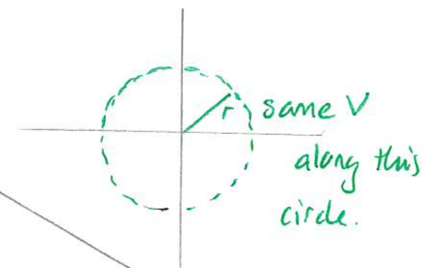
Thurs: Read 11.2, 7.3

Fri: HW by 5pm

Particles in a central potential

A central potential is one which only depends on the radial distance from the origin. So, in spherical co-ordinates, (r, θ, ϕ),

$$V = V(r)$$



In classical physics one can show:

> The angular momentum of a particle in a central potential
>
> $$\vec{L} = \vec{r} \times \vec{p}$$
>
> is conserved and the energy is
>
> $$E = \frac{p_r^2}{2m} + \frac{1}{2mr^2}\vec{L}^2 + V(r)$$
>
> where p_r is the radial component of momentum and $\vec{L}^2 = \vec{L}\cdot\vec{L}$

This reduces the problem of describing energies from a three variable problem $((x,y,z)$ or $(r,\theta,\phi))$ to a single variable problem.

In order to translate to quantum physics we will need to describe angular momentum in terms of operators.

Quantum angular momentum

In classical physics the angular momentum components are

$$L_x = y p_z - z p_y$$

$$L_y = z p_x - x p_z$$

$$L_z = x p_y - y p_x$$

Thus the comparable observable operators in quantum theory are

$$\boxed{\begin{aligned} \hat{L}_x &= \hat{y}\hat{p}_z - \hat{z}\hat{p}_y \\ \hat{L}_y &= \hat{z}\hat{p}_x - \hat{x}\hat{p}_z \\ \hat{L}_z &= \hat{x} p_y - \hat{y}\hat{p}_x \end{aligned}}$$

We will need to:

1) construct the $\hat{L}^2$ operator
2) find possible eigenstates and eigenvalues of angular momentum.

The key results that generate these are:

$$\boxed{\begin{aligned} [\hat{L}_x, \hat{L}_y] &= i\hbar L_z \\ [\hat{L}_y, \hat{L}_z] &= i\hbar \hat{L}_y \\ [\hat{L}_z, \hat{L}_x] &= i\hbar \hat{L}_x \end{aligned}}$$

These can be proved by working directly with the definitions of the angular momentum operators and the commutation rules for position and momentum operators.

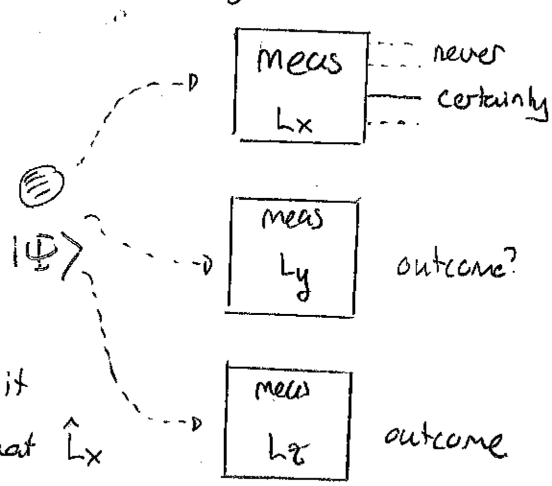
We can form the "square of the angular momentum" observable

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

and then algebra with commutators yields

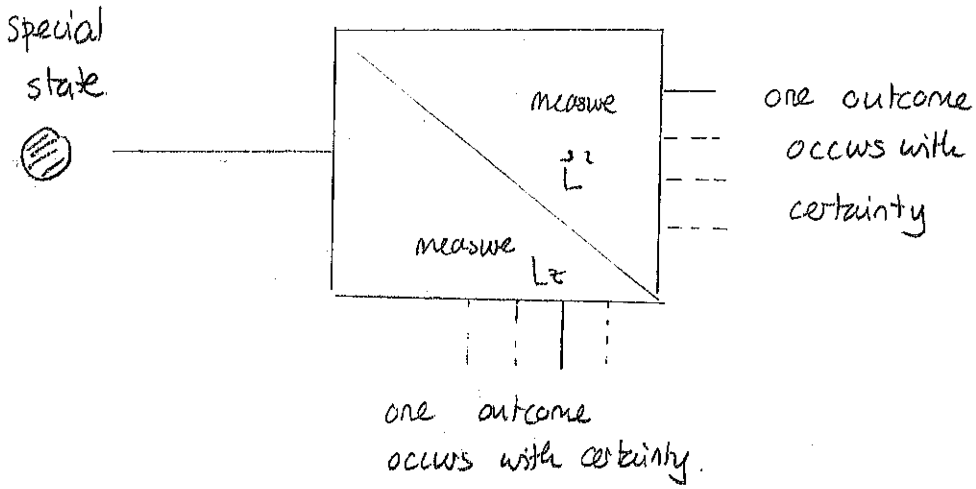
$$\boxed{\begin{aligned} [\hat{L}^2, \hat{L}_x] &= 0 \\ [\hat{L}^2, \hat{L}_y] &= 0 \\ [\hat{L}^2, \hat{L}_z] &= 0 \end{aligned}}$$

We can now use this operator algebra to describe the outcomes of measurements. We could imagine preparing a particle in a state and then measuring any of the components of angular momentum. Suppose that the state yields a definite outcome for L_x with certainty. Can such a state always be chosen to yield a definite outcome of L_y with certainty?
In general this is not true and if it were always so one can prove that $\hat{L}_x$ and $\hat{L}_y$ would commute. Since they do not we are restricted as follows:



There are no states which will yield definite outcomes for measurement of each component of momentum. In general there are states which yield a definite outcome for one component only

But there are states that yield definite outcomes for $\hat{L}^2$ and $\hat{L}_x$ or $\hat{L}^2$ and $\hat{L}_y$ or $\hat{L}^2$ and $\hat{L}_z$. The latter is the conventional choice.



Angular momentum operators on wavefunctions: spherical co-ordinates

In Cartesian co-ordinates angular momentum operators translate to:

$$\hat{L}_x \sim i\hbar\left[z\frac{\partial}{\partial y} - y\frac{\partial}{\partial z}\right]$$

$$\hat{L}_y \sim i\hbar\left[x\frac{\partial}{\partial z} - z\frac{\partial}{\partial x}\right]$$

$$\hat{L}_z \sim i\hbar\left[y\frac{\partial}{\partial x} - x\frac{\partial}{\partial y}\right]$$

We can translate these into spherical co-ordinates using

$$\frac{\partial}{\partial x} = \frac{\partial r}{\partial x}\frac{\partial}{\partial r} + \frac{\partial \theta}{\partial x}\frac{\partial}{\partial \theta} + \frac{\partial \phi}{\partial x}\frac{\partial}{\partial \phi}$$

$$\vdots$$

$$r = (x^2+y^2+z^2)^{1/2}$$

$$\theta = \arctan\left(\frac{\sqrt{x^2+y^2}}{z}\right)$$

$$\phi = \arctan\left(\frac{y}{x}\right)$$

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

$$y = r\sin\phi\sin\theta$$

$$z = r\cos\theta$$

Thus

$$\frac{\partial r}{\partial x} = \frac{1}{2}\frac{2x}{(x^2+y^2+z^2)^{1/2}} = \frac{\cos\phi\sin\theta}{r}$$

etc...

These eventually give:

$$\boxed{\begin{aligned}
\hat{L}_x &\leadsto i\hbar\left[\sin\phi\frac{\partial}{\partial\theta} + \frac{\cos\theta\cos\phi}{\sin\theta}\frac{\partial}{\partial\phi}\right] \\
\hat{L}_y &\leadsto i\hbar\left[-\cos\phi\frac{\partial}{\partial\theta} + \frac{\cos\theta\sin\phi}{\sin\theta}\frac{\partial}{\partial\phi}\right] \\
\hat{L}_z &\leadsto -i\hbar\frac{\partial}{\partial\phi} \\
\hat{L}^2 &\leadsto -\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]
\end{aligned}}$$

<u>Proof</u>:

$$\frac{\partial r}{\partial x} = \cos\phi\sin\theta \qquad \frac{\partial r}{\partial y} = \sin\phi\sin\theta \qquad \frac{\partial r}{\partial z} = \cos\theta$$

$$\frac{\partial\theta}{\partial x} = \frac{\cos\theta\cos\phi}{r} \qquad \frac{\partial\theta}{\partial y} = \frac{\cos\theta\sin\phi}{r} \qquad \frac{\partial\theta}{\partial z} = -\frac{\sin\theta}{r}$$

$$\frac{\partial\phi}{\partial x} = -\frac{\sin\phi}{r\sin\theta} \qquad \frac{\partial\phi}{\partial y} = \qquad \frac{\partial\phi}{\partial z} = 0$$

Thus

$$\frac{\partial}{\partial x} = \frac{\partial r}{\partial x}\frac{\partial}{\partial r} + \frac{\partial\theta}{\partial x}\frac{\partial}{\partial\theta} + \frac{\partial\phi}{\partial x}\frac{\partial}{\partial\phi}$$

$$= \cos\phi\sin\theta\frac{\partial}{\partial r} + \frac{\cos\phi\cos\theta}{r}\frac{\partial}{\partial\theta} - \frac{\sin\phi}{r\sin\theta}\frac{\partial}{\partial\phi}$$

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

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

Thus

$$L_x \leadsto -i\hbar\left[y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right] = -i\hbar\left[r\sin\phi\sin\theta\left(\cos\theta\frac{\partial}{\partial r}\right) - \sin\phi\sin^2\theta\frac{\partial}{\partial\theta}\right.$$

$$\left. - r\cos\theta\left(\sin\phi\sin\theta\frac{\partial}{\partial r} + \frac{\sin\phi\cos\theta}{r}\frac{\partial}{\partial\theta} + \frac{\cos\phi}{r\sin\theta}\frac{\partial}{\partial\phi}\right)\right]$$

$$\Rightarrow \quad L_x \leadsto -i\hbar \left[-\sin\phi \frac{\partial}{\partial\theta} - \frac{\cos\theta\cos\phi}{\sin\theta} \frac{\partial}{\partial\phi} \right]$$

$$= i\hbar \left[\sin\phi \frac{\partial}{\partial\theta} + \frac{\cos\theta\cos\phi}{\sin\theta} \frac{\partial}{\partial\phi} \right]$$

The others follow by similar manipulations.

1 **Angular momentum and wavefunctions: spherical coordinates**

Suppose that

$$|\Psi\rangle \leftrightarrow \Psi(r,\theta,\phi) = R(r)\frac{1}{\sqrt{4\pi}}\, e^{i\alpha\phi}$$

where α is a real constant and $R(r)$ is a normalized radial function.

a) Determine the wavefunction for $\hat{L}_x\,|\Psi\rangle$ in spherical coordinates.

b) Determine $\langle L_x\rangle$.

Answer:

a) $$\hat{L}_x|\Psi\rangle \leadsto i\hbar\left[\sin\phi\frac{\partial}{\partial\theta} + \frac{\cos\theta}{\sin\theta}\cos\phi\frac{\partial}{\partial\phi}\right]R(r)\frac{1}{\sqrt{4\pi}}\, e^{i\alpha\phi}$$

$$= i\hbar\, R(r)\frac{1}{\sqrt{4\pi}}\,\frac{\cos\theta}{\sin\theta}\cos\phi\,(i\alpha)\, e^{i\alpha\phi}$$

$$= \underbrace{-\alpha\hbar\, R(r)\frac{1}{\sqrt{4\pi}}\,\frac{\cos\theta}{\sin\theta}\cos\phi\, e^{i\alpha\phi}}$$

b) $$\langle\Psi|\hat{L}_x|\Psi\rangle = \int_0^\infty dr\int_0^\pi d\theta\int_0^{2\pi} d\phi\; r^2\sin\theta\;\Psi^*(r,\theta,\phi)\,(-\alpha\hbar)\,R(r)\frac{1}{\sqrt{4\pi}}\,\frac{\cos\theta}{\sin\theta}\cos\phi\, e^{i\alpha\phi}$$

$$= -\alpha\hbar\int_0^\infty dr\int_0^\pi d\theta\int_0^{2\pi} d\phi\; r^2\cancel{\sin\theta}\; R^2(r)\,\frac{1}{4\pi}\,\cancel{e^{-i\alpha\phi}}\,\frac{\cos\theta}{\cancel{\sin\theta}}\cos\phi\,\cancel{e^{i\alpha\phi}}$$

$$= -\frac{\alpha\hbar}{4\pi}\underbrace{\int_0^\infty R^2(r)\, r^2 dr}_{1}\;\underbrace{\int_0^\pi \cos\theta\, d\theta}_{0}\;\underbrace{\int_0^{2\pi}\cos\phi\, d\phi}_{0} = 0$$

Angular momentum and central potentials

In a central potential situation, the Hamiltonian is

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

where $\hat{r}$ is a function of $\hat{x}^2 + \hat{y}^2 + \hat{z}^2$. We can show that

$$\boxed{\begin{array}{ll} \left[\hat{L}_i, \hat{p}_x^2 + \hat{p}_y^2 + \hat{p}_z^2\right] = 0 & \text{for } i = x, y, z \\ \left[\hat{L}_i, \hat{x}^2 + \hat{y}^2 + \hat{z}^2\right] = 0 & \text{for } i = x, y, z. \end{array}}$$

HW exercise

It immediately follows that

$$\left.\begin{array}{l} \left[\hat{L}_i^2, \hat{p}_x^2 + \hat{p}_y^2 + \hat{p}_z^2\right] = 0 \\ \left[\hat{L}_i^2, \hat{x}^2 + \hat{y}^2 + \hat{z}^2\right] = 0 \end{array}\right\} \Rightarrow \begin{array}{l} \left[\hat{\vec{L}}^2, \hat{x}^2 + \hat{y}^2 + \hat{z}^2\right] = 0 \\ \left[\hat{\vec{L}}^2, \hat{p}_x^2 + \hat{p}_y^2 + \hat{p}_z^2\right] = 0 \end{array}$$

These imply:

$$\boxed{\begin{array}{l} \text{For a particle in a central potential} \\ \left[\hat{H}, \hat{L}_i\right] = 0 \qquad i = x, y, z \\ \left[\hat{H}, \hat{\vec{L}}^2\right] = 0 \end{array}}$$

2 Time evolution of angular momentum expectation values

Suppose that an ensemble of particles are each in a central potential and that the initial state of each is the same.

a) The angular momentum component L_x is measured at a later time. Determine how $\langle L_x \rangle$ varies with time. Repeat this for the other components.

b) The magnitude of the angular momentum square is measured at a later time. Determine how $\langle \mathbf{L}^2 \rangle$ varies with time. Repeat this for the other components.

c) What does this imply for the conservation of angular momentum for a particle in a central potential.

Answers: a)

$$\frac{d}{dt}\langle L_x\rangle = \langle \Psi | \cancel{\frac{\partial \hat{L}_x}{\partial t}}^{\,0} | \Psi \rangle + \frac{i}{\hbar}\langle \Psi | \underbrace{[\hat{H}, \hat{L}_x]}_{0} | \Psi \rangle$$

$$\Rightarrow \frac{d}{dt}\langle L_x\rangle = 0$$

similarly $\quad \frac{d}{dt}\langle L_y\rangle = \frac{d}{dt}\langle L_z\rangle = 0$

b) $$\frac{d}{dt}\langle \hat{L}^2\rangle = \langle \Psi | \cancel{\frac{\partial \hat{L}^2}{\partial t}}^{\,0} | \Psi \rangle + \frac{i}{\hbar}\langle \Psi | \cancel{[\hat{H}, \hat{L}^2]}^{\,0} | \Psi \rangle$$

Thus

$$\frac{d\langle \hat{L}^2\rangle}{dt} = 0$$

c) It appears that

$$\frac{d\langle L_x\rangle}{dt} = \frac{d\langle L_y\rangle}{dt} = \frac{d\langle L_z\rangle}{dt} = 0 \quad \text{AND} \quad \frac{d\langle \hat{L}^2\rangle}{dt} = 0$$

This is equivalent to conservation of angular momentum

This has an important consequence for possible states of the system. We can always find three observables that commute: e.g.

$\hat{H} \rightsquigarrow$ energy $\rightsquigarrow E$

$\hat{L}^2 \rightsquigarrow$ total angular momentum squared $\rightsquigarrow \Lambda$

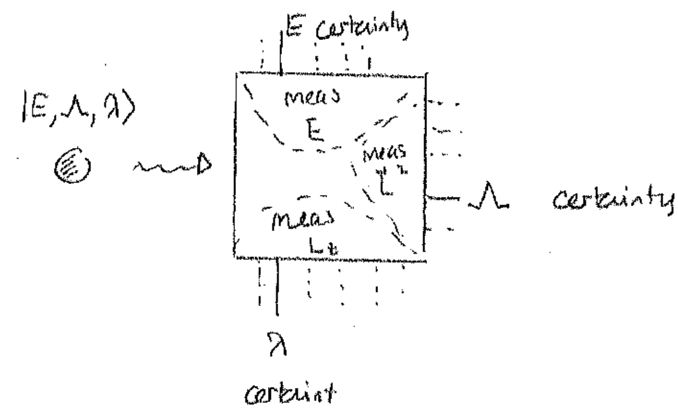
$\hat{L}_z \rightsquigarrow$ one component of angular momentum $\rightsquigarrow \lambda$

So we have states $|E, \Lambda, \lambda\rangle$ s.t.

$$\hat{H}\,|E,\Lambda,\lambda\rangle = E\,|E,\Lambda,\lambda\rangle$$
$$\hat{L}^2\,|E,\Lambda,\lambda\rangle = \Lambda\,|E,\Lambda,\lambda\rangle$$

etc....

We could construct a measuring device that could measure all three quantities



Radial component of momentum

We aim to determine an operator corresponding to the radial component of momentum. If we denote this by $\hat{p}_r$ then the eventual goal will be to construct an operator such that

$\hat{p}_r$ commutes with angular momentum observables

Hamiltonian has the form

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

Note that $\hat{r}$ and $\hat{\vec{L}}^2$ commute and the order in which $\frac{1}{2m\hat{r}^2}$ $\hat{\vec{L}}^2$ appear does not matter.

In order to define such an operator we consider the classical expression as a guide. In general

$$\vec{p} = p_x\hat{i} + p_y\hat{j} + p_z\hat{k} = p_r\hat{r} + p_\theta\hat{\theta} + p_\phi\hat{\phi}$$

We can then show:

In classical physics

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

Proof: Here

$$\hat{i} = \sin\theta\cos\phi\,\hat{r} + \cos\theta\cos\phi\,\hat{\theta} - \sin\phi\,\hat{\phi}$$
$$\hat{j} = \sin\theta\sin\phi\,\hat{r} + \cos\theta\sin\phi\,\hat{\theta} + \cos\phi\,\hat{\phi}$$
$$\hat{k} = \cos\theta\,\hat{r} - \sin\theta\,\hat{\theta}$$

Then:

$$\vec{p} = \left[p_x\sin\theta\cos\phi + p_y\sin\theta\sin\phi + p_z\cos\theta\right]\hat{r}$$
$$+\left[\quad \cdots\cdots \quad\right]\hat{\theta}$$
$$+\left[\quad \cdots \quad\right]\hat{\phi}$$

So $p_r = p_x\sin\theta\cos\phi + p_y\sin\theta\sin\phi + p_z\cos\theta$

But $x = r\sin\theta\cos\phi \Rightarrow \sin\theta\cos\phi = \frac{x}{r}$

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

$z = r\cos\theta \Rightarrow \cos\theta = z/r$

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

We might then attempt to define a radial momentum operator as

$$\hat{p}_r = \frac{\hat{x}}{\hat{r}}\hat{p}_x + \cdots$$

However, there is an ambiguity since classically $\frac{x}{r}p_x = p_x\frac{x}{r}$ and in quantum theory

$$\frac{\hat{x}}{\hat{r}}\hat{p}_x \neq \hat{p}_x\frac{\hat{x}}{\hat{r}}$$

We therefore attempt the following definition.

The observable for the radial component of momentum is

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

With this definition we can eventually show that:

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

2) $[\hat{L}_i, \hat{p}_r] = 0$

3) $[\hat{\vec{L}}^2, \hat{p}_r] = 0$

Thus the Hamiltonian becomes:

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