Lec11

- Intro to Quantum Mechanics

- Numerical solution of Schödinger's equation

Why/when quantum ?

- Newton's laws give a *very* accurate description of the behavior of everyday objects/motions.

- But they fail miserably to describe atoms !

- This was a *crisis* for physics at turn of century ...

  - Eg Laws of EM + Newton's mechanics predicts atoms should be *unstable*

  - Electrons classically have any energy but see only *discrete* energies

  - Energy of electromagnetic waves in vacuum infinite! Diffraction of electrons..

  - Photoelectric effect − light waves like particles !

Resolution

- Radical. Took many physicists about 20 years to discover.

- Discovered twice. Schrödinger, Heisenberg (1926).

- Arguably become the most well tested and accurate scientific theory (Quantum electrodynamics)

Basics

- Discard notion that microscopic objects like electrons can a well defined position, velocity etc.

- Not a practical issue but one of principle!

- Instead think of them as being described by a *wavefunction* Ψ(x,t). Like a usual wave in sense that electron is not *localized* like a classical particle.

- But this is a *probability wave*. $|\Psi(x,t)|^2$ yields probability of finding particle at (x,t).

- Dynamics: replace Newton's laws (simple ordinary differential equations) by Schrödnger's equation (partial differential equation)

Schrödinger's equation

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

- Equation looks like a funny wave equation (but only first order in t)

- Involves square root of minus 1 (i). In general Ψ is *complex*! Hence need $|\Psi|^2$ for positive *real* probability

- New fundamental constant introduced $\hbar = 1.05 \times 10^{-34}$ Js. Planck's constant.

Stationary states

- Put $\Psi = \phi(x)e^{-iEt/\hbar}$. Plug into equation. Find *time independent* Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{\partial^2\phi}{\partial x^2} + V\phi = E\phi$$

- Such a wavefunction describes the allowed state of say electron in an atom with E being its energy.

- Try to solve schematically. In general only certain energies *allowed*!

Allowed energies

Rewrite equation:

$$\frac{d^2\phi}{dt^2} = \left[\frac{2m\,(V(x) - E)}{\hbar^2}\right]\phi$$

- For a *bound* state need $V > E$ at large x.

- In which case this equation develops *exponential* solutions

  $$\phi \sim e^{\kappa x}, e^{-\kappa x}$$

  with $\kappa^2 = \frac{2m(V(x)-E)}{\hbar^2}$.

- For small x $V < E$ and generate oscillatory solutions

  $$\phi \sim \sin \kappa x, \cos \kappa x$$

Allowed energies II

- Need $\int_{-\infty}^{\infty} dx \phi^2(x) = 1$. Probability.

- Thus need to choose correct solution as $x \to \pm\infty$.

- Inside will get oscillations.

- Must smoothly match at boundary.

- Requires that E be very carefully chosen. In general discrete set of possible E's - energy level quantization.

How to solve numerically ?

Rewrite equations:

$$\begin{aligned} \frac{d\phi}{dx} &= p \\ \frac{dp}{dx} &= \left[\frac{2m\left(V(x)-E\right)}{\hbar^2}\right]\phi \end{aligned}$$

Consider case $V(-x) = V(x)$. Can show $\phi(x)$ is either even or odd function.

In former case choose $\phi(0) = 1$ and $p(0) = 0$

Choose some E and integrate equations using Euler/leapfrog.

Look at $|\phi(x)|$ for large $|x|$, If it is growing will not be able to impose $\int \phi^2 = 1$.

Choose another E and try again.

Shooting method.

What happens

- Find only discrete set of E work. So both wavefunction and E are output from calculation!

- $E_0 > V_{\text{min}}$. Otherwise cannot match with large x asymptotics. Particle cannot be stationary at minimum of potential. Quantum fluctuations even for zero temperature.

- E increases with number of oscillations.

- Find E using bisection algorithm ...

Summary

- In QM speak only of probabilities. Throw out notion that particles have simultaneously well-defined positions and momenta (Heisenberg uncertainty principle: $\delta x \delta p \geq \hbar$.)

- Probabilities gotten by solving Schrödinger equation. Can be solved using same algorithm as used for Newton's equations!

- For bound state problems find discrete spectrum of allowed energies/states.

- Many other things we haven't talked about: scattering, making quantum observations, relativity, many particles, approximation methods, operators, connection to classical physics, ...