Phys 231 2021

Lecture 31

Tues: HW by 5pm

Weds: Read 7.2

Quantum Theory in Three Dimensions

In most situations the location of a particle requires more than one spatial co-ordinate and we need to extend quantum theory to such multi-dimensional situations. Examples of these include:

1) free particles in three dimensions
2) particles in three dimensional wells
3) three dimensional harmonic oscillator
4) electrons inside atoms.

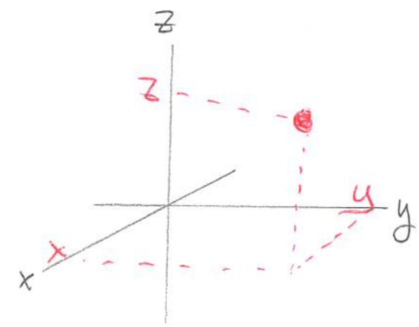
The basic concepts and structure of quantum theory will be unaltered. However, new features will appear. For example:

1) there are often multiple distinct states with the same energy
2) there are situations where symmetries are present and these are important for conserved quantities and also the structure of states.

Basic notation and concepts of probabilities

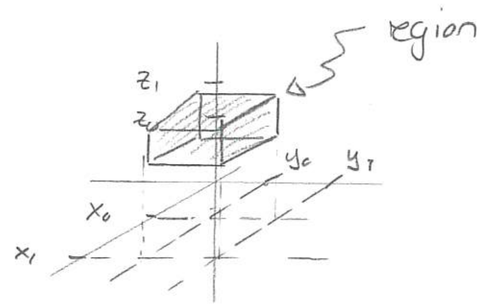
In three dimensions a position measurement gives an outcome that consists of three numbers, or co-ordinates:

$$(x,y,z) \equiv \vec{r} \equiv x\hat{i} + y\hat{j} + z\hat{k}$$



We will then consider the probability with which various position measurement outcomes occur. Again these are expressed in terms of ranges of outcomes. So the most general probability assignment is:

$$\text{Prob}\left(x_0 \le x \le x_1 \text{ AND } y_0 \le y \le y_1 \text{ AND } z_0 \le z \le z_1\right)$$



which describes the probability with which the particle will be in a certain three dimensional region. Such probabilities can be calculated by a probability density $P(x,y,z)$ whose purpose is to compute such probabilities:

$$\text{Prob}\left(x_0 \le x \le x_1 \text{ AND } y_0 \le y \le y_1 \text{ AND } z_0 \le z \le z_1\right) = \int_{z_0}^{z_1}\int_{y_0}^{y_1}\int_{x_0}^{x_1} P(x,y,z)\,dx\,dy\,dz$$

We abbreviate the probability density

$$P(x,y,z) = P(\vec{r})$$

and the volume element $dV = dx\,dy\,dz$.

So we would write

$$\int_{z_0}^{z_1}\int_{y_0}^{y_1}\int_{x_0}^{x_1} P(x,y,z)\,dx\,dy\,dz \equiv \int_{\text{region}} P(\vec{r})\,dV$$

This is shorthand for the l.h.s.

The probability must be normalized over all space. Thus

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} P(x,y,z)\,dx\,dy\,dz = \int_{\text{allspace}} P(\vec{r})\,dV = 1$$

We can also use this probability density to compute (marginal) probabilities such as

$$\text{Prob}\left(x_0 \le x \le x_1 \text{ REGARDLESS of } y,z\right) = \int_{z=-\infty}^{\infty}\int_{y=-\infty}^{\infty}\int_{x_0}^{x_1} P(x,y,z)\,dx\,dy\,dz.$$

Wavefunctions for three dimensions

In quantum theory the probability density is determined by a wavefunction, which, in general, is a function of three co-ordinates and time. Thus

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

This gives a time independent probability density

$$\boxed{P(x,y,z,t) \equiv P(\vec{r},t) = |\Psi(x,y,z,t)|^2 = |\Psi(\vec{r},t)|^2}$$

Then this is normalized if

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} |\Psi(x,y,z,t)|^2 \, dx\, dy\, dz = 1$$

and is used to determine probabilities via:

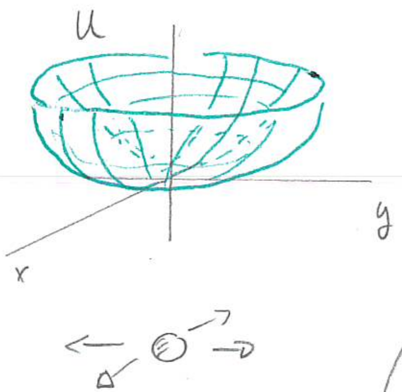
$$\text{Prob}(x_0 \le x \le x_1 \text{ AND } y_0 \le y \le y_1 \text{ AND } z_0 \le z \le z_1) = \int_{z_0}^{z_1}\int_{y_0}^{y_1}\int_{x_0}^{x_1} |\Psi(x,y,z,t)|^2 \, dx\, dy\, dz$$

Quiz 1
- all
- square roots

Schrödinger equation in three dimensions

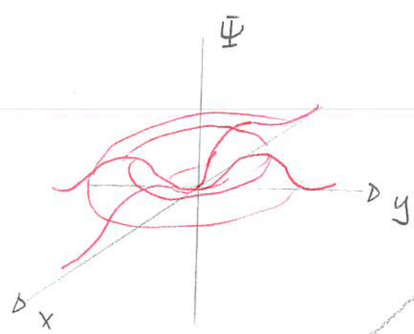
The method for determining the suitable wavefunction is similar to the one dimensional case:

specify potential $U(x,y,z)$



particle mass m

→ Particle is described by three dimensional complex wavefunction $\Psi(x,y,z,t)$



↳ Wavefunction satisfies three dimensional Schrödinger equation

The three dimensional Schrödinger equation is:

$$-\frac{\hbar^2}{2m}\left[\frac{\partial^2\Psi}{\partial x^2}+\frac{\partial^2\Psi}{\partial y^2}+\frac{\partial^2\Psi}{\partial z^2}\right]+U(x,y,z)\,\Psi(x,y,z,t)=-i\hbar\frac{\partial}{\partial t}\Psi(x,y,z,t)$$

There is a short-hand notation for the combination of spatial derivatives. The "del squared" operator is defined as

$$\nabla^2 := \frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}$$

and thus

$$\nabla^2\Psi = \frac{\partial^2\Psi}{\partial x^2}+\frac{\partial^2\Psi}{\partial y^2}+\frac{\partial^2\Psi}{\partial z^2}$$

Then the Schrödinger equation becomes

$$-\frac{\hbar^2}{2m}\nabla^2\Psi + U\Psi = -i\hbar\frac{\partial\Psi}{\partial t}$$

Again we can split the time and spatial parts. This gives stationary states or energy eigenstates with a particular energy E.

$$\Psi(\vec{r},t) = \psi(\vec{r})e^{-iEt/\hbar}$$

and the stationary state $\psi(\vec{r})$ only depends on spatial co-ordinates and satisfies the three dimensional time-independent Schrödinger equation:

$$-\frac{\hbar^2}{2m}\nabla^2\psi + U(\vec{r})\psi(\vec{r}) = E\psi(\vec{r}) \Leftrightarrow -\frac{\hbar^2}{2m}\left[\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}+\frac{\partial^2\psi}{\partial z^2}\right]+U(x,y,z)\psi(x,y,z) = E\psi(x,y,z)$$

Free particle in three dimensions

The TISE for a free particle in three dimensions is:

$$\frac{-\hbar^2}{2m}\left[\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}+\frac{\partial^2\psi}{\partial z^2}\right] = E\psi$$

We can consider various candidate solutions, guided by comparable one dimensional solutions, i.e. $\psi(x) = Ae^{ikx}$

Quiz 2

For ψ_1,

$$\frac{\partial^2\psi_1}{\partial x^2} = A(i2)^2 e^{i2x} \qquad \frac{\partial^2\psi_1}{\partial y^2} = A(i)^2 e^{iy}$$

substitution gives:

$$\frac{-\hbar^2}{2m}\left[A(-4)\, e^{i2x} + A(-1)e^{iy}\right] = E\left[Ae^{i2x} + Ae^{iy}\right]$$

$$\Rightarrow \quad \frac{\hbar^2}{2m}\left[4e^{i2x} + e^{iy}\right] = E\left(e^{i2x} + e^{iy}\right)$$

different / cannot cancel

For ψ_2 we get:

$$-\frac{\hbar^2}{2m}\left[\frac{\partial^2\psi_2}{\partial x^2}+\frac{\partial^2\psi_2}{\partial y^2}+\frac{\partial^2\psi_2}{\partial z^2}\right] = -\frac{\hbar^2}{2m}\left[A(-4)\,e^{i2x}e^{iy} - Ae^{i2x}e^{iy}\right] = EAe\cdots$$

$$\Rightarrow \quad \frac{\hbar^2}{2m}5\, e^{i2x}e^{iy} = E e^{i2x}e^{iy}$$

Thus we see that the product of two basic one dimensional wavefunctions is a solution but the sum is not. We will see this throughout.