact with each other. That is, they are "invisible" to each other.
Since their wavefunctions overlap/superpose (and this does NOT imply that the particles interact!), there is only 1 wavefunction in the well. It is the wavefunction of the *system* of two particles.
That is, it does not make sense to describe the 2 particles' wavefunctions separately.
How to handle this mathematically:

Label particle 1's position $= x_1$
Label particle 1's momentum $= p_1$
Label particle 2's position $= x_2$
Label particle 2's momentum $= p_2$
Suppose the particles can be in energy levels n_1 and n_2.
The Hamiltonian for this system is

$$H = \frac{p_1^2}{2m} + V(x_1) + \frac{p_2^2}{2m} + V(x_2) = H(x_1) + H(x_2)$$

Note we indicate that the particles are non-interacting by not having a $V(x_1 - x_2)$ term.

Suppose we want to find $\psi_{n_1 n_2}(x_1, x_2)$ and $E_{n_1 n_2}(x_1, x_2)$.

Since the H is separable, we GUESS that $\psi_{n_1 n_2}(x_1, x_2)$ can be written as the product:

$$\psi_{n_1 n_2}(x_1, x_2) = \psi_{n_1}(x_1) \cdot \psi_{n_2}(x_2)$$

where $\psi_{n_1}(x_1)$ is the solution of $H(x_1)\psi_{n_1}(x_1) = E_{n_1}\psi_{n_1}(x_1)$

and $\psi_{n_1}(x_1)$ is the solution of $H(x_1)\psi_{n_1}(x_1) = E_{n_1}\psi_{n_1}(x_1)$

For the infinite square well, $\psi_n = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right)$ and $\mathrm{E}_n = \frac{n^2\pi^2\hbar^2}{2ma^2}$

Note the "n" indicates the level number, not the particle number!

Check whether the GUESS works:

$$H\psi_{n_1 n_2}(x_1, x_2) = \left[H(x_1) + H(x_2)\right]\psi_{n_1 n_2}(x_1, x_2)$$

$$= \left\{\frac{p_1^2}{2m} + V(x_1)\right\}\psi_{n_1}(x_1) \cdot \psi_{n_2}(x_2) + \left\{\frac{p_2^2}{2m} + V(x_2)\right\}\psi_{n_1}(x_1) \cdot \psi_{n_2}(x_2)$$

$\psi(x_2)$ is unaffected by x_1 or $\frac{\partial}{\partial x_1}$. $\psi(x_1)$ is unaffected by x_2 or $\frac{\partial}{\partial x_2}$.

$$= \psi_{n_2}(x_2) H(x_1)\psi_{n_1}(x_1) + \psi_{n1}(x_1) H(x_2)\psi_{n_2}(x_2)$$

So $H\psi_{n_1 n_2}\left(x_1,x_2\right)=\psi_{n_2}\left(x_2\right)\underbrace{H(x_1)\psi_{n_1}\left(x_1\right)}_{\substack{\downarrow \\ E_{n_1}\psi_{n_1}\left(x_1\right)}}+\psi_{n1}\left(x_1\right)\underbrace{H(x_2)\psi_{n_2}\left(x_2\right)}_{\substack{\downarrow \\ E_{n_2}\psi_{n_2}\left(x_2\right)}}$

$=\left(E_{n_1}+E_{n2}\right)\psi_{n1}\psi_{n2}$

$=\left[\frac{\left(n_1^2+n_2^2\right)\pi^2\hbar^2}{2ma^2}\right]\sqrt{\frac{2}{a}}\sin\left(\frac{n_1\pi x_1}{a}\right)\sqrt{\frac{2}{a}}\sin\left(\frac{n_2\pi x_2}{a}\right)$

So we confirm that:

(i) $\psi_{n_1 n_2}\left(x_1,x_2\right)=\psi_{n_1}\left(x_1\right)\cdot\psi_{n_2}\left(x_2\right)$ is an eigenfunction of $H=H(x_1)+H(x_2)$

(ii) Its eigenvalue is $\left(E_{n_1}+E_{n_2}\right)$.

THIS math formula describes a system in which

Particle 1 is in energy level n_1 (we know this because n_1 is the argument of the sine that has x_1)

$-and-$

Particle 2 is in energy level n_2 (we know this because n_2 is the argument of the sine that has x_2).

Notice that we would get the SAME total energy, $\frac{\left(n_1^2+n_2^2\right)\pi^2\hbar^2}{2ma^2}$, if

Particle 1 were in energy level n_2 and Particle 2 were in level n_1.

So we say that "$\psi_{n_1 n_2}(x_1, x_2)$ is degenerate in energy with $\psi_{n_1 n_2}(x_2, x_1)$."
The degeneracy reflects the effect of exchanging the positions (levels) of the 2 particles, so it is called "exchange degeneracy."

III. The Exchange Operator

We just considered two 2-particle wavefunctions:

$\psi_{n_1 n_2}(x_1,x_2)$: Particle 1 in level n_1, Particle 2 in level n_2

$\psi_{n_1 n_2}(x_2,x_1)$: Particle 1 in level n_2, Particle 2 in level n_1

Define the Exchange Operator: P_{12} (not Parity!) which represents the effect that exchanging the positions of the particles has upon their total wavefunction.

Mathematically the effect of P_{12} is:

$$P_{12}\psi_{n_1 n_2}(x_1,x_2)=\psi_{n_1 n_2}(x_2,x_1)$$

Notice that because $E\left(\psi_{n_1 n_2}(x_1,x_2)\right)=E\left(\psi_{n_1 n_2}(x_2,x_1)\right)=\text{"}E\text{"}$, we expect $\left[H,P_{12}\right]=0.$

Show this:

$$\begin{aligned}\left[H,P_{12}\right]\psi_{n_1 n_2}(x_1,x_2) &= HP_{12}\psi_{n_1 n_2}(x_1,x_2)-P_{12}H\psi_{n_1 n_2}(x_1,x_2)\\ &= H\psi_{n_1 n_2}(x_2,x_1)-P_{12}E\psi_{n_1 n_2}(x_1,x_2)\\ &= E\psi_{n_1 n_2}(x_2,x_1)-EP_{12}\psi_{n_1 n_2}(x_1,x_2)\\ &= E\psi_{n_1 n_2}(x_2,x_1)-E\psi_{n_1 n_2}(x_2,x_1)\\ &= 0\end{aligned}$$

We showed (Goswami p. 122) that if 2 operators commute, they have simultaneous eigenfunctions. Find those eigenfunctions for H and P_{12} :

Notice: $\psi_{n_1 n_2}(x_1,x_2)$ is an eigenfunction of H : $H\psi_{n_1 n_2}(x_1,x_2)=\left[\frac{(n_1^2+n_2^2)\pi^2\hbar^2}{2ma^2}\right]\psi_{n_1 n_2}(x_1,x_2)$

But it is NOT an eigenfunction of P_{12} : $P_{12}\psi_{n_1 n_2}(x_1,x_2)=\psi_{n_1 n_2}(x_2,x_1)$.

because these are not the same.

Similarly $\psi_{n_1 n_2}(x_2,x_1)$ is an eigenfunction of H but not of P_{12}.

How many eigenfunctions do we expect for P_{12}? 2....because $(P_{12})^2\psi=+1\psi$, for arbitrary ψ.

The eigenvalues of P_{12} must be ± 1.

These are the 2 simultaneous eigenfunctions of P_{12} and H :

$\psi^{(s)}_{n_1 n_2}\equiv\frac{1}{\sqrt{2}}\left[\psi_{n_1}(x_1)\psi_{n_2}(x_2)+\psi_{n_1}(x_2)\psi_{n_2}(x_1)\right]$ The "symmetric ψ" has eigenfunction +1 under operator P_{12}.

$\psi^{(a)}_{n_1 n_2}\equiv\frac{1}{\sqrt{2}}\left[\psi_{n_1}(x_1)\psi_{n_2}(x_2)-\psi_{n_1}(x_2)\psi_{n_2}(x_1)\right]$ The "antisymmetric ψ" has eigenfunction -1 under operator P_{12}.

Facts about symmetric and antisymmetric:

(1) Mathematically it seems that if you have 2 particles, they should be free to arrange their ψ's in either the $\psi^{(s)}$ or the $\psi^{(a)}$ combined state so that if you had an ensemble of pairs of particles, and you could somehow detect whether they were in $\psi^{(s)}$ or $\psi^{(a)}$, you would find half in each. (Of course we cannot measure ψ directly. We can only measure $|\psi|^2=$ probability.

(2) A surprising fact about nature is that they choose NOT to do this.

Each kind of particle always picks $\psi^{(s)}$ or $\psi^{(a)}$.

Example: electrons always pick $\psi^{(a)}$, photons always pick $\psi^{(s)}$.

(iii) How do we know this?

Example for the electrons:

(1) We determine indirectly that they satisfy the Pauli Exclusion Principle. That is, if we try to add more and more electrons to an atom, they enter higher and higher energy levels and "refuse" to be all in the $\underbrace{\text{same level}}_{\text{same } \psi}$.

So we have experimental data that 2 e's will not occupy the same state. Now check how occupying the same state would affect their combined ψ:

Suppose that 2e's were in $\psi^{(s)} : \psi^{(s)}_{n_1 n_2} \equiv \frac{1}{\sqrt{2}}\left[\psi_{n_1}(x_1)\psi_{n_2}(x_2) + \psi_{n_1}(x_2)\psi_{n_2}(x_1)\right]$.

Force them to be in the same state, n_1 :

$$\psi^{(s)}_{n_1 n_1} \equiv \frac{1}{\sqrt{2}}\left[\psi_{n_1}(x_1)\psi_{n_1}(x_2) + \psi_{n_1}(x_2)\psi_{n_1}(x_1)\right]$$

$$= \sqrt{2}\psi_{n_1}(x_1)\psi_{n_1}(x_2).$$

Now suppose that 2 e's are in $\psi^{(a)} = \frac{1}{\sqrt{2}}\left[\psi_{n_1}(x_1)\psi_{n_2}(x_2) - \psi_{n_1}(x_2)\psi_{n_2}(x_1)\right]$.

Force them to be in the same state n_1 :

Then we have $\psi^{(a)}_{n_1 n_1} \equiv \frac{1}{\sqrt{2}}\left[\psi_{n_1}(x_1)\psi_{n_1}(x_2) - \psi_{n_1}(x_2)\psi_{n_1}(x_1)\right] = 0.$

Conclusion:

If we do not know whether 2 e's are in $\psi^{(s)}$ or $\psi^{(a)}$ and we try to force them to be in the same state, they will not do it. Their way of "refusing" to do it is to maintain a ψ_{total} that becomes 0 if we force that situation. The kind of ψ_{total} that can become 0 under this situation is $\psi^{(a)}$.

So we conclude: pairs of e's always arrange themselves in antisymmetric combined ψ's.

Similarly, photons preferentiall occupy the same energy level. We conclude that they arrange themselves in symmetric combined ψ's.

(iv) There is a direct connection between the spin of a particle and the symmetry of the ψ's it makes with other particles that are identical to it.

Spin	$\boldsymbol{\psi_{\text{total}}}$	**Name**	**Examples**
half integer (1/2)	$\psi^{(a)}$	fermion	electron, quark
integer (0,1)	$\psi^{(s)}$	boson	photon, $W^{\pm}$, Z, gluon

Outline

I. System of 2 interacting particles in 1 dimension
II. System of 1 particle in 2 dimensions
III. Multi (>2) particle systems in 3 dimensions

Please read Goswami Chapter 11.

I. Systems of 2 interacting particles in one dimension

Allow them to have different masses, m_1 and m_2.

In this case $H = \frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2} + V\left(x_1 - x_2\right)$.

Find the eigenvalues E and eigenvectors $\psi(x_1 x_2)$ for this H.

Note there is no reason to expect these $\psi(x_1 x_2)$ to be the product $\psi(x_1)\cdot\psi(x_2)$ that occured for separable (that is, non-interacting) H.

So we want to solve the equation:

$$\left(-\frac{\hbar^2}{2m_1}\frac{\partial^2}{\partial x_1^2} - \frac{\hbar^2}{2m_1}\frac{\partial^2}{\partial x_1^2}\right)\psi(x_1 x_2) + V\left(x_1 - x_2\right)\psi(x_1 x_2) = E\psi(x_1 x_2)$$

The way to solve this is to define:

$$x \equiv x_1 - x_2 \qquad \text{"Eq. 1"}$$

$$X \equiv \frac{m_1 x_1 + m_2 x_2}{m_1 + m_2} \qquad \text{"Eq. 2"}$$

$$\frac{1}{\mu} \equiv \frac{1}{m_1} + \frac{1}{m_2}$$

$$M \equiv m_1 + m_2$$

Rewrite the Schroedinger Equation in terms of these variables:

$$\frac{\partial}{\partial x_1} = \frac{\partial x}{\partial x_1}\frac{\partial}{\partial x} + \frac{\partial X}{\partial x_1}\frac{\partial}{\partial X} = 1\frac{\partial}{\partial x} + \left(\frac{m_1}{m_1+m_2}\right)\frac{\partial}{\partial X}$$

$$\frac{\partial^2}{\partial x_1^2} = \frac{\partial}{\partial x_1}\left[\frac{\partial}{\partial x} + \left(\frac{m_1}{m_1+m_2}\right)\frac{\partial}{\partial X}\right] = \frac{\partial x}{\partial x_1}\frac{\partial}{\partial x}\left[\frac{\partial}{\partial x} + \left(\frac{m_1}{m_1+m_2}\right)\frac{\partial}{\partial X}\right] + \frac{\partial X}{\partial x_1}\frac{\partial}{\partial X}\left[\frac{\partial}{\partial x} + \left(\frac{m_1}{m_1+m_2}\right)\frac{\partial}{\partial X}\right]$$

$$= 1\left[\frac{\partial^2}{\partial x^2} + \left(\frac{m_1}{m_1+m_2}\right)\frac{\partial^2}{\partial x \partial X}\right] + \left(\frac{m_1}{m_1+m_2}\right)\left[\frac{\partial^2}{\partial x \partial X} + \left(\frac{m_1}{m_1+m_2}\right)\frac{\partial^2}{\partial X^2}\right]$$

$$= \frac{\partial^2}{\partial x^2} + \frac{2m_1}{m_1+m_2}\frac{\partial^2}{\partial x \partial X} + \left(\frac{m_1}{m_1+m_2}\right)^2\frac{\partial^2}{\partial X^2}$$

Similarly,

$$\frac{\partial}{\partial x_2} = \frac{\partial x}{\partial x_2}\frac{\partial}{\partial x} + \frac{\partial X}{\partial x_2}\frac{\partial}{\partial X} = -1\frac{\partial}{\partial x} + \left(\frac{m_2}{m_1+m_2}\right)\frac{\partial}{\partial X}$$

$$\frac{\partial^2}{\partial x_2^2} = \frac{\partial}{\partial x_2}\left[-\frac{\partial}{\partial x} + \left(\frac{m_2}{m_1+m_2}\right)\frac{\partial}{\partial X}\right] = \frac{\partial x}{\partial x_2}\frac{\partial}{\partial x}\left[-\frac{\partial}{\partial x} + \left(\frac{m_2}{m_1+m_2}\right)\frac{\partial}{\partial X}\right] + \frac{\partial X}{\partial x_1}\frac{\partial}{\partial X}\left[-\frac{\partial}{\partial x} + \left(\frac{m_2}{m_1+m_2}\right)\frac{\partial}{\partial X}\right]$$

$$= -1\left[\frac{\partial^2}{\partial x^2} + \left(\frac{m_2}{m_1+m_2}\right)\frac{\partial^2}{\partial x \partial X}\right] + \left(\frac{m_2}{m_1+m_2}\right)\left[-\frac{\partial^2}{\partial x \partial X} + \left(\frac{m_2}{m_1+m_2}\right)\frac{\partial^2}{\partial X^2}\right]$$

$$= \frac{\partial^2}{\partial x^2} - \frac{2m_2}{m_1+m_2}\frac{\partial^2}{\partial x \partial X} + \left(\frac{m_2}{m_1+m_2}\right)^2\frac{\partial^2}{\partial X^2}$$

Also $V(x_1 - x_2) \rightarrow V(x)$ and $\psi(x_1, x_2) = \psi(x, X)$.

Substitute all of this into the Schroedinger Equation:

$$-\frac{\hbar^2}{2m_1}\left[\frac{\partial^2}{\partial x^2} + \left(\frac{2m_1}{m_1+m_2}\right)\frac{\partial^2}{\partial x \partial X} + \left(\frac{m_1}{m_1+m_2}\right)^2 \frac{\partial^2}{\partial X^2}\right]\psi$$

$$-\frac{\hbar^2}{2m_2}\left[\frac{\partial^2}{\partial x^2} - \left(\frac{2m_2}{m_1+m_2}\right)\frac{\partial^2}{\partial x \partial X} + \left(\frac{m_2}{m_1+m_2}\right)^2 \frac{\partial^2}{\partial X^2}\right]\psi + V\psi = E\psi$$

$$\left[-\frac{\hbar^2}{2}\left(\frac{1}{m_1} + \frac{1}{m_2}\right)\frac{\partial^2}{\partial x^2} - \frac{\hbar^2}{2}\left(\frac{1}{m_1+m_2}\right)\frac{\partial^2}{\partial X^2} + V\right]\psi = E\psi$$

$$\left[-\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial x^2} - \frac{\hbar^2}{2M}\frac{\partial^2}{\partial X^2} + V\right]\psi(x,X) = E\psi(x,X)$$

$$\left[\underbrace{-\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial x^2} + V(x)}_{H(x)} \underbrace{- \frac{\hbar^2}{2M}\frac{\partial^2}{\partial X^2}}_{H(X)}\right]\psi(x,X) = E\psi(x,X)$$

Now the Hamiltonian is separable into functions of x and X, so we expect the ψ to be expressible as a product: $\psi(x,X) = U(X) \cdot u(x)$

Substitute this $U(X) \cdot u(x)$ above. We get:

$$H(x)U(X)u(x) + H(X)U(X)u(x) = EU(X)u(x)$$

$$U(X)H(x)u(x) + u(x)H(X)U(X) = EU(X)u(x)$$

$$\frac{U(X)H(x)u(x)}{U(X)u(x)} + \frac{u(x)H(X)U(X)}{U(X)u(x)} = \frac{EU(X)u(x)}{U(X)u(x)}$$

$$\frac{1}{u(x)}H(x)u(x) + \frac{1}{U(X)}H(X)U(X) = E$$

$$\underbrace{\frac{1}{u(x)}H(x)u(x)}_{\text{fn of } x \text{ only}} = \underbrace{E - \frac{1}{U(X)}H(X)U(X)}_{\text{fn of } X \text{ only}}$$

These functions can be equal only if both equal the same constant. Call it E_{rel}

Then we have

$$\frac{1}{u(x)}H(x)u(x) = E_{rel} \Rightarrow \left[\frac{-\hbar^2}{2\mu}\frac{\partial^2}{\partial x^2} + V(x)\right]u(x) = E_{rel}u(x)$$

$-and-$

$$E - \frac{1}{U(X)}H(X)U(X) \Rightarrow \underbrace{\left(E - E_{rel}\right)}_{\text{This is } E_{cm}}U(X) = \frac{-\hbar^2}{2M}\frac{\partial^2}{\partial X^2}U(X)$$

Conclusions about this:

(1) The X equation concerns the motion of the center of mass. Note that there is no V acting on the center of mass.

(2) The x equation concerns the motion of the reduced mass (this is mathematically equivalent to a body of finite mass orbiting in the V of an immobile, infinitely massive other body. Since the reduced mass does respond to the V, the V is in that equation.

(3) When the Schroedinger Equation is expressed in terms of $u(x)U(X)$, the motion of M and μ are decoupled, independent. But when the Schroedinger Equation is expressed in terms of (x_1, x_2), the behaviors of the real physical particles (m_1, m_2) cannot be decoupled. They remain really physically correlated, even when separated by great distances. This implies a philosophical question: are the 2 particles truly correlated---for example, does measuring the position of m_1 disrupt the momentum of m_2? This is the Einstein-Podolsky-Rosen (EPR) Paradox.

II. System of 1 particle in 2 dimensions

First convert 1-dimensional concepts to 2-dimensional concepts:

Concept	**1 - d**	**2 - d**
Free particle ψ	$\frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar}$	$\frac{1}{\sqrt{2\pi\hbar}} e^{ip_x x/\hbar} \cdot \frac{1}{\sqrt{2\pi\hbar}} e^{ip_y y/\hbar} = \frac{1}{2\pi\hbar} e^{i\left(p_x x + p_y y\right)/\hbar}$
p_x	$-i\hbar \frac{\partial}{\partial x}$	$-i\hbar\left(\frac{\partial}{\partial x}\right)\hat{x} - i\hbar\left(\frac{\partial}{\partial y}\right)\hat{y} = -i\hbar\vec{\nabla}_{2-d}$
p_y	$-i\hbar \frac{\partial}{\partial y}$	
V	$V(x)$	$V(\vec{r})$ where $\vec{r} = x\hat{x} + y\hat{y}$
H	$\frac{p_x^2}{2m} + V(x)$	$\frac{\lvert p\rvert^2}{2m} + V(\vec{r}) = \frac{-\hbar^2}{2m}\vec{\nabla}^2_{2-d} + V(\vec{r})$

Consider a particle in a 2-dimensional square well:

$$\mathrm{V}(x,y) = \begin{cases} 0 & \text{if } 0 \le x \le a \quad \text{and} \quad 0 \le y \le a \\ \infty & \text{if } x < 0,\ x > a \quad \text{or} \quad y < 0,\ y > a \end{cases}$$

The infinite walls cause the particle to be completely confined by the well, so we solve the Schroedinger Equation for the region inside only.

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,y)}{\partial x^2} - \frac{\hbar^2}{2m}\frac{\partial^2\psi(x,y)}{\partial y^2} = E\psi(x,y)$$

$$\frac{\partial^2\psi(x,y)}{\partial x^2} + \frac{\partial^2\psi(x,y)}{\partial y^2} = \frac{-2mE}{\hbar^2}\psi(x,y)$$

Reduce this to 2 ordinary differential equations by separation of variables.

GUESS that $\psi(x,y) = u(x)\cdot v(y)$.

Make this substitution, then divide through by $\psi = uv$.

$$\frac{\partial^2\left[u(x)v(y)\right]}{\partial x^2} + \frac{\partial^2\left[u(x)v(y)\right]}{\partial y^2} = \frac{-2mE}{\hbar^2}u(x)v(y)$$

$$\frac{\dfrac{v(y)\partial^2\left[u(x)\right]}{\partial x^2}}{u(x)v(y)} + \frac{\dfrac{u(x)\partial^2\left[v(y)\right]}{\partial y^2}}{u(x)v(y)} = \frac{\dfrac{-2mE}{\hbar^2}u(x)v(y)}{u(x)v(y)}$$

$$\frac{1}{u(x)}\frac{\partial^2 u(x)}{\partial x^2} + \frac{1}{v(y)}\frac{\partial^2 v(y)}{\partial y^2} = \frac{-2mE}{\hbar^2}$$

$$\frac{1}{u(x)}\frac{\partial^2 u(x)}{\partial x^2} = \frac{-2mE}{\hbar^2} - \frac{1}{v(y)}\frac{\partial^2 v(y)}{\partial y^2}$$

This can be solved for arbitrary u, v if each side equals a constant.

Call that constant "$\dfrac{-2mE^x}{\hbar^2}$". Then we have

$$\frac{1}{u(x)}\frac{\partial^2 u(x)}{\partial x^2} = -\frac{2mE^x}{\hbar^2} \qquad \Rightarrow \qquad u(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right) \quad \text{and} \quad E^x = \frac{n^2\pi^2\hbar^2}{2ma^2}$$

$-and-$

$$\frac{-2mE}{\hbar^2} - \frac{1}{v(y)}\frac{\partial^2 v(y)}{\partial y^2} = -\frac{2mE^x}{\hbar^2} \quad \Rightarrow \frac{1}{v(y)}\frac{\partial^2 v(y)}{\partial y^2} = \frac{-2m}{\hbar^2}\underbrace{\left(E - E^x\right)}_{\text{call this } E^y}$$

$$\frac{1}{v(y)}\frac{\partial^2 v(y)}{\partial y^2}=\frac{-2mE^y}{\hbar^2} \qquad \Rightarrow v(y)=\sqrt{\frac{2}{a}}\sin\left(\frac{n'\pi y}{a}\right) \quad \text{and} \quad E^y=\frac{n'^2\pi^2\hbar^2}{2ma^2}$$

So $E=E^x+E^y=\frac{\left(n^2+n'^2\right)\pi^2\hbar^2}{2ma^2}$

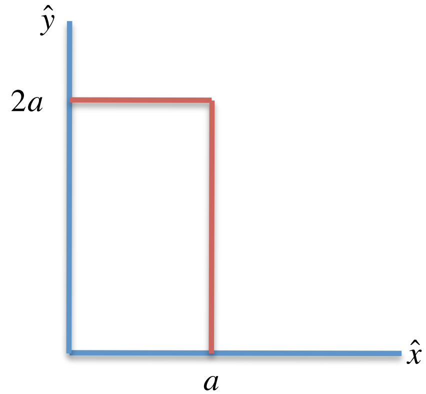
and $\psi(x,y)=u(x)v(y)=\frac{2}{a}\sin\left(\frac{n\pi x}{a}\right)\sin\left(\frac{n'\pi y}{a}\right)$

This ψ describes a particle with:
n-th level excitation of its x-direction component, and
n'-th level excitation of its y-direction component.

Notice it would have the same energy if its
x-component were at level n' and its y-component were at level n.

This is called symmetry degeneracy.

Now suppose that the well is not square, perhaps it has rectangular cross-section $a \times 2a$



In this case we would get $E = \left(\frac{n^2}{4} + n'^2 \right) \frac{\pi^2 \hbar^2}{m a^2}$.

So we would have the same E for $(n = 2,\ n' = 2)$ and $(n = 4,\ n' = 1)$.

This is called accidental degeneracy.

III. Multi (>2) particle systems in 3-dimensions

Modify existing formulas:

(1) Convert from **1 - d** to **3 - d :**

	1-d	3-d
position	x	$\vec{r}$
ψ	$\psi(x)$	$\psi(\vec{r})$
p	$-i\hbar\dfrac{\partial}{\partial x}$	$-i\hbar\vec{\nabla}_{3-d} = -i\hbar\left(\dfrac{\partial}{\partial x}\hat{x} + \dfrac{\partial}{\partial y}\hat{y} + \dfrac{\partial}{\partial z}\hat{z}\right)$
V	$V(x)$	$V(\vec{r})$

(2) Consider N particles located at positions $\vec{r}_1,\ \vec{r}_2, ...\vec{r}_N$ which may interact:

For 2 particles, $V(\vec{r}_1) + V(\vec{r}_2) \rightarrow V(\vec{r}_1, \vec{r}_2)$ which is usually $V(\vec{r}_1 - \vec{r}_2)$.

Extrapolate to N particles, all 2-body interactions, and sum:

$$
\begin{aligned}
V(\vec{r}_1,\vec{r}_2) \rightarrow\ & V(\vec{r}_1,\vec{r}_2) + V(\vec{r}_1,\vec{r}_3) + ... + V(\vec{r}_1,\vec{r}_N) \\
& + V(\vec{r}_2,\vec{r}_3) + V(\vec{r}_2,\vec{r}_4) + ... + V(\vec{r}_2,\vec{r}_N) \\
& + ... \\
& + V(\vec{r}_{N-1},\vec{r}_N)
\end{aligned}
$$

$$\sum_{i>j}\sum_{j} V(r_i, r_j)$$

(3) Convert Hamiltonian from 1 particle to N particles: $H(p,\ m,\ V) \rightarrow H(p_i, m_i, V_i \quad \text{for all } 1 \le i \le N)$

The resulting Schroedinger Equation for N interacting particles in 3-dimensions is:

$$-\sum_{i=1}^{N}\frac{\hbar^2}{2m_i}\nabla_i^2\psi\left(\vec{r}_1,\vec{r}_2,\ldots,\vec{r}_N\right)+\sum_{i>j}\sum_{j=1}^{N}V\left(r_i,r_j\right)\psi\left(\vec{r}_1,\vec{r}_2,\ldots,\vec{r}_N\right)=i\hbar\frac{\partial}{\partial t}\psi\left(\vec{r}_1,\vec{r}_2,\ldots,\vec{r}_N\right)$$

Outline

I. Angular momentum introduction
II. Angular momentum commutators
III. Representing the L operators and the $|\lambda,m'\rangle$ wavefunctions in r-θ-ϕ space.

I. Angular momentum introduction

1. Why is this important?

Any physical system that has rotational motion has energy associated with that motion. That rotation must somehow be reflected in the Hamiltonian in order to correctly and fully describe the system's energy (which is quantized by it). The rotation is also reflected in the ψ, so the rotational status is input to the system's characteristic as $\psi^{(\text{symmetric})}$ or $\psi^{(\text{antisymmetric})}$. Thus the rotational behavior influences the system's response to the Pauli Exclusion Principle.

2. This gives us a motivation to discuss how to invent a Hamiltonian. Whenever possible, people create quantum mechanical Hamiltonians by writing down the classical Hamiltonian for a system and then calling everything but known constants operators.

How to find the quantum mechanical Hamiltonian for a particle that is orbiting at a constant radius R about a point in 3-dimensions.

$$\vec{L}_{classical} = \vec{r} \times \vec{p}, \text{ so}$$

$$L^2 = (\vec{r} \times \vec{p}) \bullet (\vec{r} \times \vec{p}) = \underbrace{(\vec{r} \cdot \vec{r})}_{R^2} \underbrace{(\vec{p} \cdot \vec{p})}_{p^2} - \underbrace{(\vec{r} \cdot \vec{p})}_{0} \underbrace{(\vec{p} \cdot \vec{r})}_{0} \quad \text{if R is constant, the motion } \vec{\text{p}} \text{ is } \perp \text{ to it.}$$

$$\text{So } L^2 = R^2 p^2, \quad \text{and } p^2 = \frac{L^2}{R^2}$$

Notice: since this particle is compelled to remain at constant distance R, it cannot fall inward, so it has no potential energy, only kinetic energy.

So $H_{classical} = \dfrac{p^2}{2m}$ only

$$= \frac{1}{2m}\frac{L^2}{R^2}$$

Recall moment of interia $I = mR^2$

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

To convert this to a quantum mechanical operator, notice that while I is a constant (like mass), L can be an operator.

So $\mathrm{H}_{QM} = \dfrac{L_{op}^2}{2I}$

To convert $L_{classical} \to L_{op}$, notice

$\vec{L} = \vec{r} \times \vec{p}$ implies $L_x = yp_z - zp_y$

$$L_y = zp_x - xp_z$$

$$L_z = xp_y - yp_x$$

and $L^2 = L_x^2 + L_y^2 + L_z^2$

Replace the p_i by $-i\hbar\dfrac{\partial}{\partial x_i}$ and treat the x_i as operators (so respect the commutation rules).

II. Angular momentum commutation rules

Begin by developing foundational commutators:

$$\left[L_x, z\right] = \left[\left(yp_z - zp_y\right), z\right] = \underbrace{\left[yp_z, z\right]}_{} - \underbrace{\left[zp_y, z\right]}_{}$$

$$= 0 \text{ because } \left[z, z\right] = 0 \text{ and } \left[f(y), z\right] = 0$$

$$yp_z z - zyp_z$$

$$yp_z z - yzp_z$$

$$y\left[p_z, z\right]$$

$$y(-i\hbar)$$

$$\left[L_x, z\right] = -i\hbar y$$

Also:

$$\left[L_x, p_z\right] = \left[\left(yp_z - zp_y\right), p_z\right] = \underbrace{\left[yp_z, p_z\right]}_{} - \underbrace{\left[zp_y, p_z\right]}_{}$$

$$= 0 \text{ because } \left[z, z\right] = 0 \text{ and } \left[f(y), z\right] = 0$$

$$-\left\{zp_y p_z - p_z zp_y\right\}$$

$$-\left\{zp_z p_y - p_z zp_y\right\}$$

$$-\left[z, p_z\right] p_y$$

$$-(i\hbar) p_y$$

$$\left[L_x, p_z\right] = -i\hbar p_y$$

Also $\left[L_x, x\right] = \left[L_x, p_x\right] = 0$

function of y, z only

Use these to find $\left[L_i, L_j\right]$:

$$\left[L_x, L_y\right] = \left[L_x, (zp_x - xp_z)\right] = \left[L_x, zp_x\right] - \left[L_x, xp_z\right]$$

$$= \left\{L_x zp_x - zp_x L_x\right\} - \left\{L_x xp_z - xp_z L_x\right\}$$

$$= \underbrace{\left[L_x, z\right]} p_x - x \underbrace{\left[L_x, p_z\right]}$$

$$= (-i\hbar y)\, p_x - x\left(-i\hbar p_y\right)$$

$$= -i\hbar\left(yp_x - xp_y\right)$$

$$\left[L_x, L_y\right] = \text{-}i\hbar L_z$$

Similarly,

$$\left.\begin{aligned}\left[L_y, L_z\right] &= \text{-}i\hbar L_x \\ \left[L_z, L_x\right] &= \text{-}i\hbar L_y\end{aligned}\right\} \text{ we get these by permuting } x \to y \to z \to x$$

Recall that if 2 operators have a nonzero commutator, they cannot be measured simultaneously. They have an uncertainty relation that shows how measurement of one compromises measurement of the other:

$$\Delta A \Delta B \geq \frac{\left|\left\langle [A,B] \right\rangle\right|}{2i}$$

The L commutators indicate that we cannot simultaneously know all 3 components of a particle's angular momentum. For example,

$$\Delta L_x \Delta L_y \geq \frac{\left|\left\langle \left[L_x, L_y \right] \right\rangle\right|}{2i} = \frac{\left|\left\langle \left[L_x, L_y \right] \right\rangle\right|}{2i} = \frac{\left\langle \left| i\hbar L_z \right| \right\rangle}{2i} = \frac{\hbar}{2}\left\langle L_z \right\rangle$$

and similarly for $x \to y \to z \to x$

Now consider $L^2 = L_x^2 + L_y^2 + L_z^2$

$$\left[L^2, L_z\right] = \left[\left(L_x^2 + L_y^2 + L_z^2\right), L_z\right]$$

$$= \left[L_x^2, L_z\right] + \left[L_y^2, L_z\right] + \underbrace{\left[L_z^2, L_z\right]}_{\downarrow \atop 0}$$

$$= L_x L_x L_z - \underbrace{L_z L_x}_{\downarrow \atop i\hbar L_y + L_x L_z} L_x + L_y L_y L_z - \underbrace{L_z L_y}_{\downarrow \atop L_y L_z - i\hbar L_x} L_y$$

$$= \underbrace{L_x L_x L_z} - i\hbar L_y L_x \underbrace{- L_x L_z L_x} + \underbrace{L_y L_y L_z - L_y L_z L_y} + i\hbar L_x L_y$$

$$L_x\left[L_x, L_z\right] \qquad\qquad L_y\left[L_y, L_z\right]$$

$$L_x\left(-i\hbar L_y\right) \qquad\qquad L_y\left(i\hbar L_x\right)$$

$$= -i\hbar L_x L_y - i\hbar L_y L_x + i\hbar L_y L_x + i\hbar L_x L_y = 0$$

Similarly, $\left[L^2, L_x\right] = \left[L^2, L_y\right] = 0$

Conclusions about this:

1) We cannot simultaneously know L_x, L_y, and L_z, but we CAN simultaneously know L^2 (but not L) and any one of the L_i.

2) The convention is to choose (or define) the L_i that we measure simultaneously as L^2 and L_z.

3) Recall that operators that commute have simultaneous eigenvectors.
Label the eigenvectors $|\lambda m'\rangle$ where
λ is the eigenvalue of L^2 : $\qquad L^2|\lambda m'\rangle = \lambda|\lambda m'\rangle$
and m' is the eigenvalue of L_z : $\qquad L_z|\lambda m'\rangle = m'|\lambda m'\rangle$

III. Representing the L operators and $|\lambda m'\rangle$ in r-θ-ϕ space

Notice $|\lambda m'\rangle$ is a Hilbert space ket that describes an object with L^2 eigenvalue λ and L_z eigenvalue m'.

Project it into coordinate space: $\langle \text{x-space}|\lambda m'\rangle$

and choose r-θ-ϕ (that is, spherical) coordinates: $\langle \theta\phi|\lambda m'\rangle$

No "r" is needed because angular momentum concerns angular motion without change in radius.

Plan for this section:

(i) Find $\vec{L}(r,\ \theta,\ \phi)$

(ii) Find $L_z(r,\ \theta,\ \phi) = \vec{L}\cdot\hat{z}$

(iii) Find $L^2(r,\ \theta,\ \phi) = \vec{L}\cdot\vec{L}$

(iv) Substitute in $L_z\langle \theta\phi|\lambda m'\rangle = m'\langle \theta\phi|\lambda m'\rangle$ to get

(a) restrictions on m' and λ

(b) the form of $\langle \theta\phi|\lambda m'\rangle$

Carry out the plan:

(i) Find $\vec{L}(r,\ \theta,\ \phi)$

$$\vec{L} = \vec{r} \times \vec{p} = \vec{r} \times \left(-i\hbar\vec{\nabla}\right)$$

Recall $\vec{r} = r\hat{r}$

$$\vec{\nabla} = \hat{r}\frac{\partial}{\partial r} + \hat{\theta}\frac{1}{r}\frac{\partial}{\partial \theta} + \hat{\phi}\frac{1}{r\sin\theta}\frac{\partial}{\partial \phi}$$

So $\vec{L} = -i\hbar r\hat{r} \times \left[\hat{r}\frac{\partial}{\partial r} + \hat{\theta}\frac{1}{r}\frac{\partial}{\partial \theta} + \hat{\phi}\frac{1}{r\sin\theta}\frac{\partial}{\partial \phi}\right]$

$$= -i\hbar r\left\{\underbrace{\hat{r}\times\hat{r}}_{0}\frac{\partial}{\partial r} + \underbrace{\hat{r}\times\hat{\theta}}_{\hat{\phi}}\frac{1}{r}\frac{\partial}{\partial \theta} + \underbrace{\hat{r}\times\hat{\phi}}_{-\hat{\theta}}\frac{1}{r\sin\theta}\frac{\partial}{\partial \phi}\right\}$$

$$\vec{L} = -i\hbar\left\{\hat{\phi}\frac{\partial}{\partial \theta} - \hat{\theta}\frac{1}{\sin\theta}\frac{\partial}{\partial \phi}\right\}$$

(ii) Find $L_z = \vec{L}\cdot\hat{z}$ Recall $\hat{z} = \hat{r}\cos\theta - \hat{\theta}\sin\theta$

So $L_z = \left[\hat{r}\cos\theta - \hat{\theta}\sin\theta\right]\cdot\left(-i\hbar\right)\left[\hat{\phi}\frac{\partial}{\partial \theta} - \hat{\theta}\frac{1}{\sin\theta}\frac{\partial}{\partial \phi}\right]$

$$= -i\hbar\left\{\underbrace{\hat{r}\cdot\hat{\phi}}_{0}\cos\theta\frac{\partial}{\partial \theta} - \underbrace{\hat{\theta}\cdot\hat{\phi}}_{0}\sin\theta\frac{\partial}{\partial \theta} - \underbrace{\hat{r}\cdot\hat{\theta}}_{0}\frac{\cos\theta}{\sin\theta}\frac{\partial}{\partial \phi} + \underbrace{\hat{\theta}\cdot\hat{\theta}}_{1}\frac{\sin\theta}{\sin\theta}\frac{\partial}{\partial \phi}\right\} = -i\hbar\frac{\partial}{\partial \phi}$$

(iii) Find $L^2 = \vec{L}\cdot\vec{L}$

$$= \left(-i\hbar\right)\left[\hat{\phi}\frac{\partial}{\partial\theta} - \hat{\theta}\frac{1}{\sin\theta}\frac{\partial}{\partial\phi}\right]\cdot\left(-i\hbar\right)\left[\hat{\phi}\frac{\partial}{\partial\theta} - \hat{\theta}\frac{1}{\sin\theta}\frac{\partial}{\partial\phi}\right]$$

$$= -\hbar^2\left\{\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right\}$$

(iv.a) Find restrictions that these forms impose upon m':

Begin with $L_z\left|\lambda m'\right\rangle = m'\left|\lambda m'\right\rangle$. Apply $\left\langle\theta\phi\right|$ to both sides:

$$\left\langle\theta\phi\right|L_z\left|\lambda m'\right\rangle = \left\langle\theta\phi\right|m'\left|\lambda m'\right\rangle$$

Let L_z act to the left. Move scalar m' outside the integral.

$$-i\hbar\frac{\partial}{\partial\phi}\left\langle\theta\phi|\lambda m'\right\rangle = m'\left\langle\theta\phi|\lambda m'\right\rangle$$

$$\frac{\partial}{\partial\phi}\left\langle\theta\phi|\lambda m'\right\rangle = \frac{im'}{\hbar}\left\langle\theta\phi|\lambda m'\right\rangle$$ Integrate:

$$\left\langle\theta\phi|\lambda m'\right\rangle = f(\theta)\cdot e^{\frac{im'\phi}{\hbar}}$$ We don't yet know what $f(\theta)$ is. Call it "$P(\theta)$".

Notice that $\left\langle\theta\phi|\lambda m'\right\rangle$ is a wavefunction. (We could call it "$\Psi_{\lambda m'}\left(\theta,\phi\right)$".)

Like all quantum mechanically meaningful wavefunctions it must have the properties:

	Does f(q) meet these?	**Does the j portion meet these?**
(i) continuous	We will force this	yes
(ii) square-integrable	We will force this	yes
(iii) single-valued	We will force this	*

* only if we insist that $\langle \theta\phi + 2\pi | \lambda m' \rangle = \langle \theta\phi | \lambda m' \rangle$:

$$e^{\frac{im'(\phi+2\pi)}{\hbar}} = e^{\frac{im'\phi}{\hbar}} = \cos\frac{m'\phi}{\hbar} + i\sin\frac{m'\phi}{\hbar}$$

This works if $\dfrac{m'}{\hbar} = ...-3,-2,-1,0,1,2,3,...$

So $m' = m\hbar$ where $m = -3,-2,-1,0,1,2,3,...$

This is the restriction on what m' can be.

Then,

(1) $L_z |\lambda m'\rangle = m\hbar |\lambda m'\rangle$. We now rename this ket as $|\lambda m\rangle$ because either m or m' uniquely specify the state.

(2) $\langle \theta\phi | \lambda m \rangle = e^{im\hbar\phi/\hbar} P(\theta) = e^{im\phi} P(\theta)$.

(iv.b) Now find f(θ) to get the full $\langle \theta\phi | \lambda m \rangle$

Do this by demanding that $P(\theta)$ produces a $\langle \theta\phi | \lambda m \rangle$ that satisfies the original eigenvalue equation that defined the $|\lambda m\rangle$:

$$L^2 |\lambda m\rangle = \lambda |\lambda m\rangle$$

$$\langle \theta\phi | L^2 |\lambda m\rangle = \lambda \langle \theta\phi | \lambda m\rangle$$

Substitute: (i) $\langle \theta\phi | L^2 = -\hbar^2 \left\{ \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2} \right\} \langle \theta\phi |$

(ii) $\langle \theta\phi | \lambda m\rangle = e^{im\phi}P(\theta)$

$$-\hbar^2 \left\{ \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2} \right\} e^{im\phi}P(\theta) = \lambda e^{im\phi}P(\theta)$$

$$-\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)e^{im\phi}P(\theta) - \frac{1}{\sin^2\theta}\underbrace{\frac{\partial^2 e^{im\phi}}{\partial\phi^2}}_{\downarrow}P(\theta) = \frac{\lambda}{\hbar}e^{im\phi}P(\theta)$$

$$\text{-}\, m^2 e^{im\phi}$$

$$-\frac{e^{im\phi}}{\sin\theta}\frac{\partial}{\partial\theta}\left\{\sin\theta\frac{\partial P(\theta)}{\partial\theta}\right\} + \frac{m^2 e^{im\phi}}{\sin^2\theta}P(\theta) = \frac{\lambda}{\hbar}e^{im\phi}P(\theta).$$

Cancel all the $e^{im\phi}$'s

Define $\zeta \equiv \cos\theta$

then $\sin^2\theta = 1-\zeta^2$

and $\dfrac{\partial}{\partial\theta} = \dfrac{\partial\zeta}{\partial\theta}\dfrac{\partial}{\partial\zeta} = -\sin\theta\dfrac{\partial}{\partial\zeta}$

so $\dfrac{1}{\sin\theta}\dfrac{\partial}{\partial\theta} = -\dfrac{\partial}{\partial\zeta}$

For consistency, rename $\mathrm{P}(\theta) \to P(\zeta)$.

Make all these substitutions to get:

$$\frac{\partial}{\partial\zeta}\left\{\underbrace{\sin\theta\sin\theta}_{\substack{\downarrow \\ 1-\zeta^2}}\underbrace{\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}}_{\substack{\downarrow \\ -\frac{\partial}{\partial\zeta}}}P(\zeta)\right\} + \frac{m^2}{1-\zeta^2}P(\zeta) = \frac{\lambda}{\hbar^2}P(\zeta)$$

$$\frac{\partial}{\partial\zeta}\left(1-\zeta^2\right)\left(-\frac{\partial}{\partial\zeta}\right)P(\zeta) + \frac{m^2}{1-\zeta^2}P(\zeta) = \frac{\lambda}{\hbar^2}P(\zeta)$$

$$0 = \frac{\partial}{\partial\zeta}\left(1-\zeta^2\right)\frac{\partial}{\partial\zeta}P(\zeta) + \left[\frac{\lambda}{\hbar^2} - \frac{m^2}{1-\zeta^2}\right]P(\zeta) \qquad \text{Eq. 1}$$

This is solved by

$$P^m(\zeta) = \left(1-\zeta^2\right)^{m/2} \frac{d^m}{d\zeta^m} P_\ell(\zeta)$$

Associated Legendre function

$$P_\ell(\zeta) \equiv \frac{1}{2^\ell \ell!} \frac{d^\ell}{d\zeta^\ell} \left(\zeta^2 - 1\right)^\ell$$

Rewrite this as

$$P_\ell^m(\zeta) = \frac{1}{2^\ell \ell!} \left(1-\zeta^2\right)^{m/2} \frac{d^{\ell+m}}{d\zeta^{\ell+m}} \left(\zeta^2 - 1\right)^\ell$$

Notice: because of the form of this derivative, $P_\ell^m = 0$ unless $\ell \geq |m|$

Facts about the P_ℓ^m :

(i) They are orthogonal if they have the same m:

$$\int_{-1}^{+1} P_\ell^m(\zeta) P_{\ell'}^m(\zeta) d\zeta = \delta_{\ell\ell'}$$

(ii) Normalization:

$$\int_{-1}^{+1} d\zeta \left|P_\ell^m\right|^2 = \frac{2}{2\ell+1}\frac{(\ell+m)!}{(l-m)!}$$

(iii) Alternative form:

$$P_\ell^m(\zeta) = \frac{(-1)^m}{2^\ell}\frac{(\ell+m)!}{\ell!(l-m)!}\left(1\text{-}\zeta^2\right)^{-m/2}\frac{d^{\ell-m}}{d\zeta^{\ell-m}}\left(\zeta^2-1\right)^\ell$$

(iv) They imply a surprising quantization condition. Consider the case where $m = 0$. Then the equation they solve becomes

$$\frac{\partial}{\partial\zeta}\left(1\text{-}\zeta^2\right)\frac{\partial}{\partial\zeta}P(\zeta) + \left[\frac{\lambda}{\hbar^2}\right]P(\zeta) = 0$$

Suppose that we did not have the $\mathrm{P}(\zeta)$ and wanted to solve this equation with the series technique. We could guess:

$$P(\zeta) = \sum_{n=0}^{\infty} c_n \zeta^n$$

Then $\dfrac{dP}{d\zeta} = \sum_{n=1}^{\infty} n c_n \zeta^{n-1}$

$$\left(1-\zeta^2\right)\frac{dP}{d\zeta} = \sum_{n=1}^{\infty} n c_n \zeta^{n-1} - \sum_{n=1}^{\infty} n c_n \zeta^{n+1}$$

$$\frac{d}{d\zeta}\left(1-\zeta^2\right)\frac{dP}{d\zeta} = \sum_{n=2}^{\infty} n(n-1) c_n \zeta^{n-2} - \sum_{n=1}^{\infty} n(n+1) c_n \zeta^{n}$$

Substitute these back in:

$$\sum_{n=2}^{\infty} n(n-1) c_n \zeta^{n-2} - \sum_{n=1}^{\infty} n(n+1) c_n \zeta^{n} + \frac{\lambda}{\hbar^2}\sum_{n=0}^{\infty} c_n \zeta^n = 0$$

Collect terms with like powers of ζ:

$$\zeta^0: \quad 2\cdot 1\cdot c_2 \qquad\qquad + \frac{\lambda}{\hbar^2} c_0 = 0$$

$$\zeta^1: \quad 3\cdot 2\cdot c_3 - 1\cdot 2\cdot c_1 + \frac{\lambda}{\hbar^2} c_1 = 0$$

$$\zeta^2: \quad 4\cdot 3\cdot c_4 - 2\cdot 3\cdot c_2 + \frac{\lambda}{\hbar^2} c_2 = 0$$

...

$$\zeta^n: \quad (n+2)(n+1) c_{n+2} - \left\{ n(n+1) - \frac{\lambda}{\hbar^2} \right\} c_n = 0$$

This implies the recursion relation:

$$c_{n+2} = \frac{\left(n(n+1) - \dfrac{\lambda}{\hbar^2}\right)}{(n+2)(n+1)} c_n$$

As n $\to \infty$, this P(ζ) series $\propto \zeta^n$, so it diverges. Force it to truncate at some $n = \ell$ as follows. Notice that since n $\in \{0,1,2,...\}$ by definition of the P$_\ell$ series, then also $\ell \in \{0,1,2,...\}$. So λ must be (integer)$\cdot \hbar^2$.

(1) Set $\lambda = \ell(\ell+1)\hbar^2$.

Then $$c_{\ell+2} = \frac{\left(\ell(\ell+1) - \dfrac{\ell(\ell+1)\hbar^2}{\hbar^2}\right)}{(\ell+2)(\ell+1)} c_\ell = 0$$

(2) If ℓ is odd, set $c_0 = 0$; if ℓ is even, set $c_1 = 0$

(3) Because $\lambda \sim \ell$, relabel $|\lambda m\rangle \to |\ell m\rangle$

Summarize all the restrictions on m' and λ:

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

(ii) $L_z |\ell m\rangle = m\hbar |\ell m\rangle$, where $m = 0,\ \pm 1,\ \pm 2,\ ..., \pm \ell$

Outline

I. Graphical representation of angular momentum
II. Spherical harmonics
III. The rigid rotator
IV. Generalized angular momentum

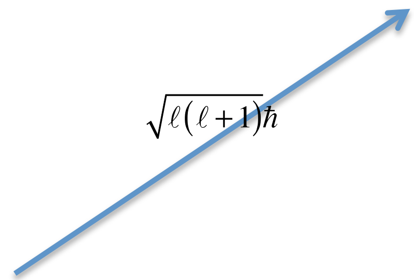
I. Graphical representation of angular momentum

Represent $\vec{\text{L}}$ as a vector (using the arrow)

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

$|L| = \sqrt{\ell(\ell+1)}\hbar$

Draw a vector of length $\sqrt{\ell(\ell+1)}\hbar$:

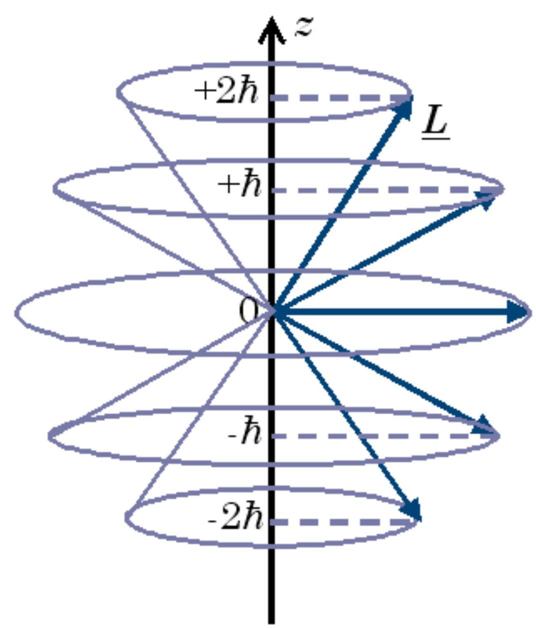


$\vec{L}$ has a limited number of orientations permitted to it relative to the z-axis: $L_z = m\hbar$, where $|m| \le \ell$.

Example:

if $\ell = 2$, then $L_z = 2\hbar,\ 1\hbar,\ 0\hbar,\ -1\hbar,\ -2\hbar$

but $L = \sqrt{2(2+1)}\hbar = 2.45\hbar$



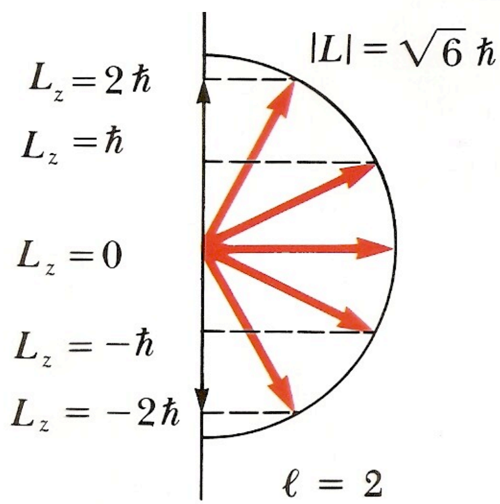
Notice:

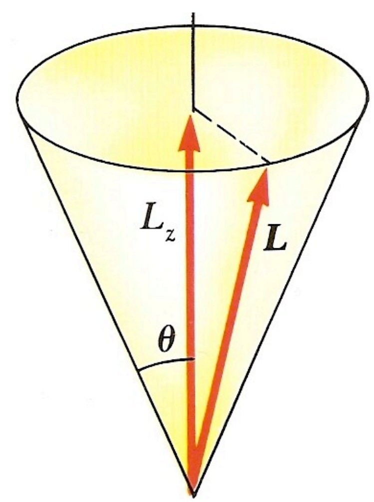
(i) The length of L is quantized

(ii) The direction of L is quantized. It behaves as if it must "fit" into specific "slots" in space relative to the z-axis. There are $2\ell+1$ slots available.

(iii) L can never align exactly with the z-axis: $m\hbar < \sqrt{\ell(\ell+1)}\hbar$. So L_x or L_y is always nonzero.

(iv) Only 1 component is quantized. We choose to call it L_z. L_x and L_y can take any values consistent with the requirement that $L_x^2 + L_y^2 + L_z^2 = L^2$.





II. Spherical harmonics

Recall we found that $\langle \theta\phi | \lambda m \rangle \sim P_\ell^m(\cos\theta)\cdot\exp(im\phi)$. Insert the normalization term N_ℓ^m. Then

$\langle \theta\phi | \lambda m \rangle = N_\ell^m P_\ell^m(\cos\theta)\cdot\exp(im\phi)$

Facts about the $\langle \theta\phi | \lambda m \rangle$:

(i) These are the simultaneous eigenfunctions of L^2 and L_z.

(ii) They are a family of mathematical functions called "spherical harmonics."

(iii) Alternative symbol: $Y_{\ell m}(\theta,\phi) = \langle \theta\phi | \lambda m \rangle$

(iv) Normalization:

for $m \geq 0$, $N_\ell^m = \left[\dfrac{2\ell+1}{4\pi} \dfrac{(\ell-m)!}{(\ell+m)!} \right]^{1/2} (-1)^m$

for $m < 0$ $Y_{\ell m} = (-1)^m Y^*_{\ell,-m}$

negative

(v) $\displaystyle\sum_{m=-\ell}^{+\ell} |Y_{\ell m}|^2 = \frac{2\ell+1}{4\pi}$

(vi) Parity:

Recall the parity operation reflects every coordinate through the origin. In rectangular coordinates, that means

$$x \to -x,\ y \to -y,\ z \to -z.$$ Notice this is not really the same as mirroring.

In spherical coordinates:

$$r \to -r$$
$$\theta \to \pi - \theta$$
$$\phi \to \pi + \phi$$

Recall $Y_{\ell m}(\theta,\phi) \sim e^{im\phi}\left(1-\cos^2\theta\right)^{-m/2} \dfrac{d^{\ell-m}}{d\cos\theta^{\ell-m}}\left(\cos^2\theta - 1\right)^{\ell}$

So $Y_{\ell m}(\pi-\theta,\pi+\phi) = \underbrace{e^{im(\pi+\phi)}}\left(1-\underbrace{\cos^2(\pi-\theta)}\right)^{-m/2} \underbrace{\dfrac{d^{\ell-m}}{d\cos(\pi-\theta)^{\ell-m}}}\left(\underbrace{\cos^2(\pi-\theta)}-1\right)^{\ell}$

$$e^{im\pi}e^{im\phi} = \overbrace{(-1)^m e^{im\phi}} \qquad \cos^2\theta \qquad \underbrace{\frac{d^{\ell-m}}{d\cos(-\theta)^{\ell-m}}\left(\overbrace{\cos^2\theta}-1\right)^{\ell}}$$

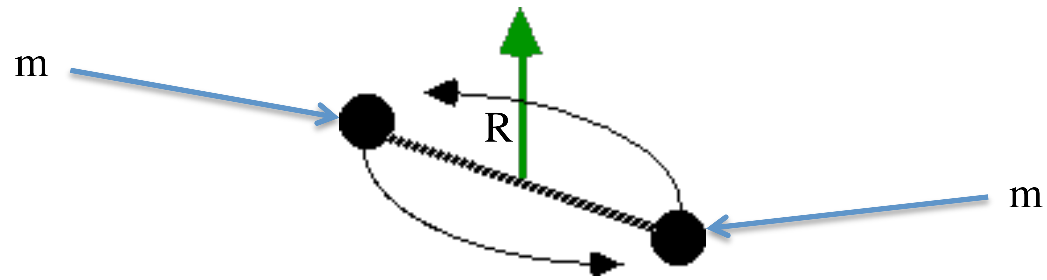
$$(-1)^{\ell-m}\left(\cos^2\theta-1\right)^{\ell}$$

$$Y_{\ell m}(\pi-\theta,\pi+\phi) = (-1)^m\ (-1)^{\ell-m}\ e^{im\phi}\ \mathrm{P}_{\ell}^{m} = (-1)^{\ell}\, Y_{\ell m}$$

Conclusion: $PY_{\ell m} = (-1)^{\ell} Y_{\ell m}$.....an eigenvalue equation.

The $Y_{\ell m}$'s are simultaneous eigenfunctions of Parity and L^2. We expect to find that $\left[P, L^2\right] = 0$.

III. An example use of L^2 in quantum mechanics: the rigidly rotating molecule



Recall $H = \dfrac{L^2}{2I}$

$H|\psi\rangle = E|\psi\rangle$

$\dfrac{L^2}{2I}|\psi\rangle = E|\psi\rangle$ Since we know that the eigenfunctions of L^2 are the $|\ell m\rangle$, replace $|\psi\rangle \to |\ell m\rangle$

$E = \dfrac{1}{2I}\langle \ell m|L^2|\ell m\rangle$

$E_\ell = \dfrac{1}{2I}\ell(\ell+1)\hbar^2$

Recall each ℓ-type level has $2\ell+1$ m-type sublevels.

All $2\ell+1$ of them have the same energy: $\dfrac{1}{2I}\ell(\ell+1)\hbar^2$. This is a degeneracy.

If we observe the spectrum of a molecular substance and find that the spectral lines are separated by a pattern involving whole numbers ℓ like this, we know that the molecules have rotational excitation (as distinguished from, for example, vibrational excitation, which would give a pattern of lines separated by $\hbar\omega\left(n+\dfrac{1}{2}\right)$.

IV. Generalized angular momentum

Recall we have operators L_x, L_y, and L_z whose action on a wavefunction represents the act of measuring the states' angular momentum components.
Generalize these to include the possibility of other forms (that is, spin) of angular momentum.

The generalized angular momentum operators are called
J_x, J_y, and J_z

Later we will see that J and L are related by $\vec{J} = \vec{L} + \vec{S}$

Because the J's are generalized versions of the L's we can include in their definition the following:

(1) $\left[J_x, J_y\right] = i\hbar J_z$ and $x \to y \to z \to x$

(2) $J^2 = J_x^2 + J_y^2 + J_z^2$

(3) Because of relations (1) and (2), it will turn out that $\left[J^2, J_i\right] = 0$ (we will focus on $i = z$).

Then J^2 and J_z have simultaneous eigenfunctions.

Call these $\left|\lambda_J m_J'\right\rangle$, NOT NECESSARILY the same as $\left|\ell m\right\rangle$

So $J^2\left|\lambda_J m_J'\right\rangle = \lambda_J\left|\lambda_J m_J'\right\rangle$

and $J_z\left|\lambda_J m_J'\right\rangle = m_J'\left|\lambda_J m_J'\right\rangle$

We don't yet say what $m_J\,'$ is. Especially, we do not yet see whether it is an integer. However divide $\hbar$ out of it to define a related number:

Let $m_J\,' \equiv m_J \hbar$ where m_J is unknown, not necessarily integer

Then we can rename $\left|\lambda_J m_J\,'\right\rangle \rightarrow \left|\lambda_J m_J\right\rangle$

Question: What are λ_J, m_J, and $\left|\lambda_J m_J\right\rangle$?

*Why we CANNOT find them in the way we found λ, m, and so forth for the L operators: When we were examining the L's we found λ, m', and $\left|\lambda m'\right\rangle$ by guessing that the form of L_{op} mimics the form of $\vec{L}_{classical} = \vec{r} \times \vec{p}$. Then we substituted $L_{op}(r,p) = L(\theta,\phi)$ and solved the equation $L^2\left|\ \right\rangle = \lambda\left|\ \right\rangle$. Here J is an operator which we define ONLY on the basis of having commutation relations similar to those of the L's. We have NOT said "$J = r \times p$".

So we cannot get $J(\theta,\phi)$. We only know the J's in the Hilbert space of $\left|\lambda_J m_J\right\rangle$, not in $\left\langle \theta\phi \middle| \lambda_J m_J\right\rangle$. To find λ_J, m_J, and $\left|\lambda_J m_J\right\rangle$, we need to define ladder operators for the states of J.

Outline

I. Angular momentum ladder operators
II. Finding m_J and λ_J
III. Normalizing the $|\lambda_J m_J\rangle$
IV. L_z is the generator of rotations
V. Conservation of angular momentum in quantum mechanics

I. Angular momentum ladder operators

Define $J_+ \equiv J_x + iJ_y$ and

$$J_- \equiv J_x - iJ_y$$

To demonstrate that these are raising and lowering operators, we will need to use their commutators. Work out the commutators here:

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

BY DEFINITION of the J's

$$= \hbar(iJ_y + J_x)$$

$$[J_z, J_+] = \hbar J_+$$

Similarly,

$$[J_z, J_-] = -\hbar J_-$$

$$[J_+, J_-] = 2\hbar J_z$$

Also notice $J_+J_- = (J_x + iJ_y)(J_x - iJ_y) = \underbrace{J_x^2 + J_y^2}_{J^2 - J_z^2} + i\underbrace{(J_yJ_x - J_xJ_y)}_{-i\hbar J_z}$

Thus $J_+J_- = J^2 - J_z^2 + \hbar J_z$

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

Now show that J_+ and J_- are ladder operators:

Consider $J_z J_+ \left|\lambda_J m_J\right\rangle$

$$\text{Recall } \left[J_z, J_+\right] = \hbar J_+, \text{ so}$$

$$J_z J_+ - J_+ J_z = \hbar J_+$$

$$\text{So } J_z J_+ = J_+ J_z + \hbar J_+ = J_+\left(J_z + \hbar\right). \text{ Use this:}$$

$$\begin{aligned} J_z J_+ \left|\lambda_J m_J\right\rangle &= J_+\left(J_z + \hbar\right)\left|\lambda_J m_J\right\rangle \\ &= J_+\left\{J_z\left|\lambda_J m_J\right\rangle + \hbar\left|\lambda_J m_J\right\rangle\right\} \\ &= J_+\left\{m_J\hbar\left|\lambda_J m_J\right\rangle + \hbar\left|\lambda_J m_J\right\rangle\right\} \\ &= \left(m_J + 1\right)\hbar J_+\left|\lambda_J m_J\right\rangle \end{aligned}$$

We interpret this to mean that J_+ acting on $\left|\lambda_J m_J\right\rangle$ raises the m_J level by 1 (to $m_J + 1$). This is evident when J_z acts on the result. The definition of J_z is "the operator that extracts the m-eigenvalue," and we see that J_z extracts eigenvalue $m_J + 1$. So J_+ is a raising operator which raises the eigenvalue of J_z by $1\hbar$.

Similarly,

$J_z J_- \left|\lambda_J m_J\right\rangle = \left(m_J - 1\right)\hbar J_+ \left|\lambda_J m_J\right\rangle$, so J_- is a lowering operator which lowers the eigenvalue of J_z by $1\hbar$.

Notice that J_+ and J_- have no effect upon λ, which is the eigenvalue of J^2.

This allows us to predict that $\left[J^2, J_+\right] = 0$. Check it---it is true.

Summarizing:

$$J_+ \left|\lambda_J, m_J\right\rangle = c_{\lambda_J m_J} \left|\lambda_J, m_J + 1\right\rangle$$

$$J_- \left|\lambda_J, m_J\right\rangle = d_{\lambda_J m_J} \left|\lambda_J, m_J - 1\right\rangle$$

These normalizations ($c_{\lambda_J m_J}$, $d_{\lambda_J m_J}$) have not yet been specified.

Note, if we are working on a problem in which we are explicitly considering $J = L$ (that is, we know that spin is not involved), then we can call these operators L_+ and L_-.

II. Finding m_J and λ_J

First we show that m is bounded. That means, there exists an $m_{J_{MAX}} < \infty$ and an $m_{J_{MIN}} < -\infty$.

To see this, note

the length of a component is $\leq$ the length of its vector:

$$|L_z| \leq |L|$$

$$\text{eigenvalue } m\hbar \leq \text{eigenvalue } \sqrt{\lambda}$$

To find $\mathrm{m}_{J_{MAX}}$:

By definition of "max," there can be no state with higher m than $m_{\max}$. To enforce this, insist that J_+ cannot raise a state with $\left|\lambda_J, m_{J_{MAX}}\right\rangle$ higher. Demand

$$J_+\left|\lambda_J, m_{J_{MAX}}\right\rangle = 0.$$

Apply J_- to both sides:

$$\underbrace{J_- J_+}\left|\lambda_J, m_{J_{MAX}}\right\rangle = J_- 0 = 0$$

$$\overbrace{\left(J^2 - J_z^2 - \hbar J_z\right)}\left|\lambda_J, m_{J_{MAX}}\right\rangle = 0$$

$$\lambda_J - m_{J_{MAX}}^2\hbar^2 - \hbar\left(m_{J_{MAX}}\hbar\right)\left|\lambda_J, m_{J_{MAX}}\right\rangle = 0$$

$$\lambda_J - m_{J_{MAX}}\left(m_{J_{MAX}} + 1\right)\hbar^2 = 0 \qquad \text{"Eq. 1"}$$

Similarly begin with $J_{-}\left|\lambda_J, m_{J_{MIN}}\right\rangle = 0.$

Apply J_{+} to both sides to get

$\lambda_J - m_{J_{MIN}}\left(m_{J_{MIN}} - 1\right)\hbar^2 = 0$ "Eq. 2"

Eliminate λ_J from Eq. 1 and Eq 2. to get

$$m_{J_{MAX}}\left(m_{J_{MAX}} + 1\right)\hbar^2 = m_{J_{MIN}}\left(m_{J_{MIN}} - 1\right)\hbar^2$$

This has 2 solutions:

$m_{J_{MIN}} = \left(m_{J_{MAX}} + 1\right)$ and $m_{J_{MIN}} = -m_{J_{MAX}}$

Impossible by the definitions of $m_{J_{MIN}}$ and $m_{J_{MAX}}$.

So this is the only solution.
Name $m_{J_{MIN}} = "-j"$.
Then $m_{J_{MAX}} = +j$

Now substitute $m_{J_{MAX}} = j$ into Eq. 1 to get

$$\lambda_J = j\left(j+1\right)\hbar^2$$

What values can j take?

Note that if we begin at level $m_{J_{MIN}}$, we can arrive at $m_{J_{MAX}}$ by applying J_z some number of times.

So $m_{J_{MAX}} - m_{J_{MIN}} =$ integer (or 0)

j - (- j) = integer

$2j$ = integer

$j = \dfrac{\text{integer}}{2}$ Not like the ℓ from L!

We will see that J concerns spin "S" (when it is half-integer) and orbital angular momentum "L" (when it is whole-integer).

III. Normalizing the $\left|\lambda_J, m_J\right\rangle$

First, since λ=λ(j), we can rename the states $\left|j, m_J\right\rangle$

Then to be clear we should call the eigenvectors of L^2 the $\left|\ell, m_\ell\right\rangle$

Note subscript

We want to find $c_{\lambda_J m_J} \equiv c_{jm}$ which is defined through $J_+\left|\lambda_J, m_J\right\rangle = c_{\lambda_J m_J}\left|\lambda_J, m_J+1\right\rangle$

and $d_{\lambda_J m_J} \equiv d_{jm}$ which is defined through $J_-\left|\lambda_J, m_J\right\rangle = d_{\lambda_J m_J}\left|\lambda_J, m_J-1\right\rangle$

To get c_{jm} : Find $\langle jm|J_- J_+|jm\rangle = \langle jm|J^2 - J_z^2 - \hbar J_z|jm\rangle$ Note $J_- = J_+^\dagger$.

$\langle jm|J_+^\dagger J_+|jm\rangle = \langle jm|J^2 - J_z^2 - \hbar J_z|jm\rangle$ Apply $J_+^\dagger$ to the left, all other operators to the right.

$\left\langle J_+^\dagger jm\middle|J_+ jm\right\rangle = \langle jm|J^2 - J_z^2 - \hbar J_z|jm\rangle$

$\left\langle c_{Jm}^* j, m+1\middle|c_{Jm} j, m\_1\right\rangle = \langle jm|j(j+1)\hbar^2 - m_J^2\hbar^2 - \hbar m_J\hbar|jm\rangle$

$$|c_{Jm}|^2 \underbrace{\langle j, m+1|j, m\_1\rangle}_{\text{Require }=1} = j(j+1)\hbar^2 - m_J^2\hbar^2 - \hbar m_J\hbar \underbrace{\langle jm|jm\rangle}_{\text{Require }=1}$$

$|c_{Jm}|^2 = \left[j(j+1) - m_J^2 - m_J\right]\hbar^2$

So $c_{Jm} = \hbar\sqrt{j(j+1) - m_J(m_J+1)}$

Similarly, $d_{Jm} = \hbar\sqrt{j(j+1) - m_J(m_J-1)}$

IV. L_z is the generator of rotations in space

Recall that:

(i) $p = -i\hbar \frac{\partial}{\partial x}$ is the generator of translations in space: $f(x+x_0) = e^{ipx_0/\hbar} f(x)$

(ii) $H = +i\hbar \frac{\partial}{\partial t}$ is the generator of translations in time: $\psi(t+t_0) = e^{-iHt_0/\hbar}\psi(t)$

Now show that L_z is the generator of rotations:

Consider $f(\phi+\phi_0)$. Expand in a Taylor Series for small ϕ_0 :

$$f(\phi+\phi_0) = \sum_{n=0}^{\infty} \frac{1}{n!}\phi_0^n \frac{\partial^n f(\phi)}{\partial \phi^n}$$

But $L_z = -i\hbar \frac{\partial}{\partial \phi}$, so $\frac{\partial}{\partial \phi} = \frac{i}{\hbar} L_z$

$$= \underbrace{\sum_{n=0}^{\infty} \frac{1}{n!}\phi_0^n \left(\frac{i}{\hbar}\right)^n (L_z)^n}\, f(\phi)$$

This is the exponential series.

$$f(\phi+\phi_0) = e^{iL_z\phi_0/\hbar} f(\phi)$$

V. Conservation of angular momentum in quantum mechanics

Recall we showed that for any Hermitian operator Q,

$$\frac{d\langle Q\rangle}{dt} = \frac{i}{\hbar}\langle [H,Q]\rangle + \left\langle \frac{\partial Q}{\partial t}\right\rangle$$

So if $Q \neq Q(t)$, Q is conserved if $[H,Q]=0$.

$L_i \neq L_i(t)$.

Evaluate $[H,L_i]$ for $V = V(r = r_1 - r_2)$

$$[H,L_x] = \left[\left(\frac{p^2}{2m} + V(r)\right), L_x\right]$$

$$= \frac{1}{2m}[p^2, L_x] + [V(r), L_x]$$

$$= \frac{1}{2m}\{[p_x^2, L_x] + [p_y^2, L_x] + [p_z^2, L_x]\} + [V(r), L_x]$$

Recall that for any commutator involving products, $[AB,C] = ABC - CAB$

Add to the righthand side: $0 = -ACB + ACB$

$[AB,C] = ABC - ACB + ACB - CAB$

$[AB,C] = A[B,C] + [A,C]B$

$$[H,L_x] = \frac{1}{2m}\{p_x[p_x,L_x] + [p_x,L_x]p_x + p_y[p_y,L_x] + [p_y,L_x]p_y + p_z[p_z,L_x] + [p_z,L_x]p_z\} + [V(r),L_x]$$

$$[H,L_x]=\frac{1}{2m}\left\{p_x\cdot 0+0\cdot p_x+p_y\cdot(-i\hbar p_z)+(-i\hbar p_z)\cdot p_y+p_z\cdot(i\hbar p_y)+(i\hbar p_y)\cdot p_z\right\}+[V(r),L_x]$$

$$=\frac{i\hbar}{2m}\underbrace{\left\{-p_yp_z-p_zp_y+p_zp_y+p_yp_z\right\}}_{0}+\underbrace{[V(r),L_x]}_{[V(r),(yp_z-zp_y)]}$$

$$=\qquad \mathrm{y}[V(r),p_z]+\underbrace{[V(r),y]}_{0}p_z-z[V(r),p_y]+\underbrace{[V(r),z]}_{0}p_y$$

Another useful commutator identity: Recall $[x,p]=i\hbar$.

Notice $[x^2,p]=x[x,p]+[x,p]x=2i\hbar x$.

Then by induction, $[x^n,p]=ni\hbar x^{n-1}$.

Consider a general function $f(x)=\sum_n a_n x^n$.

Then $[f,p]=\sum_n a_n[x^n,p]=\sum_n a_n ni\hbar x^{n-1}=i\hbar\sum_n a_n nx^{n-1}=i\hbar\frac{\partial f}{\partial x}$

So $[H,L_x]=y\left(i\hbar\frac{\partial V}{\partial z}\right)-z\left(i\hbar\frac{\partial V}{\partial y}\right)=i\hbar\left\{\vec{r}\times\vec{\nabla}V\right\}_x$

Thus $\frac{d\langle L_x\rangle}{dt}=\frac{i}{\hbar}\left\langle i\hbar\left\{\vec{r}\times\vec{\nabla}V\right\}_x\right\rangle=-\left\langle\left\{\vec{r}\times\vec{\nabla}V\right\}_x\right\rangle$

Apply this to the full vector $\vec{L} = L_x \hat{x} + L_y \hat{y} + L_z \hat{z}$:

$$\frac{d\vec{L}}{dt} = -\left\langle \vec{r} \times \vec{\nabla} V \right\rangle$$

$$\vec{r} = r\hat{r}$$

$$\text{If } V = V(r),\ \vec{\nabla} V = \frac{\partial V}{\partial r}\hat{r}$$

$$\frac{d\vec{L}}{dt} = -\left\langle r \frac{\partial V}{\partial r} \underbrace{\hat{r} \times \hat{r}}_{0} \right\rangle = 0.$$