Thurs: Exam II

Covers: Class 11 - 21 - April 13

~~Bring~~ HW 11 - 20

Time evolution of spin-$\frac{1}{2}$, particles in one dimension, harmonic oscillator, interferometers

Bring: Calculator

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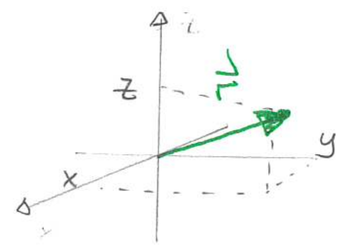
Study: 2007, 2022 All questions

Particles in three dimensions

In general particles are located in three dimensional space. Thus we expect that the outcome of a position measurement is three co-ordinates

particle $\rightsquigarrow$ $\boxed{\text{Measure position}}$ $\rightsquigarrow$ outcome $(x,y,z) = \vec{r}$ ← abbreviation



The formalism of one dimensional quantum theory generalizes to three dimensions with the basic assumption:

> The position co-ordinates x, y, z are independent
> The momentum " p_x, p_y, p_z " "

Then

State $|\Psi(t)\rangle$

Position measurements

Position wavefunction

$$\Psi(x,y,z,t) \equiv \Psi(\vec{r},t)$$

↪ $\vec{r} = x\hat{x} + y\hat{y} + z\hat{z}$

Probabilities of outcomes:

$$\boxed{\begin{aligned}&\text{Prob}\Big[\, x_a \leq x \leq x_b \text{ AND } y_a \leq y \leq y_b \text{ AND } z_a \leq z \leq z_b \,\Big] \\ &= \int_{x_a}^{x_b} dx \int_{y_a}^{y_b} dy \int_{z_a}^{z_b} dz \, |\Psi(x,y,z,t)|^2\end{aligned}}$$

Momentum measurements

Momentum wavefunction

$$\tilde{\Psi}(p_x,p_y,p_z,t) \equiv \tilde{\Psi}(\vec{p},t)$$

↪ $p_x\hat{x} + p_y\hat{y} + p_z\hat{z} = \vec{p}$

Probabilities of outcomes

$$\boxed{\begin{aligned}&\text{Prob}\Big[\, p_{xa} \leq p_x \leq p_{xb} \text{ AND } p_{ya} \leq p_y \leq p_{yb} \text{ AND } p_{za} \leq p_z \leq p_{zb} \,\Big] \\ &= \int_{p_{xa}}^{p_{xb}} dp_x \int_{p_{ya}}^{p_{yb}} dp_y \int_{p_{zb}}^{p_{zb}} dp_z \, |\tilde{\Psi}(p_x,p_y,p_z,t)|^2\end{aligned}}$$

To convert between the position and momentum wavefunctions

$$\tilde{\Psi}(p_x, p_y, p_z, t) = \frac{1}{(2\pi\hbar)^{3/2}} \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy \int_{-\infty}^{\infty} dz \; e^{-ip_x x/\hbar} e^{-ip_y y/\hbar} e^{-ip_z z/\hbar} \Psi(x,y,z,t)$$

and with $\vec{p} \cdot \vec{r} = p_x x + p_y y + p_z z$ we get

$$\boxed{\begin{aligned} \tilde{\Psi}(\vec{p}, t) &= \frac{1}{(2\pi\hbar)^{3/2}} \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy \int_{-\infty}^{\infty} dz \; e^{-i\vec{p}\cdot\vec{r}/\hbar} \Psi(\vec{r}, t) \\ \Psi(\vec{r}, t) &= \frac{1}{(2\pi\hbar)^{3/2}} \int_{-\infty}^{\infty} dp_x \int_{-\infty}^{\infty} dp_y \int_{-\infty}^{\infty} dp_z \; e^{i\vec{p}\cdot\vec{r}/\hbar} \tilde{\Psi}(\vec{p}, t) \end{aligned}}$$

Position operators

We will need to describe position and momentum operators so that:

1) we can describe position and momentum measurements
2) describe angular momentum, $\vec{L} = \vec{r} \times \vec{p}$
3) describe energies.

There will be three independent position operators

$\hat{x} \rightsquigarrow$ describes measurements of x component of position
$\hat{y} \rightsquigarrow$ " " " y " " "
$\hat{z} \rightsquigarrow$ " " " z " " "

These are independent and this is encoded via

$$\boxed{[\hat{x}, \hat{y}] = [\hat{y}, \hat{z}] = [\hat{z}, \hat{x}] = 0}$$

The formalism of these results in the following important rules:

If $|\Psi\rangle \rightsquigarrow \Psi(x,y,z)$ then
$|\Phi\rangle \rightsquigarrow \Phi(x,y,z)$

$$\langle \Phi | \Psi \rangle = \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy \int_{-\infty}^{\infty} dz \; \Phi^*(x,y,z) \, \Psi(x,y,z)$$

Formal proof: There are position eigenstates that are simultaneously eigenstates of all three operators: These are $|x,y,z\rangle \equiv |\vec{r}\rangle$ and

$$\boxed{\begin{aligned} \hat{x}|x,y,z\rangle &= x\,|x,y,z\rangle \\ \hat{y}\,|x,y,z\rangle &= y\,|x,y,z\rangle \\ \hat{z}\,|x,y,z\rangle &= z\,|x,y,z\rangle \end{aligned}}$$

Then

$$\boxed{\langle\vec{r},\vec{r}\,'\rangle = \langle x,y,z|x',y',z'\rangle = \delta(x-x')\,\delta(y-y')\,\delta(z-z') = \delta^3(\vec{r}-\vec{r}\,')}$$

and

$$\boxed{\int_{-\infty}^{\infty}dx\int_{-\infty}^{\infty}dy\int_{-\infty}^{\infty}dz\;|x,y,z\rangle\langle x,y,z| = \hat{I} \quad \Rightarrow \quad \int d^3\vec{r}\,|\vec{r}\rangle\langle\vec{r}| = \hat{I}}$$

Formally

$$\Psi(x,y,z) = \langle\vec{r}|\Psi\rangle$$

Then

$$\langle\Phi|\Psi\rangle = \langle\Phi|\underbrace{\int d^3\vec{r}\,|\vec{r}\rangle\langle\vec{r}|}_{\hat{I}}|\Psi\rangle = \int d^3\vec{r}\;\langle\Phi|\vec{r}\rangle\langle\vec{r}|\Psi\rangle$$

$$= \int_{-\infty}^{\infty}dx\int_{-\infty}^{\infty}dy\int_{-\infty}^{\infty}dz\;\Phi^*(x,y,z)\,\Psi(x,y,z)$$

End proof ∎

If $|\Psi\rangle \rightsquigarrow \Psi(x,y,z)$ then

$\hat{x}|\Psi\rangle \rightsquigarrow x\,\Psi(x,y,z)$

$\hat{y}|\Psi\rangle \rightsquigarrow y\,\Psi(x,y,z)$

$\hat{z}|\Psi\rangle \rightsquigarrow z\,\Psi(x,y,z)$

Formal derivation:

$$\hat{x}|\Psi\rangle \rightsquigarrow \text{wavefunction } \langle x,y,z|\,\hat{x}\,|\Psi\rangle$$

$$= x\langle x,y,z|\Psi\rangle \equiv x\,\Psi(x,y,z)$$

Similarly for the others

End derivation ⊠

If f is a function of position measurement outcomes, i.e. $f = f(x,y,z)$, then for a system in state $|\Psi\rangle$

$$\langle f\rangle = \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy \int_{-\infty}^{\infty} dz\; \Psi^*(x,y,z)\, f(x,y,z)\, \Psi(x,y,z) = \langle\Psi|\, f(\hat{x},\hat{y},\hat{z})\,|\Psi\rangle$$

Formal derivation: The left hand equality is the definition. The right hand equality uses the series for f

$$f(x,y,z) = \sum_{lmn} a_{lmn}\, x^l y^m z^n$$

Then $f(\hat{x},\hat{y},\hat{z}) = \sum_{lmn} a_{lmn}\, \hat{x}^l \hat{y}^m \hat{z}^n$ since the constituent operators all commute. Now

$$\langle\Psi|\, f(\hat{x},\hat{y},\hat{z})\,|\Psi\rangle = \langle\Psi|\, f(\hat{x},\hat{y},\hat{z}) \iiint |x,y,z\rangle\langle x,y,z|\Psi\rangle$$

$$= \langle\Psi| \iiint f(\hat{x},\hat{y},\hat{z})\,|x,y,z\rangle\, \Psi(x,y,z)$$

$$= \quad \ldots \quad \text{end result}$$

End derivation.

Momentum operators.

Similarly there are three independent momentum operators

$\hat{p}_x \rightsquigarrow$ describes measurements of p_x

$\hat{p}_y \rightsquigarrow$ " " " p_y etc...

These satisfy

$$\boxed{[\hat{p}_x, \hat{p}_y] = [\hat{p}_y, \hat{p}_z] = [\hat{p}_z, \hat{p}_x] = 0}$$

In terms of wavefunctions.

If $|\Psi\rangle \rightsquigarrow \Psi(x,y,z)$ then

$$\hat{p}_x|\Psi\rangle \rightsquigarrow -i\hbar \frac{\partial \Psi(x,y,z)}{\partial x}$$

$$\hat{p}_y|\Psi\rangle \rightsquigarrow -i\hbar \frac{\partial}{\partial y}\Psi(x,y,z)$$

$$\hat{p}_z|\Psi\rangle \rightsquigarrow -i\hbar \frac{\partial}{\partial z}\Psi(x,y,z)$$

Then we can consider a particle with momentum $\vec{p}$. The wavefunction for this state is

$\vec{p} = p_x\hat{x} + p_y\hat{y} + p_z\hat{z}$

$$\Psi_{\vec{p}}(\vec{r}) = \frac{1}{(2\pi\hbar)^{3/2}} e^{i\vec{p}\cdot\vec{r}/\hbar}$$

$$\Psi_{\vec{p}}(x,y,z) = \frac{1}{(2\pi\hbar)^{3/2}} \underbrace{e^{ip_x x/\hbar} e^{ip_y y/\hbar} e^{ip_z z/\hbar}}_{\text{product of for } F(x)G(y)H(z)}$$

We can show that

$$[\hat{x},\hat{y}] = [\hat{y},\hat{z}] = [\hat{z},\hat{x}] = 0 \qquad [\hat{x},\hat{p}_x] = i\hbar\hat{I} \qquad [\hat{x},\hat{p}_y] = [\hat{x},\hat{p}_z] = 0$$

$$[\hat{p}_x,\hat{p}_y] = [\hat{p}_y,\hat{p}_z] = [\hat{p}_z,\hat{p}_x] = 0 \qquad [\hat{y},\hat{p}_y] = i\hbar\hat{I} \qquad [\hat{y},\hat{p}_x] = [\hat{y},\hat{p}_z] = 0$$

$$[\hat{z},\hat{p}_z] = i\hbar\hat{I} \qquad [\hat{z},\hat{p}_x] = [\hat{z},\hat{p}_y] = 0$$

Energy eigenstates

In general, we consider a particle subject to a known potential and aim to find the energy eigenstates. The procedure is.

Analogous classical system

$$KE = \frac{p_x^2}{2m} + \frac{p_y^2}{2m} + \frac{p_z^2}{2m} = \frac{\vec{p}\cdot\vec{p}}{2m} \equiv \frac{\vec{p}^2}{2m}$$

$$PE = V(x,y,z)$$

$\hookrightarrow$ Construct Hamiltonian

$$\hat{H} = \frac{\hat{p}_x^2}{2m} + \frac{\hat{p}_y^2}{2m} + \frac{\hat{p}_z^2}{2m} + V(\hat{x},\hat{y},\hat{z})$$

$\rightarrow$ Note that if

$|\Psi\rangle \rightsquigarrow \Psi(x,y,z)$

then

$V(\hat{x},\hat{y},\hat{z})|\Psi\rangle \rightsquigarrow V(x,y,z)\Psi(x,y,z)$

$\hookrightarrow$ Find energy eigenstates by solving the TISE

$$\hat{H}|\phi_E\rangle = E|\phi_E\rangle$$

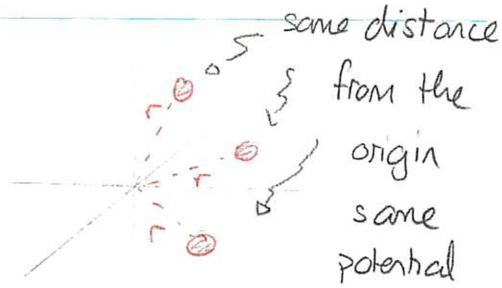
$$\Updownarrow$$

$$\boxed{-\frac{\hbar^2}{2m}\left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right]\phi_E(x,y,z) + V(x,y,z)\,\phi_E(x,y,z) = E\,\phi_E(x,y,z)}$$

We could apply this to three-dimensional system such as a three dimensional infinite well. We will consider a special class of such systems – those where the potential is spherically symmetric.

Particles in a central potential

An important class of systems of particles in three dimensions is that where the potential is spherically symmetrical. The classical version of such a system is described by a potential that only depends on the radial distance from the origin. Thus $V = V(r)$. Examples are:



1) Coulomb potential

$$V(r) = k\,\frac{q_1 q_2}{r}$$

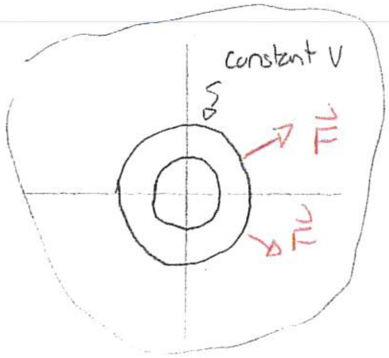
2) Three dimensional harmonic oscillator

$$V = \frac{1}{2} m\omega^2 (x^2 + y^2 + z^2) = \frac{1}{2} m \omega^2 r^2$$

Whenever $V = V(r)$ we say that the potential is a central potential. We first consider some of the consequences of this for the dynamics of the particle. In general:

Given potential V ⇝ Force is $\vec{F} = -\vec{\nabla} V$ ⇝ Torque $\vec{\tau} = \vec{r} \times \vec{F}$ → Angular momentum $\vec{L} = \vec{r} \times \vec{p}$ satisfies $\frac{d\vec{L}}{dt} = \vec{\tau}_{net}$

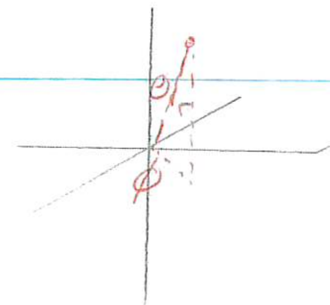
Illustrated in two dimensions



$\vec{\nabla} V$ perpendicular to contours $\Rightarrow$ Force is radially in/out ⇝ $\vec{F}$ and $\vec{r}$ parallel/opposite, $\vec{\tau} = 0$ → Angular momentum is constant

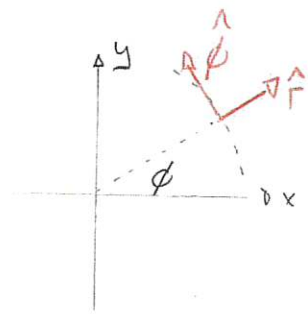
Spherical co-ordinates

The spherical symmetry means that it will be preferable to use spherical co-ordinates rather than Cartesian co-ordinates. In this case we have three co-ordinates: r, θ, ϕ such that

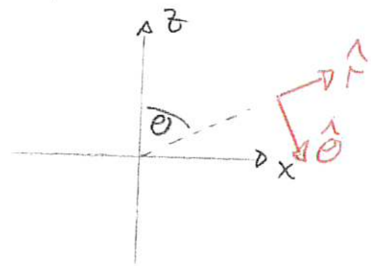


$$x = r\cos\phi \sin\theta$$
$$y = r\sin\phi \sin\theta$$
$$z = r\cos\theta$$

These are accompanied by three spherical unit vectors $\hat{r}, \hat{\theta}, \hat{\phi}$ and we have



$$\hat{r} = \cos\phi\sin\theta\,\hat{x} + \sin\phi\sin\theta\,\hat{y} + \cos\theta\,\hat{z}$$
$$\hat{\theta} = \cos\phi\cos\theta\,\hat{x} + \sin\phi\cos\theta\,\hat{y} - \sin\theta\,\hat{z}$$
$$\hat{\phi} = -\sin\phi\,\hat{x} + \cos\phi\,\hat{y}$$



We can verify that these are orthonormal and

$$\hat{r} \times \hat{\theta} = \hat{\phi} \qquad \hat{\theta} \times \hat{\phi} = \hat{r} \qquad \hat{\phi} \times \hat{r} = \hat{\theta}$$

In general any vector can be expressed as

$$\vec{A} = A_r\,\hat{r} + A_\theta\,\hat{\theta} + A_\phi\,\hat{\phi}$$

We now need to convert all of the mathematics into spherical co-ordinates. This includes all of the probability calculations and quantum mechanical observable operators.

1 Classical particle in a central potential

The classical particle in a central potential has energy

$$E = \frac{\mathbf{p}^2}{2m} + V(r)$$

where the potential, V, only depends on r.

a) Using

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

and the definition of angular momentum

$$\mathbf{L} = \mathbf{r} \times \mathbf{p},$$

show that

$$\mathbf{p}^2 = p_r^2 + \frac{1}{r^2}\mathbf{L}^2.$$

b) Express the energy in terms of radial momentum p_r and angular momentum.

Answer: a) $\vec{r} = r\hat{r}$

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

$$\Rightarrow \vec{r} \times \vec{p} = r\hat{r} \times \left[p_r \hat{r} + p_\theta \hat{\theta} + p_\phi \hat{\phi} \right]$$

$$= r p_r \cancel{\hat{r} \times \hat{r}}^{\,0} + r p_\theta \underbrace{\hat{r} \times \hat{\theta}}_{\hat{\phi}} + r p_\phi \underbrace{\hat{r} \times \hat{\phi}}_{-\hat{\theta}} = r p_\theta \hat{\phi} - r p_\phi \hat{\theta}$$

Then

$$\vec{L}^2 = (r p_\theta)^2 + (r p_\phi)^2 = r^2 (p_\theta^2 + p_\phi^2)$$

$$\vec{p}^2 = p_r^2 + p_\theta^2 + p_\phi^2 = p_r^2 + \frac{1}{r^2} \vec{L}^2$$

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

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

The previous derivation shows that one can express the energy as:

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

If the angular momentum is conserved then $\vec{L}^2$ is effectively a parameter and this reduces the energy to an expression that depends on the radial variable only.

Quantum treatment

In quantum theory we will need to:

Define angular momentum operators and determine their algebraic properties

Reconstruct the Hamiltonian in terms of angular momentum operators

Show that the Hamiltonian commutes with some angular momentum operators

Find eigenstates that are simultaneously energy and angular momentum eigenstates

Use these to simplify the Hamiltonian and analyze its radial behavior separately.

Eventually we will obtain a complete set of energy eigenstates that partly describe angular momentum

Wave functions in spherical co-ordinates

In general we will express wavefunctions using spherical co-ordinates. So

$$|\Psi\rangle \rightsquigarrow \Psi(r,\theta,\phi)$$

We can use these to determine probabilities by noting that

$$dx\,dy\,dz \to r^2 \sin\theta \, dr\, d\theta\, d\phi$$

Then we have a inner product:

$$\boxed{\langle \Phi|\Psi\rangle = \int_0^\infty dr \int_0^{2\pi} d\phi \int_0^{\pi} d\theta \; r^2 \sin\theta \; \Phi^*(r,\theta,\phi)\,\Psi(r,\theta,\phi)}$$

and a probability interpretation

$$\boxed{\begin{aligned}&\text{Prob}\left(r_a \leq r \leq r_b \text{ AND } \theta_a \leq \theta \leq \theta_b \text{ AND } \phi_a \leq \phi \leq \phi_b\right)\\ &= \int_{r_a}^{r_b} dr \int_{\theta_a}^{\theta_b} d\theta \int_{\phi_a}^{\phi_b} d\phi \; r^2 \sin\theta \; |\Psi(r,\theta,\phi)|^2\end{aligned}}$$

Angular momentum operators

The classical angular momentum is

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

and we can use Cartesian co-ordinate expressions for the components of these to determine expressions for comparable quantum angular momentum operators.

2 Angular momentum operators: definition

The classical angular momentum is

$$\mathbf{L} = \mathbf{r} \times \mathbf{p}$$

where

$$\mathbf{r} = x\,\hat{\mathbf{i}} + y\,\hat{\mathbf{j}} + z\,\hat{\mathbf{k}}$$
$$\mathbf{p} = p_x\,\hat{\mathbf{i}} + p_y\,\hat{\mathbf{j}} + p_z\,\hat{\mathbf{k}}.$$

a) Determine expressions for each component of angular momentum in terms of the various components of position and momentum.

b) Use these to define an observable operator for each component of angular momentum. Are there any issues with the order of the constituents when doing this?

c) Determine the outcome of the operation of $\hat{L}_z$ on the position wavefunction

$$\Psi(x, y, z) = A\,(x + iy)$$

where A is a constant.

Answer:

a) $$\vec{L} = (x\hat{i} + y\hat{j} + z\hat{k}) \times (p_x\hat{i} + p_y\hat{j} + p_z\hat{k})$$

$$= x p_y \underbrace{\hat{i}\times\hat{j}}_{\hat{k}} + x p_z \underbrace{\hat{i}\times\hat{k}}_{-\hat{j}} + y p_x \underbrace{\hat{j}\times\hat{i}}_{-\hat{k}} + y p_z \underbrace{\hat{j}\times\hat{k}}_{\hat{i}} + z p_x \underbrace{\hat{k}\times\hat{i}}_{\hat{j}} + z p_y \underbrace{\hat{k}\times\hat{j}}_{-\hat{i}}$$

$$= (y p_z - z p_y)\,\hat{i} + (z p_x - x p_z)\,\hat{j} + (x p_y - y p_x)\,\hat{k}$$

$$\Rightarrow \quad L_x = y p_z - z p_y$$
$$L_y = z p_x - x p_z$$
$$L_z = x p_y - y p_x$$

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

(Note $\hat{y}\hat{p}_z = \hat{p}_z\hat{y}$ so order doesn't matter)

c) $\hat{L}_z |\Psi\rangle \rightsquigarrow \left[x\left(-i\hbar\frac{\partial}{\partial y}\right) - y\left(-i\hbar\frac{\partial}{\partial x}\right)\right]\Psi(x,y,z)$

$$= -i\hbar\left[x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right]A(x+iy)$$

$$= -i\hbar\left[xAi - Ay\right]$$

$$= \hbar A(x+iy)$$

$$= \hbar\,\Psi(x,y,z)$$

$\therefore$ This is an eigenstate with eigenvalue $\hbar$.