



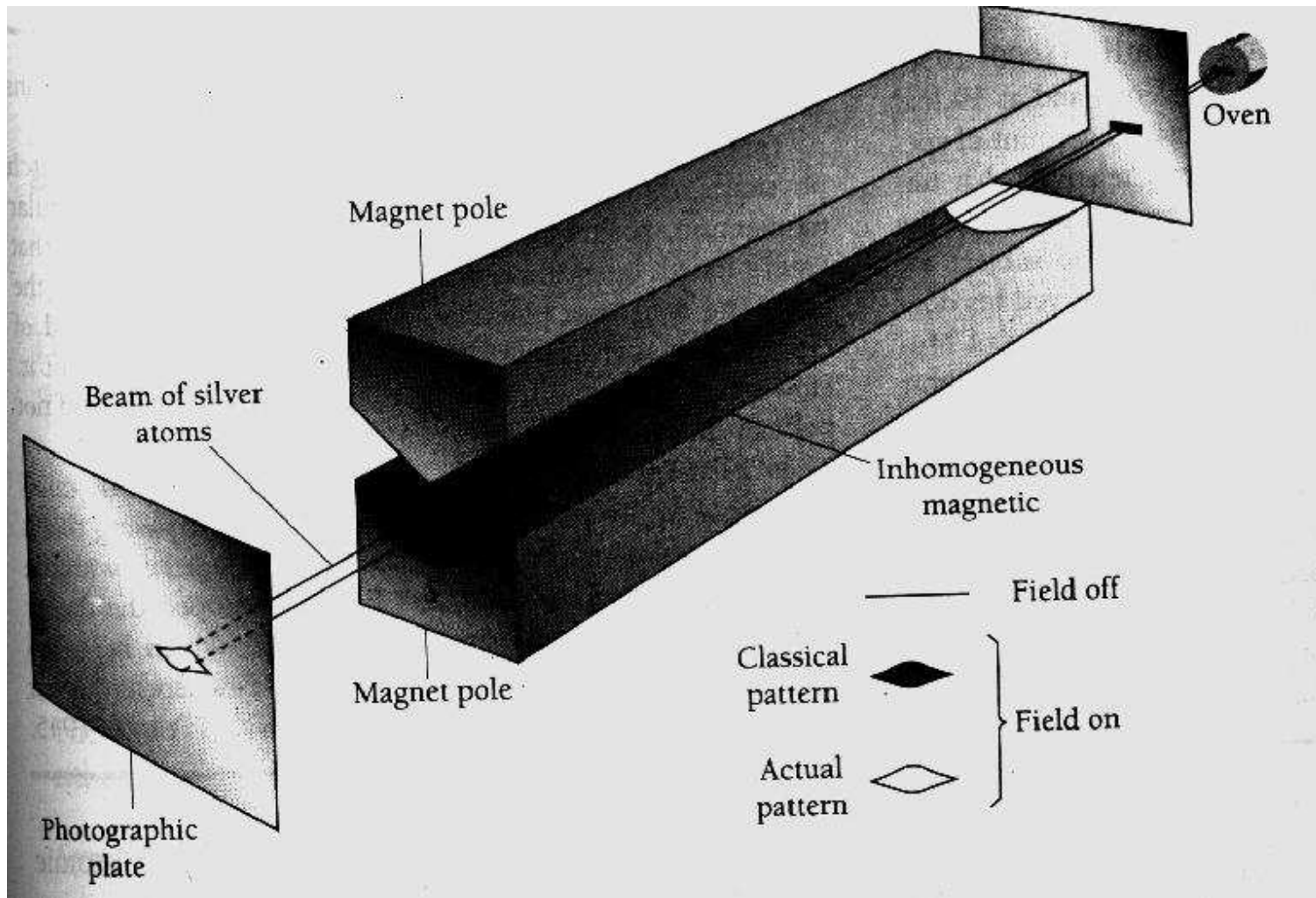
Quantum Mechanics Basics



Why Quantum Mechanics?

- Ultraviolet catastrophe
- Photoelectric effect
- Stability of atoms
- Spectrum of atoms
- Specific heat anomaly
- The “success” Drudé model
- The Stern-Gerlach Experiment

The Stern-Gerlach Experiment



Beiser



Stern-Gerlach contd.

- Silver atoms emanate from an oven and go through a weakly inhomogeneous magnetic field $B(z)e_z$ - Call this the “Z-filter”
- Each atom has an intrinsic magnetic moment μ
- Force on the atom $\sim \cos \theta$ (θ is the angle between μ and e_z)
- Classically we would expect a smeared distribution of atoms
- What is seen is that the beam splits into two! Call this this $+z$ beam and $-z$ beam!
- Suppose $+z$ beam is passed through another Z-filter, what happens? How about X-filter?



The Stern-Gerlach Surprise

- If the $+z$ beam is passed through an Z -filter, it comes out as a single beam
- If the $+z$ beam is passed through an X -filter, it splits into two beams!! A $+x$ and a $-x$!!!!
- Why should the beam split into two in the first place? And, why should the $+z$ split into a $+x$ and a $-x$???
- The answers to these questions lie in quantum mechanics!



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!
- And, what is with Stern-Gerlach?
- ...
- 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) 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,

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



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**

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 form 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 experiment 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 experiments performed on identical copies of systems!



Meaning of the Wavefunction

- We cannot predict the outcome of a single experiment! We can predict outcome of a collection of single experiments 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 an experiment
- In general, the wavefunction with depend on time; thus the time evolution of the state of the particle is given by $\psi(x, t)$
- This may be understood in analogy with the veena string!



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)
- The expected value of outcome of measurement of A is given by $\langle A \rangle = \int_{-L}^L \psi^*(x) A \psi(x) dx$
- The uncertainty in the measurement of A is given by $\langle (A - \langle A \rangle)^2 \rangle = \Delta A^2$
- The process of measurement of A in a single experiment will change ψ to an eigenstate of A !! You **CANNOT** be an innocent observer in quantum mechanics, if you observe you **WILL** change the state of the system! This is what happens in Stern-Gerlach!



Examples of Physical Observables

- **Position** – X , $\langle X \rangle = \int_{-L}^L \psi^*(x)x\psi(x)dx$
- **Momentum** – P , $\langle P \rangle = \int_{-L}^L \psi^*(x)P\psi(x)dx$
- **Electric potential of particle** – $V_E(X) = \frac{1}{4\pi\epsilon_0} \frac{1}{X}$
- **Kinetic energy of particle** – $\frac{P^2}{2m}$
- **Hamiltonian (Total Energy)** – $\frac{P^2}{2m} + V(X)$, 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:

$$\begin{aligned} X\psi &\equiv x(-i\hbar \frac{\partial}{\partial x})\psi(x) = -i\hbar x \frac{\partial \psi}{\partial x}, & PX\psi &\equiv (-i\hbar \frac{\partial}{\partial x})x\psi(x) = -i\hbar(\psi(x) + x \frac{\partial \psi}{\partial x}) \\ [X, P]\psi &= i\hbar\psi \end{aligned}$$

- 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 experiment; “experiment” in quantum mechanics means an “ensemble” of experiments**
- **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**