Example: Uncertainty in momentum

Electron confined in a region of width 1×10^{-10} m.

a) Calculate uncertainty in momentum.

$$\Delta x = 1\times10^{-10}\,m$$

$$\Delta p_x = \frac{\hbar}{\Delta x} = \frac{1.055\times10^{-34}\,J.s}{1\times10^{-10}\,m} = 1.1\times10^{-24}\,\frac{kg.m}{s}$$

b) Kinetic energy associated with this uncertainty

$$K = \frac{(\Delta p_x)^2}{2m} = \frac{(1.1\times10^{-24})^2}{2(9.11\times10^{-31})}$$

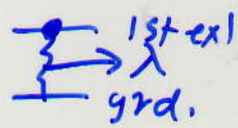
$$= 6.1\times10^{-19}\,J = 3.8\,eV$$

Region is roughly size of an atom. Electron has roughly this much energy in an atom.

$\Rightarrow$ Uncertainty principle gives order of magnitude values of relevant quantities.

Example: Uncertainty in energy and time

Sodium atom remains in its lowest excited state for 1.6×10^{-8} s before making transition to ground state.



a) Uncertainty in energy of the excited state?

$$\Delta E = \frac{\hbar}{\Delta t} = \frac{1.055\times10^{-34}\,J.s}{1.6\times10^{-8}\,s} = 6.6\times10^{-27}\,J$$

$$= 4.1\times10^{-8}\,eV$$

b) Spectral width of radiation of $\lambda = 589$ nm + of energy $E = 2.105$ eV

$$\frac{\Delta\lambda}{\lambda} = \frac{\Delta E}{E} \Rightarrow \Delta\lambda = \frac{\Delta E}{E}\lambda = \frac{4.1\times10^{-8}}{2.105}\times 589\,nm = \underline{0.000011\,nm}$$

Lecture 17

Final Exam

Monday, August 30
4:00 PM – 6:00 PM
Room: Disque 108

Make up lab:

Tuesday, Wednesday, Thusday
Next week

Please e-mail ~~to~~
Dr. Joseph Trout
at: st9217c3@drexel.edu
~~Let him Know~~
to schedule a time

Wave Function

Last time we have established particle-wave duality of matter. What is the nature of the particle wave and what is the corresponding wave function?

For EM waves:	E, B fields
Four sound waves:	Pressure
For String waves	dispacement
For water waves	displacement

All these wave functions satisfy the same wave equation

$$\frac{\partial^2 f(x,t)}{\partial x^2} = \frac{1}{v^2} \frac{\partial^2 f(x,t)}{\partial t^2}$$

Where $f(x,t) = E(x,t),\ B(x,t)$ EM wave

$= p(x,t),\ \rho(x,t)$ Sound wave

$= y(x,t)$ string or water wave

All these waves carry energy and momentum but no mass transportation

The simplest solution of wave eqn is $f(x,t) = A\cos(kx - \omega t)$

with $\omega = 2\pi f = \frac{2\pi}{T}$, $k = \frac{2\pi}{\lambda}$

This wave function is extended over all space and time

We have seen intensity or energy density at any point ~~and~~ at any instant

$$I \propto |f(x,t)|^2 \quad \text{cf: } I \propto |E|^2$$

We expect wave function representing matter to be different because matter wave carries mass and (often) electric charge in addition.

If matter wave function is $\Psi(x,y,z,t)$,
$|\Psi(x,y,z,t)|^2$ = Prob. of finding the particle at location (x,y,z) and at time t.

$\Psi(x,y,z,t)$ is called "probability amplitude".

This interpretation of $\Psi(x,y,z,t)$ would mean

$$\iiint |\Psi(x,y,z,t)|^2 \, dx\, dy\, dz = 1$$

since the particle must be found somewhere in space

$\Rightarrow$ The wave function is normalized (Max ~~Planck~~ Born)

~~S~~tationary States

We expect probability $|\psi(x,y,z,t)|^2$ to be a function of both space and time coordinates. If particle is in a stationary state of constant energy, $|\Psi|^2$ at each point is independent of time. For a particle in a state of definite energy, we can write

$$\Psi(x,y,z,t) = \psi(x,y,z)\,e^{-i\frac{E}{\hbar}t} = \psi(x,y,z)\,e^{-i\omega t}$$

Such that

$$P(x,y,z,t) = |\Psi(x,y,z,t)|^2$$

$$= \Psi^*(x,y,z,t)\,\Psi(x,y,z,t)$$

$$= \psi^*(x,y,z)\,\cancel{e^{+i\frac{E}{\hbar}t}}\,\psi(x,y,z)\,\cancel{e^{-i\frac{E}{\hbar}t}}$$

$$= \psi^*(x,y,z)\,\psi(x,y,z) = |\psi(x,y,z)|^2$$

$\Rightarrow$ Probability is independent of time for a particle in a given energy state or eigenstate.

$\Rightarrow$ A stationary state is a state of definite energy. Example: electrons in different orbits in hydrogen atom

~~We~~ The question is how do we find the matter wave function $\Psi(x,y,z,t)$? What kind of "wave" equation does it satisfy?

Schroedinger Equation

String waves and other mechanical waves (sound, water) satisfy wave eqn derived from Newton's mechanics
EM wave equation derived from Maxwell's equations.

Matter waves are described by a wave eqn advanced by Austrian physicist Irwin Schroedinger in 1926.

Schroedinger eqn. cannot be derived just Newton's laws of motion cannot be derived. Validity lies in agreement with experiment. Ψ obtained from Schroedinger eqn gives average values of all physical quantities like position, energy, momentum, angular momentum, etc. For example, average position of a particle

$$\langle x \rangle = \int_{-\infty}^{\infty} \psi^* x \psi \, dx$$

. Also, called expectation value.

Average value of any function of x

$$\langle f(x) \rangle = \int_{-\infty}^{\infty} \psi^* f(x) \psi(x) \, dx$$

These should agree with experimental values.

The Schroedinger Equation for a particle of mass m in a force field

Total energy

$$E = K + U = \frac{p^2}{2m} + U$$

Using de Broglie hypothesis

$$p = \frac{h}{\lambda} = \frac{h}{2\pi}\cdot\frac{2\pi}{\lambda} = \hbar k$$

and $E = hf = \frac{h}{2\pi}\cdot 2\pi f = \hbar\omega$

Above energy eq.

$$\hbar\omega = \frac{\hbar^2 k^2}{2m} + U(x)$$

Remembering wave eqn. for $\vec{E}$

$$\frac{\partial^2 E}{\partial x^2} = \frac{1}{c^2}\frac{\partial^2 E}{\partial t^2}$$

Choosing soln $E = E_0 \cos(kx - \omega t)$

we get $-k^2 = -\frac{\omega^2}{c^2}$

From this can conclude 1st derivative of wave function should give $\hbar\omega$ and second derivative $\frac{\hbar^2 k^2}{2m}$ for matter wave.

Schroedinger eq. should be first order in time derivative and 2nd order in position derivative. So Schroedinger wrote (1-dimension)

$$\boxed{-\frac{\hbar^2}{2m}\frac{d^2\Psi(x,t)}{dx^2} + U(x)\,\Psi(x,t) = i\hbar\frac{\partial\Psi}{\partial t}(x,t)}$$

For the stationary state of energy E

$$\Psi(x,t) = \psi(x)\,e^{-i\omega t} \quad \text{since } \omega = \frac{E}{\hbar}$$

get

$$\boxed{-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + U(x)\,\psi(x) = E\,\psi(x)}$$

where $E = \hbar\omega$

E is the total energy of the system.

We know Schroedinger eq. is correct because predictions made by using this eq. agree with expt.

Wave function for a free particle

If the particle is free $U(x) = 0$

S. eqn: $-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\,\psi(x)$

Try soln: $\psi(x) = A\cos kx + B\sin kx$

$$\frac{d\psi}{dx} = k\left[-A\sin kx + B\cos kx\right]$$

$$\frac{d^2\psi}{dx^2} = -k^2\left[A\cos kx + B\sin kx\right] = -k^2\psi$$

Substituting in S. eqn $\boxed{\frac{\hbar^2 k^2}{2m} = E}$ Allowed values of k can be found from boundary condition

Wave Function for a Free Particle

Free particle $\Rightarrow$ no barrier, no force

$\Rightarrow$ $U(x) = 0$.

Schroedinger eqn

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi \Rightarrow \frac{d^2\psi}{dx^2} + \frac{2mE}{\hbar^2}\psi = 0$$

$$\boxed{\frac{d^2\psi}{dx^2} + k^2\psi = 0} \quad \text{where} \quad k^2 \equiv \frac{2mE}{\hbar^2}$$

Most general soln.

$$\psi(x) = A e^{ikx} + B e^{-ikx} \qquad e^{\pm ikx} = \cos kx \pm i \sin kx$$

Introducing time dependence

$$\Psi(x,t) = \psi(x)\, e^{-i\omega t} = \overset{\rightarrow}{A e^{i(kx-\omega t)}} + \overset{\leftarrow}{B e^{-i(kx+\omega t)}}$$

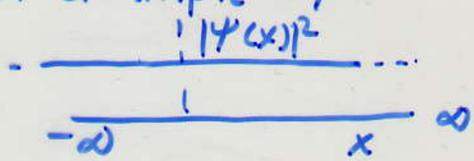
First term: wave traveling to right and second term: wave traveling to left. Concentrating on wave traveling to right ($B=0$)

$$\psi(x) = \psi_0\, e^{i(kx-\omega t)}, \text{ replacing } A \text{ by } \psi_0.$$

Prob. of finding particle at x at time t

$$P(x,t) = |\psi(x,t)|^2 = |\psi_0|^2 e^{i(kx-\omega t)} e^{-i(kx-\omega t)} = |\psi_0|^2$$

It is the same for all $x \Rightarrow$ no info. about position of particle. This is an example of <u>uncertainty principle</u>.



No forces $\Rightarrow$ p const, $\Delta p = 0$

$\Rightarrow$ $\Delta x \to \infty$ by uncertainty principle

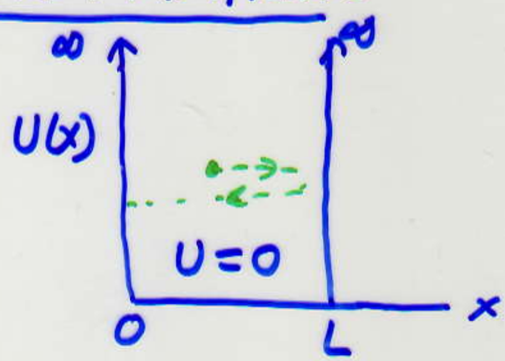
Chapter 40

Quantum Mechanics

Here we solve Schroedinger eqn for realistic physical systems with appropriate boundary conditions. This gives allowed energy values (eigenvalues) and wave functions (eigenfunctions). These can be used to calculate expectation values or average values of physical properties.

Particle in a Box or Particle in Infinite Square Well potential

$$U(x) = 0 \quad \text{for } 0<x<L$$
$$= \infty \quad \text{for } x \leq 0 \text{ or } x \geq L$$



$\Rightarrow \quad \psi(x) = 0$ at $x \leq 0$ or $x \geq L$

In region $0<x<L$, Schroedinger eqn

$$\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi = -k^2\psi$$

where $k^2 = \dfrac{2mE}{\hbar^2}$

Two independent soln : $\sin kx$ and $\cos kx$

General Solution

$$\psi(x) = A \sin kx + B \cos kx$$

Boundary conditions at $x=0$ + L and normalization condition give A, B and k.

$$\psi(0) = 0 + B = 0 \Rightarrow B = 0$$

$$\psi(x) = A \sin kx$$

$$\psi(L) = \sin kL = 0$$

$$\Rightarrow \quad kL = n\pi, \quad n = 1, 2, \cdots$$

Allowed energy levels

$$kL = \sqrt{\frac{2mE}{\hbar^2}}\, L = n\pi$$

$$\boxed{E_n = \frac{\pi^2 \hbar^2 n^2}{2mL^2}}$$

$\Rightarrow$ Energies of particles in a box are quantized.

Eigenfunctions

$$\psi_n(x) = A \sin \frac{n\pi x}{L}$$

Normalization:

$$\int_0^L |\psi_n(x)|^2 dx = A^2 \int_0^L \sin^2 \frac{n\pi x}{L}\, dx = A^2 \frac{L}{2} = 1$$

$$A = \sqrt{\frac{2}{L}}$$