Chapter 1: Introduction - Why Quantum Theory?

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The Basics: Why Quantum Theory?

- The most important question which one should ask is why quantum mechanics was needed at all!
- We had a pretty successful theory of material particles in form of Newtonian mechanics
- and the electromagnetic theory as embodied in Maxwell's equations described phenomena related to charged particles, electromagnetic waves, and their interactions very well.
- So why bother about a new theory called quantum theory?
- The fact of the matter is that at the beginning of the twentieth century it was realized that our understanding of the physics at the microscopic level was far from complete.

Why quantum theory...

- Some of the phenomena which were poorly understood were:
  1. Black body spectrum
  2. Spectra of various atoms and molecules, quantization of their energy level
  3. Photoelectric effect
  4. Compton effect and several other phenomena.
- Early explanations of these phenomena were given by different people using different approaches
- The common feature of all these approaches was the notion of "quantum".

Emergence of "Quantum"

- For example, the energy levels of the hydrogen atom were explained by Bohr using his hypothesis which implied quantization of energy.
- Black body spectrum was explained by Max Planck who assumed that the energy was quantized.
- Similarly the important assumption involved in the Einstein's work on photoelectric effect was the quantization of the energy of the light waves.
- Thus, the notion of "quantum" emerged from various directions.

Quantum Nature of light

- Planck's explanation of black body radiation and Einstein's explanation of the photoelectric effect both assumed the quantization of light energy with the smallest unit of energy being
$$E_{\text{min}} = h\nu = \hbar\omega \tag{1}$$
where h and $\hbar = \dfrac{h}{2\pi}$ are constants called the Planck's constant, while ν/ω are the frequency/ angular frequency of the radiation involved.
- Thus, it was postulated that these indivisible entities with energy $\hbar\omega$ were objects called photons and that electromagnetic radiation was composed of these objects.

Particle-like nature of light

- It was further postulated that photons also carried momentum given by

$$\vec{p} = \hbar\vec{k} \tag{2}$$

where $\vec{k} \equiv$ wave number is given by

$$\bar{k} = \frac{2\pi}{\lambda}\hat{e} \tag{3}$$

$\hat{e} \equiv$ unit vector in the direction of propagation of light.

- With momenta associated with e.m. radiation, it in fact has particle-like properties.

Wave-particle Duality of Light

- Indeed, the particle-like properties of photons were verified in the Compton's scattering experiment.
- We will discuss Compton scattering/effect in detail later on
- Thus e.m. radiation exhibits both wave-like (interference, diffraction,..) and particle-like (Blackbody radiation, Compton effect, photo-electric effect) properties.
- In other words it exhibits wave-particle duality.

De Broglie's Hypothesis

- Louis de Broglie was inspired by the success of Bohr's model of the hydrogen atom, and the ideas of wave-particle duality of e.m. radiation proposed by Einstein, Planck, and Compton
- He generalized these ideas by arguing that the wave-particle duality is a fundamental property of all matter, and not just light.
- He proposed that even material (massive) particles will also exhibit wave-like properties with the wave length

$$\lambda = \frac{h}{p}, \tag{4}$$

where p is the momentum of the particle.

- Note that this relation is equivalent to Eq.(2) defined for light.
- Louis de Broglie named the waves associated with the material particles “matter waves”.

Heisenberg's Uncertainty Principle

- Heisenberg proposed that at microscopic level there are insurmountable uncertainties associated with physical measurements which are independent of the precision of the apparatus used.
- In other words these uncertainties effectively originate from a fundamental physical law which he called the "uncertainty principle".
- The original formulation of the uncertainty principle was as follows
- If one can measure the x-component of the momentum of a particle with an uncertainty Δp
- One cannot, at the same time, know its x-position more accurately than $\Delta x = \frac{h}{\Delta p}$, where h is Planck's constant.
- This implies

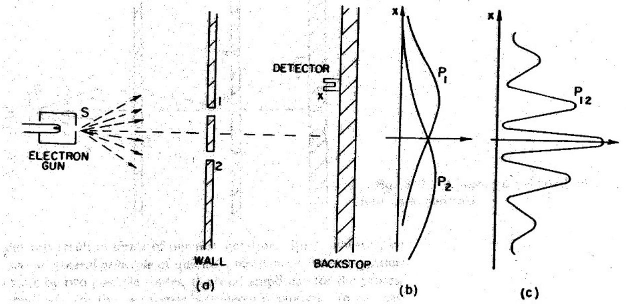
$$\Delta x \Delta p \sim h \tag{5}$$

Uncertainty principle...

- In other words, if one measures the position of an object to a great certainty, its momentum becomes uncertain, and vice versa.
- The same result applies to other components of momenta/position as well.
- We will learn that a more general formulation of the uncertainty principle involves any pair of canonically conjugate variables.
- We will also learn that the uncertainty principle and wave-particle duality are deeply related to each other.
- Next, we will discuss some experiments which illustrate the notions of wave-particle duality and the uncertainty principle.
- Then, we will discuss the connections between the particle vs wave pictures of matter

Young's Double Slit Experiment with Electrons

- Let us consider the experimental set up given below:



- Electrons emitted from a source are made to pass through a double slit arrangement and then they impinge upon a screen on which a detector is placed which is free to move along the screen.

Young's Double Slit Experiment with Electrons, contd...

- If a photographic plate is kept on the screen, then after sufficient exposure, it can be developed to observe the intensity pattern of the scattered electors.
- One finds that, similar) to the double slit experiment performed with the light, the intensity pattern exhibits dark and bright fringes.
- In other words, scattered electrons exhibit wavelike phenomenon of interference.
- This is astounding (amazing)!
- However, the detector on the screen, which can be used to detect even a single electron, reports that at any point on the screen electrons arrive only one at a time.
- This is a very paticle-like behaviour.

Young's Double Slit Experiment with Electrons, contd...

- When the experiment above is done with a very low intensity beam of electrons so that only one electron is emitted at a time, still after sufficient exposure one gets an interference pattern in the screen.
- Under those circumstances, the question is: What is interfering with what?
- Recall that in the optical experiment beams coming for different slits interfere on the screen to give rise to fringes.
- But, here we have material particles which arrive on the screen one at a time, then how can this is interference?
- Since electron is a material particle, it must be passing through either hole 1 or 2 before hitting the screen.

Young's Double Slit Experiment with Electrons, contd...

- So if we add the intensities of the elections scattered from two holes we should get the result of the double slit experiment, right?
- No, wrong!
- So we perform the experiment with holes 2/1 blocked to obtain the intensity patterns P_1/P_2.
- If the intensity patterns obtained with but the holes open is P_{12}, we note that

$$P_{12} \neq P_1 + P_2$$

- Because P_1 and P_2 are essentially Gaussian distributions centered around holes 1/2, while P_{12} exhibits interference fringes.
- Thus, when we know for sure which hole did the electron pass through, interference pattern gets wiped out.

Young's Double Slit Experiment with Electrons, contd...

- We can try a more sophisticated experiment which will not involve blocking any hole, but will be able to tell which hole a given election went through.
- We can put a detector each close to both the holes which only tracks the electrons by say "Shining light" on them but does not absorb then.
- Then by doing coincidence measurements with the detector on screen we can tell which electron passed through which hole.
- If the intensity pattern of electrons passing through hole 1/2 is P_1'/P_2', we find P_1'/P_2' similar to P_1/P_2. Moreover, if the total intensity is P_{12}', we find

$$P_{12}' = P_1' + P_2'$$

and no interference pattern.

- Thus we conclude: When the double slit experiment is performed so that we do not know which hole the individual electrons have passed through, we obtain interference pattern.
- However, whenever we repeat the experiment where we track the electrons through which hole they passed, the interference pattern is wiped out.
- Recall that in optics interference pattern is obtained whenever we can add the amplitudes of the light wave, and is not seen whenever we add the intensities.
- So if we define an 'amplitude' for each electrons journey for the source to the screen as ψ and further classify
  - $\Psi_1 \equiv$ amplitude if the electron passed through hole 1
  - $\psi_2 \equiv$ amplitude if the electron passed through hole 2

Double slite experiment...

- Then when interference pattern is obtained

$$P_{12} \propto |\psi_1 + \psi_2|^2 \equiv \text{ amplitudes are added}$$

and when we know which hole electron passed through

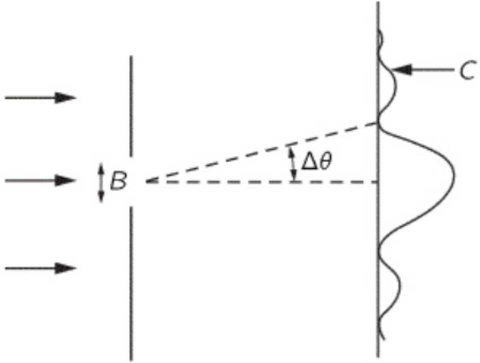
$$P_{12}' \propto \left(|\psi_1|^2 + |\psi_2|^2\right) \equiv \text{ intensities are added}$$

The deepest mystery of the nature is that how is this decision made by electrons as to which rule to follow?

- Obviously, the act of measurement disturbs the system in such a way that the interference pattern is wiped out.
- This is consistent with the spirit of the uncertainty principle, discussed earlier

Single-slit experiment and position momentum uncertainty

- Let us examine position-momentum uncertainty from an experimental point of view. We envision a beam of electrons whose position we want ascertain at a given time.



Single-slit experiment (contd.)

- We arrange a single-slit experiment for the purpose, as shown in the figure. An electron beam is emitted from a gun, and we assume that it is traveling in the $x - y$ plane.
- To measure the position of the electrons, we place a single slit of width B, at a given point, with a screen a certain distance away from the slit.
- All the electrons which hit the screen must have passed through the slit, thereby determining their x coordinates precisely when they passed through the slit.
- But what about their y coordinates?
- We further assume that the beam is well collimated so that the initial electron momenta are along the x-direction

$$\vec{p}_i = p_0 \hat{i}$$

Single-slit experiment (contd.)

- Now if the width of the slit is large the electrons will pass through it undeflected implying that $p_y \approx 0$ while they pass through the slit.
- Thus, the y component of the momentum $p_y = 0$ is known with great certainty
- But the uncertainty in the y-coordinate of those electrons is large and of the order of the slit width, i.e. $\Delta y \approx B$.
- Now to measure the y-coordinate of those electrons with greater certainty, we must make the slit as narrow as possible.
- However, once we do that electrons, will begin to diffract (or deflect) at the slit leading to the formation of a diffraction pattern at the screen.

Single-slit experiment (contd.)

- Thus, after scattering at the slit, electron also acquires a y-component of the momentum
- This means that the y-component of their momentum p_y will become uncertain, with an uncertainty, say, Δp_y.
- Assuming that the magnitude of the momentum p_0 is conserved during the scattering, its momentum after the scattering will be

$$\vec{p}_f = p_0 \cos \Delta\theta \hat{i} + p_0 \sin \Delta\theta \hat{j} \approx p_0 \hat{i} + p_0 \Delta\theta \hat{j}$$

- Thus, the uncertainty in the y component of the momentum will be $\Delta p_y \approx p_y \approx p_0 \Delta\theta$, leading to

$$\Delta\theta \approx \frac{\Delta p_y}{p_0}$$

Single-slit experiment (contd.)

- If $\Delta\theta$ corresponds to the position of the first minimum of the diffraction pattern, from the rules of diffraction of light from a single slit
$$\Delta\theta = \frac{\lambda}{B},$$
where λ is the wavelength of light.
- Using the concept of wave-particle duality if we argue that the electrons will also exhibit single-slit diffraction pattern like light, and use the previous two formulas for this case, we obtain
$$\Delta p_y \approx p_0 \frac{\lambda}{B} \tag{6}$$
where λ is the de Broglie wavelength of the electrons.

Uncertainty Principle Revisited

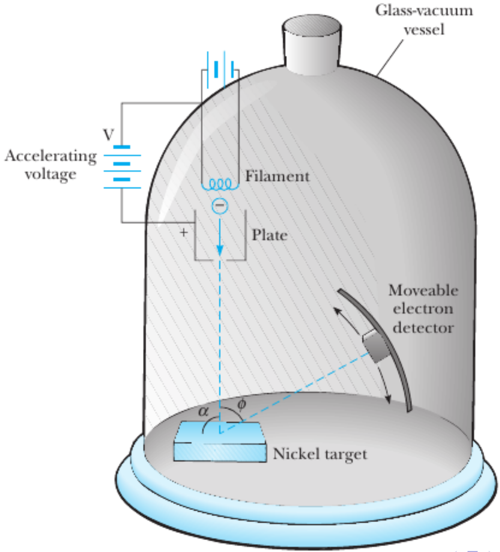
- But, the de Broglie wavelength $\lambda = \dfrac{h}{p_0}$, and the uncertainty in the y component of the position of the particle $\Delta y \approx B$ (as argued earlier), we obtain

$$\Delta p_y \approx \frac{h}{p_0}\frac{p_0}{\Delta y}$$
$$\Rightarrow \boxed{\Delta p_y \Delta y \approx h}$$

- This is precisely the Heisenberg uncertainty principle, as stated in Eq. 5 for the x components.
- Thus, we conclude that wave-particle duality of de Broglie, and the uncertainty principle of Heisenberg are fully consistent with each other.
- Next, we will discuss the Davisson-Germer experiment in which the wave nature of electrons was first confirmed

Davisson-Germer Experiment

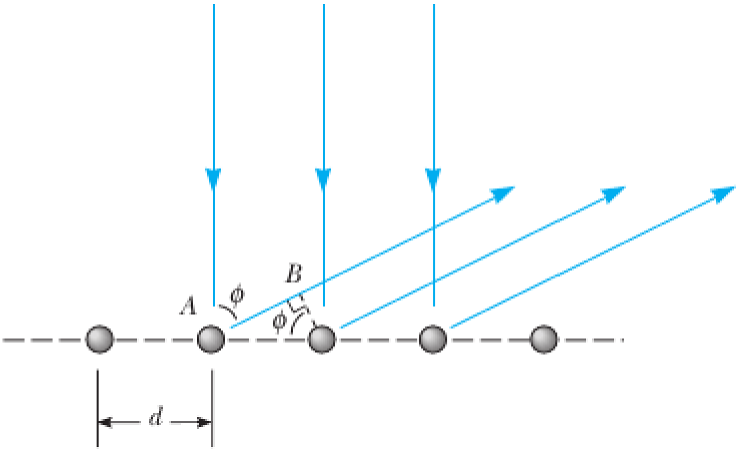
- Davisson and Germer by a beautiful diffraction experiment demonstrated the wave nature of electrons
- They used the apparatus as shown



Davisson-Germer Experiment...

- Relatively low-energy electrons were used to hit the Ni target
- Because of their low energies, electrons were scattered from the top layer of Ni
- Instead of a double slit if we use a large number ($N \to \infty$) of equidistant slits (an array), the arrangement is called "diffraction grating".
- Diffraction gratings are used quite frequently in optical experiments
- If electrons behave like waves, the periodic arrangement of the atoms on the top layer of the target (Ni) will act like a diffraction grating

Davisson-Germer Experiment...



$$AB = d \sin\phi = n\lambda$$

Davisson-Germer Experiment...

- If electrons behave like waves, they will interfere constructively/destructively to give maxima/minima in the intensity pattern after scattering, i.e., like interference fringes of light
- As shown in the figure, the condition for an intensity maximum at the scattering angle ϕ will clearly be

  $$d \sin \phi = n\lambda,$$

  where d is the interatomic spacing and λ is the de Broglie wavelength of electrons
- In the experiment electrons of kinetic energy 54 eV were used.
- Because $K = \frac{1}{2}mv^2 = \dfrac{p^2}{2m}$, we have $p = \sqrt{2mK}$
- Thus, their de Broglie wavelength λ_{dB} will be

  $$\lambda_{dB} = \frac{h}{p} = \frac{h}{\sqrt{2mK}}$$

Davisson-Germer Experiment

- Which turns out to be

$$\lambda_{dB} = \frac{6.63 \times 10^{-34}\ \text{J-s}}{\sqrt{(2 \times 9.11 \times 10^{-31}\ \text{kg})(54\ \text{V} \times 1.6 \times 10^{-19}\text{C})}}$$
$$= 1.67 \times 10^{-10}\text{m} = 1.67\ \text{Å}$$

- In the experiment, an intensity maximum was found at $\phi = 50^\circ$
- For Ni, $d = 2.15$ Å leading to (for $n = 1$)

$$\lambda = 2.15 \times \sin 50^\circ = 1.65\,\text{Å}$$

- Thus, we obtain excellent agreement between the calculated value of λ_{dB} and its measured value!
- This confirms that electrons indeed behave like waves

Electron Microscope

- Inspired by the results of Davisson-Germer experiment, Ernst Ruska invented an electron microscope in 1931
- It works on the same principles, i.e., wave nature of electrons, and yields images of tremendous magnification
- Much superior to those given by optical microscopes
- Next, we will discuss Compton's experiment, which established the particle nature of light for the first time