Fri: HW

Tues: Read.

Radial component of momentum

For a classical particle in a central potential the energy is

$$E = \frac{1}{2m} p_r^2 + \frac{1}{2mr^2} \vec{L}^2 + V(r)$$

where $\vec{L}$ is the angular momentum and

p_r is the radial component of the momentum

$$\vec{p} = p_r \hat{r} + p_\theta \hat{\theta} + p_\phi \hat{\phi}$$

The analogous quantum system is described by the Hamiltonian

$$\hat{H} = \frac{1}{2m}\left(\hat{p}_x^2 + \hat{p}_y^2 + \hat{p}_z^2\right) + V(\hat{r})$$

where $\hat{r} = \left(\hat{x}^2 + \hat{y}^2 + \hat{z}^2\right)^{1/2}$. We aim to rewrite this using the square of the magnitude of the angular momentum operator $\hat{\vec{L}}^2$ and a radial component of momentum operator $\hat{p}_r$. Ideally we want

$$\hat{H} \overset{??}{=} \frac{1}{2m}\hat{p}_r^2 + \frac{1}{2m\hat{r}^2}\hat{\vec{L}}^2 + V(\hat{r})$$

In classical physics

$$p_r = \frac{x}{r} p_x + \frac{y}{r} p_y + \frac{z}{r} p_z$$

$$= \frac{1}{2}\left(\frac{x}{r} p_x + p_x \frac{x}{r}\right) + \frac{1}{2}\left(\frac{y}{r} p_y + p_y \frac{y}{r}\right) + \frac{1}{2}\left(\frac{z}{r} p_z + p_z \frac{z}{r}\right)$$

Thus we define:

The observable operator for the radial component of momentum is

$$\hat{p}_r := \frac{1}{2}\left[\frac{\hat{x}}{\hat{r}}\hat{p}_x + \hat{p}_x\frac{\hat{x}}{\hat{r}} + \frac{\hat{y}}{\hat{r}}\hat{p}_y + \hat{p}_y\frac{\hat{y}}{\hat{r}} + \frac{\hat{z}}{\hat{r}}\hat{p}_z + \hat{p}_z\frac{\hat{z}}{\hat{r}}\right]$$

We can then do following

Start with

$$\hat{L}_x = \hat{y}\hat{p}_z - \hat{z}\hat{p}_y$$
$$\hat{L}_y = \hat{z}\hat{p}_x - \hat{x}\hat{p}_z$$
$$\hat{L}_z = \hat{x}\hat{p}_y - \hat{y}\hat{p}_x$$

→ Construct

$$\hat{\vec{L}}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$$

and express this in terms of $\hat{x}, \hat{y}, \hat{z}, \hat{p}_x, \hat{p}_y, \hat{p}_z$

Start with

$$\hat{p}_r = \frac{1}{2}\left[\frac{\hat{x}}{\hat{r}}\hat{p}_x + \hat{p}_x\frac{\hat{x}}{\hat{r}} + \dots\right]$$

→ Construct

$$\hat{p}_r^2$$

and express this in terms of $\hat{x}, \hat{y}, \hat{z}, \hat{p}_x, \hat{p}_y, \hat{p}_z$

Form $\hat{p}_r^2 + \frac{1}{\hat{r}^2}\hat{\vec{L}}^2$

We can show:

$$\boxed{\hat{p}_r^2 + \frac{1}{\hat{r}^2}\hat{\vec{L}}^2 = \hat{p}_x^2 + \hat{p}_y^2 + \hat{p}_z^2}$$

Then

$$\boxed{\hat{H} = \frac{1}{2m}\hat{p}_r^2 + \frac{1}{2m\hat{r}^2}\hat{\vec{L}}^2 + V(\hat{r})}$$

We can manipulate the radial momentum into spherical co-ordinates to get

$$\boxed{\hat{p}_r |\Psi\rangle \rightsquigarrow -i\hbar \left(\frac{\partial}{\partial r} + \frac{1}{r} \right) \Psi(r,\theta,\phi)}$$

Proof: $\hat{p}_r = \frac{1}{2}\left[\frac{\hat{x}}{\hat{r}}\hat{p}_x + \hat{p}_x \frac{\hat{x}}{\hat{r}} + \frac{\hat{y}}{\hat{r}}\hat{p}_y + \hat{p}_y \frac{\hat{y}}{\hat{r}} + \frac{\hat{z}}{\hat{r}}\hat{p}_z + \hat{p}_z \frac{\hat{z}}{\hat{r}} \right]$

Now $\left[\hat{p}_x, f(\hat{x})\right] = -i\hbar \frac{\partial f}{\partial x}\Big|_{\hat{x}}$ gives

$$\hat{p}_x \frac{\hat{x}}{\hat{r}} = \frac{\hat{x}}{\hat{r}}\hat{p}_x - i\hbar \frac{\partial}{\partial x}\left(\frac{x}{r}\right)_{\hat{x}}$$

$$= \frac{\hat{x}}{\hat{r}}\hat{p}_x - i\hbar \left[\frac{r - x^2/r}{r^2} \right]_{\hat{x}}$$

$$= \frac{\hat{x}}{\hat{r}}\hat{p}_x - i\hbar \left[\frac{1}{\hat{r}} - \frac{\hat{x}^2}{\hat{r}^3} \right]$$

Thus

$$\hat{p}_r = \frac{1}{2} 2 \left[\frac{\hat{x}}{\hat{r}}\hat{p}_x + \frac{\hat{y}}{\hat{r}}\hat{p}_y + \frac{\hat{z}}{\hat{r}}\hat{p}_z \right] - \frac{i\hbar}{2}\left[\frac{3}{\hat{r}} - \underbrace{\frac{\hat{x}^2+\hat{y}^2+\hat{z}^2}{\hat{r}^3}}_{= 1/\hat{r}^2} \right]$$

$$= \frac{\hat{x}}{\hat{r}}\hat{p}_x + \frac{\hat{y}}{\hat{r}}\hat{p}_y + \frac{\hat{z}}{\hat{r}}\hat{p}_z - i\hbar \frac{1}{\hat{r}}$$

In terms of wavefunctions this gives:

$$\hat{p}_r \rightsquigarrow -i\hbar \left[\frac{x}{r}\frac{\partial}{\partial x} + \frac{y}{r}\frac{\partial}{\partial y} + \frac{z}{r}\frac{\partial}{\partial z} + \frac{1}{r} \right]$$

Now

$$\frac{\partial}{\partial r} = \frac{\partial x}{\partial r}\frac{\partial}{\partial r} + \frac{\partial y}{\partial r}\frac{\partial}{\partial y} + \frac{\partial z}{\partial r}\frac{\partial}{\partial z}$$

and $\quad x = r\cos\phi\sin\theta \quad \Rightarrow \quad \frac{\partial x}{\partial r} = \cos\phi\sin\theta = \frac{x}{r}.$

Similarly

$$\frac{\partial y}{\partial r} = \sin\phi\sin\theta$$

$$\frac{\partial z}{\partial r} = \cos\theta$$

Thus

$$\frac{\partial}{\partial r} = \frac{x}{r}\frac{\partial}{\partial x} + \frac{y}{r}\frac{\partial}{\partial y} + \frac{z}{r}\frac{\partial}{\partial z}$$

This proves the result.

1 Radial momentum eigenstates

In spherical coordinates, the radial momentum operator is

$$\hat{p}_r \leftrightarrow -i\hbar\left[\frac{\partial}{\partial r}+\frac{1}{r}\right].$$

We seek radial momentum eigenstates, $\Psi(r,\theta,\phi)$, and their eigenvalues.

a) Express the eigenvalue equation as a differential equation for $\Psi(r,\theta,\phi)$.

b) A possible candidate for an eigenstate is

$$\Psi(r,\theta,\phi)=Ae^{i\alpha r/\hbar}$$

where α is real and A is a constant. Check whether this is an eigenstate. If so, determine the eigenvalue.

c) Another possible candidate for an eigenstate is

$$\Psi(r,\theta,\phi)=\frac{A}{r}\,e^{i\alpha r/\hbar}$$

where α is real and A is a constant. Check whether this is an eigenstate. If so, determine the eigenvalue.

Answer: a) $\hat{p}_r\Psi(r,\theta,\phi) = p\Psi(r,\theta,\phi)$

$$\Rightarrow -i\hbar\left(\frac{\partial}{\partial r}+\frac{1}{r}\right)\Psi = p\Psi \Rightarrow -i\hbar\left(\frac{\partial\Psi}{\partial r}+\frac{1}{r}\Psi\right)=p\Psi \quad \text{— (A)}$$

b) $\frac{\partial\Psi}{\partial r} = \frac{i\alpha}{\hbar}\Psi$. Then substitution into (A) gives:

$$-i\hbar\left(\frac{i\alpha}{\hbar}\cancel{\Psi}+\frac{1}{r}\cancel{\Psi}\right)=p\cancel{\Psi} \Rightarrow -i\hbar\left(\frac{i\alpha}{\hbar}+\frac{1}{r}\right)=p$$

But p cannot depend on r. So this is not an eigenstate

c) $$\frac{\partial\Psi}{\partial r} = -\frac{A}{r^2}e^{i\alpha r/\hbar}+\frac{A}{r}\left(\frac{i\alpha}{\hbar}\right)e^{i\alpha r/\hbar} \Rightarrow \frac{\partial\Psi}{\partial r} = -\frac{1}{r}\Psi+\frac{i\alpha}{\hbar}\Psi$$

Substitution into (A) gives:

$$-i\hbar\left[\cancel{-\frac{1}{r}\Psi}+\frac{i\alpha}{\hbar}\Psi+\cancel{\frac{1}{r}\Psi}\right]=p\Psi \Rightarrow \alpha\Psi=p\Psi$$

This is an eigenstate with eigenvalue α.

Separately algebra involving position and momentum commutators gives.

$$\boxed{\begin{gathered}[\hat{L}_i, \hat{p}_r] = 0 \\ [\hat{L}^2, \hat{p}_r] = 0\end{gathered}}$$

Central potential and angular momentum

Since $\hat{H}, \hat{\vec{L}}^2$ and $\hat{L}_z$ all commute with each other there exist simultaneous eigenstates

$$|\Psi\rangle = |E, \Lambda, \lambda\rangle$$

refers to $\hat{L}_z$ and L_z component.

refers to $\hat{H}$ and energy

refers to $\hat{\vec{L}}^2$ and magnitude of angular momentum

Specifically:

$$\hat{H}|\Psi\rangle = E|\Psi\rangle$$
$$\hat{\vec{L}}^2|\Psi\rangle = \Lambda|\Psi\rangle$$
$$\hat{L}_z|\Psi\rangle = \lambda|\Psi\rangle$$

Then

$$\hat{H}|\Psi\rangle = \left[\frac{1}{2m}\hat{p}_r^2 + \frac{1}{2m\hat{r}^2}\hat{\vec{L}}^2 + V(\hat{r})\right]|\Psi\rangle = E|\Psi\rangle$$

$$\Rightarrow \underbrace{\left[\frac{1}{2m}\hat{p}_r^2 + \frac{1}{2m\hat{r}^2}\Lambda + V(\hat{r})\right]}_{\text{only radial dependence!}}|\Psi\rangle = E|\Psi\rangle$$

In terms of wavefunctions this gives:

$$\left[\frac{-\hbar^2}{2m}\left(\frac{\partial}{\partial r}+\frac{1}{r}\right)^2 + \frac{1}{2mr^2}\Lambda + V(r)\right]\Psi(r,\theta,\phi) = E\,\Psi(r,\theta,\phi)$$

and with

$$\Psi(r,\theta,\phi) = R(r)\,Y(\theta,\phi)$$

this reduces to an ordinary differential equation:

$$\left[-\frac{\hbar^2}{2m}\left(\frac{d}{dr}+\frac{1}{r}\right)^2 + \frac{\Lambda}{2mr^2} + V(r)\right]R(r) = E\,R(r)$$

We do need the possible eigenvalues Λ

Angular momentum eigenvalues

The angular momentum eigenvalues will be determined by the algebraic commutator relationships between angular momentum operators and the units of angular momentum, $\hbar$.

The orbital and spin angular momentum observables satisfy the same algebraic relationships. So we consider a generic angular momentum $\vec{J}$ that could represent any combination of the two. Classically

$$\vec{J} = J_x \hat{i} + J_y \hat{j} + J_z \hat{k}$$

The associated observables satisfy

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

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

$$[\hat{J}_z, \hat{J}_x] = i\hbar J_y$$

and

Magnitude of angular momentum squared:

$$\hat{\vec{J}}^2 = \hat{J}_x^2 + \hat{J}_y^2 + \hat{J}_z^2$$

satisfies

$$[\hat{\vec{J}}^2, \hat{J}_i] = 0 \quad i = x, y, z.$$

We aim to find simultaneous eigenstates of $\hat{\vec{J}}^2$ and $\hat{J}_z$. The units of angular momentum are the same as $\hbar$. Thus we seek

State

$|j, m\rangle$

Describes $\vec{J}^2$

Describes J_z

Satisfies:

$$\hat{\vec{J}}^2 |j, m\rangle = \hbar^2 A_j |j, m\rangle$$

$$\hat{J}_z |j, m\rangle = \hbar B_m |j, m\rangle.$$

We now need to find possibilities for j, m, A_j, B_m. We will eventually show

1) good labels j, m are either integers or half integers.
2) for orbital angular momentum these must be integers

Bounds on angular momentum eigenvalues

We begin by providing bounds on the eigenvalues of angular momentum. First consider $\vec{J}^2$. Classically we expect that this cannot be negative. The same is true in quantum theory.

The eigenvalues of $\hat{\vec{J}}^2$ cannot be negative. Thus

$$A_j \geqslant 0$$

This follows from the fact that, for any state $|\Psi\rangle$, $\langle\Psi|\hat{\vec{J}}^2|\Psi\rangle \geqslant 0$. This is a consequence of

$$\langle\Psi|\hat{\vec{J}}^2|\Psi\rangle = \langle\Psi|\hat{J}_x^2|\Psi\rangle + \langle\Psi|\hat{J}_y^2|\Psi\rangle + \langle\Psi|\hat{J}_z^2|\Psi\rangle$$

and

$$\langle\Psi|\hat{J}_x^2|\Psi\rangle = \langle\Psi|\hat{J}_x\hat{J}_x|\Psi\rangle = \langle\Psi|\hat{J}_x^{+}\hat{J}_x|\Psi\rangle$$

which is the inner product of $\hat{J}_x|\Psi\rangle$ with itself. This cannot be negative.

The next question is

Given a particular eigenvalue A_j for $\vec{J}^2$ what are the bounds on B_m for J_z?

There are bounds in classical physics but the bounds in quantum physics are different.

2 Bounds on angular momentum eigenvalues

Consider a state with eigenvalue, $\hbar^2 A_j$, for $\mathbf{J}^2$.

a) If this were a classical system, what be would the range of values for J_z?

b) Consider a quantum system and suppose that there is an eigenstate of $\hat{J}_z$ whose eigenvalue squared is exactly the same as the eigenvalue of $\hat{\mathbf{J}}^2$. What does this imply about $\langle J_x^2 \rangle + \langle J_y^2 \rangle$ for this state?

Several lines of algebra involving angular momentum observables show that, for any eigenstate of $\hat{J}_z$,

$$\langle J_x \rangle = \langle J_y \rangle = 0.$$

c) What does this imply for $(\Delta J_x)^2 + (\Delta J_y)^2$ for the hypothetical state above? Is this possible?

Answer: a) For a classical system

$$\vec{J}^2 = J_x^2 + J_y^2 + J_z^2$$

If $J_x = J_y = 0$ then $J_z = \pm\sqrt{\vec{J}^2}$. Any values between these are possible thus we could have

$$-\sqrt{\vec{J}^2} \leq J_z \leq +\sqrt{\vec{J}^2} \quad \text{or} \quad -\hbar\sqrt{A_j} \leq J_z \leq +\hbar\sqrt{A_j}$$

b) $$\hat{\vec{J}}^2 = \hat{J}_x^2 + \hat{J}_y^2 + \hat{J}_z^2$$

Suppose that $|j,m\rangle$ is an eigenstate

$$\left.\begin{aligned} \hat{\vec{J}}^2 |j,m\rangle &= \hbar^2 A_j |j,m\rangle \\ \hat{J}_z |j,m\rangle &= \hbar B_m |j,m\rangle. \end{aligned}\right\} \text{ such that } \hbar^2 A_j = (\hbar B_m)^2$$

Then, for this state

$$\langle \vec{J}^2 \rangle = \langle J_x^2 \rangle + \langle J_y^2 \rangle + \langle J_z^2 \rangle$$

But $$\langle \vec{J}^2 \rangle = \langle j,m | \hat{\vec{J}}^2 | j,m \rangle = \hbar^2 A_j$$

$$\langle J_z^2 \rangle = \hbar^2 B_m^2$$

$$\Rightarrow \quad \hbar^2 A_j = \langle J_x^2 \rangle + \langle J_y^2 \rangle + \hbar^2 B_m^2$$

if these are equal then $0 = \langle J_x^2 \rangle + \langle J_y^2 \rangle$

c) $(\Delta J_x)^2 = \langle J_x^2 \rangle - \langle J_x \rangle^2$

$$\Rightarrow \quad (\Delta J_x)^2 = \langle J_x^2 \rangle$$

similarly $(\Delta J_y)^2 = \langle J_y^2 \rangle$ and this gives

$$(\Delta J_x)^2 + (\Delta J_y)^2 = \langle J_x^2 \rangle + \langle J_y^2 \rangle = 0 \qquad \Rightarrow \Delta J_x = \Delta J_y = 0$$

Now consider the uncertainty principle

$$(\Delta J_x)(\Delta J_y) \geq \frac{1}{2} \left| \langle \Psi | [\hat{J}_x, \hat{J}_y] | \Psi \rangle \right|$$

$$= \frac{1}{2} \left| \langle \Psi | (-i\hbar \hat{J}_z) | \Psi \rangle \right|$$

$$= \frac{\hbar}{2} \Big| \underbrace{\langle j, m | \hat{J}_z | j, m \rangle}_{\hbar B_m} \Big| = \frac{\hbar^2}{2} |B_m|$$

These cannot both be zero unless $B_m = 0$ and $A_j = 0$. Thus

$$\boxed{\begin{array}{l} \text{For non-zero total angular momentum, it is} \\ \text{impossible that} \\ \qquad (\text{eigenvalue of } J_z)^2 = \text{eigenvalue of } \vec{J}^2 \\ \qquad\qquad\qquad \text{or} \\ \qquad \text{eigenvalue of } J_z = \pm\sqrt{\text{eigen value of } \vec{J}^2} \end{array}}$$

By contrast, classical physics does allow this.

This leaves the question of how close $\hbar^2 B_m^2$ can approach $\hbar^2 A_j$. Or equivalently how close B_m^2 can approach A_j

A series of algebraic manipulations use:

For eigenstate $|j,m\rangle$

$$\hbar^2 A_j = (\Delta J_x)^2 + (\Delta J_y)^2 + \hbar^2 B_m^2$$

$$(\Delta J_x)(\Delta J_y) \geq \frac{\hbar^2}{2} |B_m|$$

$$\downarrow$$

$$B_m^2 \leq A_j + \underbrace{\frac{1}{2} - \sqrt{A_j + \frac{1}{4}}}_{\text{negative if } A_j > 0}$$

We can then reset A_j by define $a_j > 0$ such that.

$$A_j = a_j(a_j+1)$$

This gives

$$B_m^2 \leq a_j(a_j+1) + \frac{1}{2} - \sqrt{(a_j^2 + a_j + \frac{1}{4})}$$

$$B_m^2 \leq a_j^2 + a_j + \frac{1}{2} - \underbrace{\sqrt{(a_j + \frac{1}{2})^2}}_{a_j + \frac{1}{2}}$$

$$B_m^2 \leq a_j^2 \quad \Rightarrow \quad -a_j \leq B_m \leq a_j$$

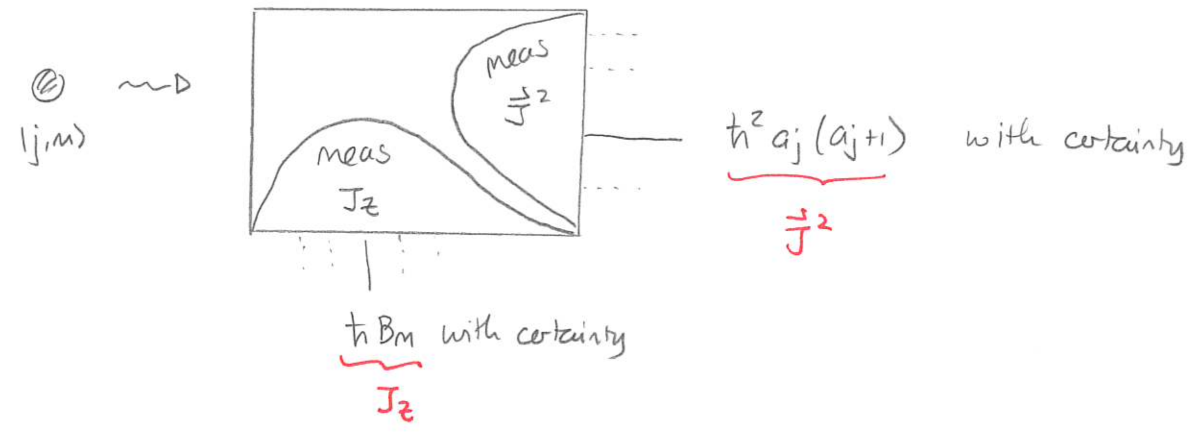
Thus:

The eigenstates $|j,m\rangle$ satisfy.

$$\hat{J}^2 |j,m\rangle = \hbar^2 a_j(a_j+1) |j,m\rangle \qquad a_j > 0$$

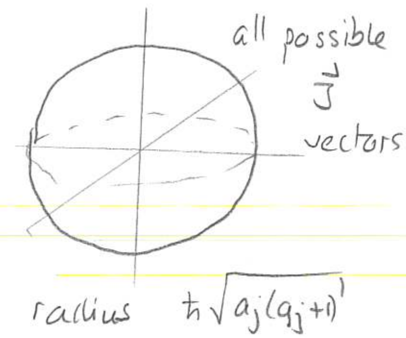
$$\hat{J}_z |j,m\rangle = \hbar B_m |j,m\rangle \qquad -a_j \leq B_m \leq a_j$$

We get a physical interpretation:



A semi-classical interpretation is:

The magnitude of $\vec{J}^2$ is determined via a_j via j. Corresponds to a vector somewhere on sphere with radius $\hbar\sqrt{a_j(a_j+1)}$

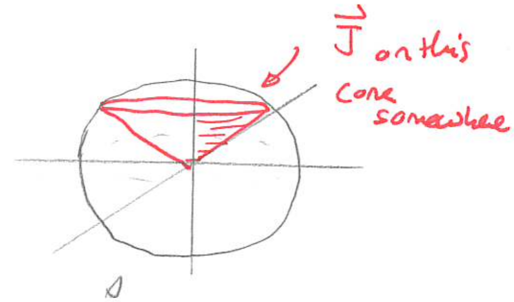


The value of J_z is determined via B_m via m.

$$J_z = \hbar B_m$$

and $|J_z| < |\vec{J}|$

$$(\Delta J_x)^2 + (\Delta J_y)^2 > 0$$



We cannot describe $\vec{J}$ any more precisely than this cone structure.