QM Basics II

UP201

IISc Bangalore

Basic Postulates of Quantum Mechanics

1. State of a Particle – Wave Functions
2. Physical Observables – Hermitian Operators
3. Outcome of Experiment – Expectation Values
4. Uncertainty Relations – Commutation Relations
5. Time Evolution – Schrödinger Equation

Some questions....

- What is really “the uncertainty principle”?
  - Why do we have metals?
  - What happens in a TEM?
- Oh, how is all this related to classical mechanics?
- Fine, but how do I solve the Scrödinger equation?

The *Essence* of Uncertainty Principle

- If state of the particle corresponds to spatial localization, then there is a large uncertainty in momentum
- In a state with expected momentum zero, spatial localization implies larger kinetic energy
- Understand this with a state $\psi(x) = \delta(x - x0)$ for free particle
  - Particle is at $x0$ with no uncertainty
  - $\langle P \rangle = 0$
  - $\langle P^2 \rangle \longrightarrow \infty$...kinetic energy blows up!

The *Essence* of Uncertainty Principle

- Moral...if you localize particle of mass m to a size scale ℓ, it will cost you kinetic energy roughly equal to $\frac{\hbar^2}{m\ell^2}$!
- The essence of metallic bonding...electrons are *delocalized* from their atomic states and are free to wander around...hence lower kinetic energy! (Of course, you can now ask...why have insulators(ionic bonds)?)
- "Resonance stabilization" in Benzene..all the way...graphite!
- Even stuff like anti-ferromagnetism has origins in this!

The *Essence* of Uncertainty Principle

- What happens in a TEM?
- Electrons are accelerated to a momentum $p_0 = \hbar k_0$...state of the electron $\psi(x) = e^{ik_0 x}$...or is it?
- Recall Gaussian distributions...
- State of the electron...superpositon of momentum states with momentum uncertainty Δk (called a Gaussian wavepacket!)

$$\begin{aligned} \psi(x) &= \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi}} e^{\frac{(k-k0)^2}{2\Delta k^2}} e^{ikx} dk \\ &\approx e^{-\frac{(x^2)\Delta k^2}{2}} e^{ik_0 x} \\ \implies \Delta x &\approx \frac{1}{\Delta k} \implies \Delta k \Delta x \approx 1 \quad \text{or} \quad \Delta p \Delta x \approx \hbar!! \end{aligned}$$

The *Essence* of Uncertainty Principle

- If Δk is large then electrons begin to behave like particles!
- The key to a good TEM (or SEM) is to keep Δk small so that electrons are in nearly a plane wave state!
- The same goes with neutrons! Or anything else...

Ahh...I want my Classical Mechanics!

- How is all this related to classical mechanics?
- Recall Hamilton's equations
- Learn the consequences of Scrödinger before solving anything
- Ehrenfest theorem!

Ok...here is your Classical Mechanics!

- Ehrenfest theorem
  - $\frac{d\langle X\rangle}{dt} = \frac{\langle P\rangle}{m}$
  - $\frac{d\langle P\rangle}{dt} = -\langle\frac{\partial V}{\partial X}\rangle$
- Proof of these are very instructive
- Classical systems consists of situations where $\hbar$ is a "small number"...hence uncertainties are small...
- We thus recover classical mechanics...phew!

How about tackling Schrödinger?

- Slight change in notation...time dependent wavefunction $\Psi(x,t)$
- Schrödinger tells $i\hbar\frac{\partial\Psi}{\partial t} = H\Psi$
- Initial condition $\Psi(x,0) = \psi^0(x)$
- Assume H is independent of time
- Separation of variables ansatz $\Psi(x,t) = \psi(x)T(t)$ (we will understand what this means in a minute!)

Tackling Schrödinger contd...

- Ansatz implies $i\hbar \frac{1}{T}\frac{\partial T}{\partial T} = \frac{H\psi}{\psi} = E$
- Argument...T part depends only on time and ψ part depends only on space and hence E must be a number (independent of t or x)
- Thus, $T(t) = Ce^{-\frac{-iEt}{\hbar}}$
- Have to solve $H\psi = E\psi$...*an eigenvalue problem*!
- States that satisfy the ansatz are *eigenstates* of the Hamiltonian operator H
- Also called *stationery states*!
- If ψ^0 is an eigenstate of H it will stay in that state...*energy is conserved!* Hence, called stationery...(prove this).

General Solution

- In general $H\psi = E\psi$ leads to a eigenvalues and eigenstates E_n and ψ_n
- Since H is Hermitian ψ_n form a basis
- Expand ψ^0 in terms of ψ_n i.e.,$\psi^0(x) = \sum_n a_n \psi_n(x)$
- Can easily verify that $\Psi(x,t) = \sum_n a_n \psi_n(x) e^{\frac{-iE_n t}{\hbar}}$ is the solution of Schrödinger
- Schrödinger tackled...need to "Diagonalize the Hamiltonian"
- Look at specific examples later...most of the QM is "just" specific examples of this!!

Summary

- The meaning of uncertainty relations
- Classical and Quantum connections
- Schrödinger tackled