



Quantum Mechanics Basics II



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 Schrödinger 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 $\psi(x) = \delta(x - x_0)$ for free particle
 - Particle is at x_0 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...superposition of momentum states with momentum uncertainty Δk (called a Gaussian wavepacket!)

$$\begin{aligned}
 \psi(x) &= \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi}} e^{-\frac{(k-k_0)^2}{2\Delta k^2}} e^{ikx} dk \\
 &\approx e^{-\frac{(x^2)\Delta k^2}{2}} e^{ik_0 x} \\
 \Rightarrow \Delta x &\approx \frac{1}{\Delta k} \Rightarrow \Delta k \Delta x \approx 1 \quad \text{or} \quad \Delta p \Delta x \approx \hbar!!
 \end{aligned}$$



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 Schrödinger before solving anything
- Ehrenfest theorem!



Ok...here is your Classical Mechanics!

- **Ehrenfest theorem**

- $$\frac{d\langle X \rangle}{dt} = \frac{\langle P \rangle}{m}$$

- $$\frac{d\langle P \rangle}{dt} = -\left\langle \frac{\partial V}{\partial X} \right\rangle$$

- **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...pew!**



How about tackling Schrödinger?

- Slight change in notation...time dependent wavefunction $\Psi(x, t)$
- Schrödinger tells $\frac{\partial \Psi}{\partial t} = H\Psi$
- 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 stationary states!
- If ψ^0 is an eigenstate of H it will stay in that state...energy is conserved! Hence, called stationary...(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