QM Basics I

UP201

IISc Bangalore

Why Quantum Mechanics?

- Ultraviolet catastrophe
- Photoelectric effect
- Stability of atoms
- Spectrum of atoms
- Specific heat anomaly

What you know already...and more!

- Bohr model of atom
- Wave-particle duality $\lambda = h/p$ or $p = \hbar k$
- Heisenberg uncertainty relation $\Delta p \Delta x \geq \hbar$
- Can understand working of an electron microscope from these...and many other things!
- Still, not clear why an atom has discrete spectrum!
- ...
- To find out, we proceed along lines of Schrödinger, Heisenberg and Dirac
- Goal: Understand how QM works in 1D...but first..

Some Probability that you Probably know with Probability 1

- x_i is an outcome of a trial with probability $P(x_i)$
- The mean value of many trials is $\langle x \rangle = \sum_i x_i P(x_i)$
- The variance (or *uncertainty*)is Δx is given by

$$(\Delta x)^2 = \langle (x - \langle x \rangle)^2 \rangle = \langle x^2 \rangle - \langle x \rangle^2$$

- If outcome is continuous, then $P(x)dx$ is the probability that the outcome will be between x and $x + dx$. Also,

$$\langle x \rangle = \int x P(x) dx$$

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

We shall be prisoners of 1D until further notice!

What is an “Electron” anyway?

- Is it a “Particle”? or is it a “wave”?
- We really don’t know! It is not a “particle” or a “wave”!!
- We think it has mass m (and may be a charge!)
- “Particle” now really means a quantum mechanical entity!
- How do we describe its *state*? Recall, in classical mechanics it is described by two numbers (x, p)!

State of a Particle

- Consider a particle in 1D "box" $(-L \leq x \leq L)$
- A *state* of the particle is described by a continuous complex valued function $\psi(x)$ called the "wavefunction"! Thus the set of all possible states of the particle from a vector (Hilbert) space
- The wavefunction satisfies $\int_{-L}^{L} \psi^*(x)\psi(x)dx = 1$
- Wavefunction cannot be measured directly...so what can we measure?
- A *single trial* to measure position will result in *any* value of x between $-L$ and L!
- "Experiment" in quantum mechanics has a different meaning! It means an collection of single trial performed on identical copies of systems!

Meaning of the Wavefunction

- We cannot predict the outcome of a *single trial*! We *can* predict outcome of a collection of *single trials* on identically prepared systems, simply called "experiment" or "observation"!
- Born interpretation : The quantity $|\psi(x)|^2 dx$ gives the probability that the particle is found between x and $x + dx$ in a trial
- In general, the wavefunction with depend on time; thus the time evolution of the state of the particle is given by $\psi(x, t)$

Physical Observables

- Back to the question...what can we measure?
- Associated with every *physical observable* (say position, momentum, kinetic energy etc.), there is a *Hermitian operator* (say A, in general)
- Let A have a set of eigenvalues a_n and corresponding eigenfunction ϕ_n^A.
- The process of measurement of A in a *single trial* will
  - Result in an eigenvalue a_n as outcome.
  - *Change* ψ to an *eigenstate of A*, and if fact if you found the result to be a_n, ψ will be changed to ϕ_n^A!! You *CANNOT* be an innocent observer in quantum mechanics, if you observe you *WILL* change the state of the system!
- What we can predict is the probability of obtaining a_n as the result of a single trial...this is given by

$$P(a_n) == |\psi_n|^2 = |(\phi_n^A, \psi)|^2$$

(Recall $\psi = \sum_n \psi_n \phi_n^A$ where the c-number $\psi_n = (\phi_n^A, \psi)$.

Physical Observables

- The mean value of A in an experiment is

$$\langle A \rangle = \sum_n a_n |\psi_n|^2 = (\psi, A\psi)$$

Proof: Note $A\phi_n^A = a_n \phi_n^A$, $(\phi_n^A, \phi_m^A) = \delta_{mn}$, $\psi = \sum_n \psi_n \phi_n^A$ and $A\psi = A\left(\sum_n \psi_n \phi_n^A\right) = \sum_n a_n \psi_n \phi_n^A$.

$$\begin{aligned}
\langle A \rangle &= \sum_n a_n \psi_n^* \psi_n \\
&= \sum_{mn} \psi_n^* \delta_{mn} a_n \psi_n \\
&= \sum_{mn} \psi_m^* (\phi_m^A, \phi_n^A) a_n \psi_n \\
&= \left(\left[\sum_m \psi_m \phi_m^A \right], A \left[\sum_n \psi_n \phi_n^A \right] \right) = (\psi, A\psi)
\end{aligned}$$

- The uncertainty in the measurement of A is given by $\langle (A - \langle A \rangle)^2 \rangle = \Delta A^2$

Examples of Physical Observables

- Position – X, $\quad \langle X \rangle = \int_{-L}^{L} \psi^*(x) x \psi(x) dx$
- Momentum – P, $\quad \langle P \rangle = \int_{-L}^{L} \psi^*(x) P \psi(x) dx$
- Electric potential of particle – $V_E(X) = \dfrac{1}{4\pi\varepsilon_0} \dfrac{1}{X}$
- Kinetic energy of particle – $\dfrac{P^2}{2m}$
- Hamiltonian (Total Energy) – $\dfrac{P^2}{2m} + V(X)$, V potential in which "particle moves"
- What are the eigenstates of the position operator?
- All good, but what *is* P?

The Momentum Operator

- The momentum operator *is* $P = -i\hbar D = -i\hbar\frac{\partial}{\partial x}$...apparently, God said this to Schrödinger!!
- What is $[X, P] = XP - PX$? This is the commutator
- Lets calculate:

$$XP\psi \equiv x(-i\hbar\frac{\partial}{\partial x})\psi(x) = -i\hbar x\frac{\partial\psi}{\partial x},$$
$$PX\psi \equiv (-i\hbar\frac{\partial}{\partial x})x\psi(x) = -i\hbar(\psi(x) + x\frac{\partial\psi}{\partial x})$$
$$\implies [X, P]\,\psi = i\hbar\psi$$

- Thus $[X, P] = i\hbar I$...this *is* the statement of uncertainty relation! AKA, canonical commutation relation!
- What are the eigenstates of the momentum operator?

Time Evolution

- And, finally, how does ψ evolve with time? If we know at $t = 0$ the state is $\psi^0(x)$, what will be the state at another time $\Psi(x,t)$?
- God also told Schrödinger

$$i\hbar \frac{\partial \Psi}{\partial t} = H\Psi$$

  where H is the Hamiltonian operator; and that is how states evolve!!
- This is a *first order linear equation* in time with a given initial condition $\Psi(x,0) = \Psi^0(x)$
- This is the analogue of Newton's Law...*cannot ask a 15 mark question to derive Schrödinger equation*...its the quantum *LAW*!

Summary

- State of a particle is described by complex valued functions
- Cannot predict outcome of a *single trial*; "experiment" in quantum mechanics means an "ensemble" of trials
- Cannot measure the wavefunction
- Physical observables are represented by operators with rules for calculating expectation values
- Momentum operator is defined in a "canonical" way which is the basis of the uncertainty relation
- Time evolution via Schrödinger equation