

CH107: Week 0 & 1

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January 3, 2023

1 Week 0: Introduction

Week 0 was the introductory lecture to the course. Here we did a recapitulation of the topics we have studied earlier, the theories which lead to the development of Quantum Mechanics.

We first studied about the Atomic Spectra and the Rydberg- Ritz Combination Principle about spectral lines. Then Rutherford's model of atom introducing nuclei and circular paths of electron.

Due to the flaw in his theory Neils Bohr Phenomenal Orbital theory was introduced, which allowed only specific energy levels. It quantised the angular momentum of electron:

$$m_e v r = \frac{n h}{2\pi}, \quad n \in \mathbb{N} \quad (1)$$

Electrons are only present in specific energy levels where they don't emit any EM Radiations. When they make transition from one state to another it emits or absorbs a photon of energy $E_a - E_b = h\nu$

We then studied about the wave particle duality. Wave was initially considered to be an electromagnetic wave but in order to explain photoelectric effect, photons and quanta were introduced $E_p = K E_M + \phi$.

Davisson-Germer Experiment later confirmed the wave-like nature of electron by the scattering of electron through nickel crystals. The wavelength could be calculated using $m\lambda = 2d \sin\theta$. An interference pattern was observed. Matter waves: de Broglie hypothesis: according to de Broglie since nature is symmetric particles also behave like waves with wavelength:

$$\lambda = \frac{h}{p} = \frac{h}{mv} \quad (2)$$

In fact the wavelength of electrons calculated from the scattering experiment was very similar to the de Broglie value.

We then studied about the Heisenberg's uncertainty principle which stated that the momentum and position of a particle cannot be predicted accurately at the same time.

$$\Delta x \cdot \Delta p \geq \frac{h}{2\pi} \quad (3)$$

2 Week 1: Schrodinger's Philosophy

Schrodinger said that a new theory was required to explain the earlier phenomena. Schrodinger used wave like equations for describing sub-atomic systems.

$$\frac{\partial^2 \Psi(x, t)}{\partial x^2} = \frac{1}{c^2} \frac{\partial^2 \psi(x, t)}{\partial t^2} \quad \text{Classical wave equation}$$

$$\Psi = C e^{i\alpha} \quad (4)$$

$$\begin{aligned} \text{Where } \alpha &= 2\pi \left(\frac{x}{\lambda} - \nu t \right) \\ &= \frac{x \cdot p - E \cdot t}{\hbar} \end{aligned}$$

Using this we derive

$$\frac{-\hbar}{i} \frac{\partial \Psi(x, t)}{\partial t} = E \Psi(x, t) \quad (5)$$

$$\frac{\hbar}{i} \frac{\partial \Psi(x, t)}{\partial x} = p_x \Psi(x, t) \quad (6)$$

We then studied the operators in quantum mechanics. The above equations are examples of basic operators in quantum mechanics. Various operators exist like for Positon, momentum, KE, PE, TE etc.

Schrodinger's Equation: Particles can be wave and waves can be particles. According to schrodinger particles can be represented as waves. In classical mechanics \hat{H} represents the total energy operator. We can therefore write $\hat{H}\psi = E\psi$. For one dimension:

$$\left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right] \psi(x) = E \cdot \psi(x) \quad (7)$$

Here schrodinger eqn is an eigen eqn.

We then studied in brief the Laws of quantum mechanics which state

1. That the state of the system is completely specified by $\Psi(r, t)$.
2. To every observable in classical mechanics, there is a linear operator in quantum mechanics
3. Only those values can be observable whose eigen values are real. In eigen eqn $\hat{A} \cdot \Psi = a \cdot \Psi$, a is the eigen value. We then studies examples of eigen function for $\Psi(x) = \sin(cx)$. Here we also studied the time dependent schrodinger's equation and how to separate the variables: time and position in the equation by using the fact that $\Psi(x, y, x, t) = \psi(x, y, z) \cdot \phi(t)$. On separating the variables and solving the equation we can conclude that $\phi(t) = e^{-\frac{Wt}{\hbar}}$ where $W = \frac{\hat{H}\Psi}{\Psi} = \frac{1}{\phi} \left(i\hbar \frac{\partial \phi}{\partial t} \right)$
4. All eigen functions are orthogonal.

$$\int_{-\infty}^{+\infty} \Psi_m^*(x) \Psi_n(x) dx = 0 \quad \text{for } m \neq n \quad (8)$$

5. The average value of the observable corresponding to operator \hat{A} is:

$$\langle a \rangle = \int \Psi^* \hat{A} \Psi dx \quad (9)$$

We studied that to find most probable value we calculate maxima of Probability distribution and for average value we integrate.

6. **Born Interpretation:** According to it probability density of finding electron was $|\Psi(x, t)|^2$ and probability is $|\Psi(x, t)|^2 dx$
Normalization of wave function is required such that integral of probability over whole space is zero.

$$\iiint \Psi^*(x, y, z) \cdot \Psi(x, y, z) dx dy dz = 1 \quad (10)$$

7. We then studied the various restriction or properties that the wave function has to follow including that it should be bounded and go to zero at infinity, must be integrable etc.

Exactly Solvable Equations

We then studied various cases of exactly solvable schrodingers equation for Free Particle, Particle in Square Well Potential.

Free Particle

Here since the particle is free we can take $V = 0$, so the equation becomes a second order linear differential equation:

$$-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi(x) = E\psi(x)$$

. On solving this equation we get a solution of the form

$$\psi(x) = A \sin\left(\frac{\sqrt{2mE}}{\hbar} x\right) + B \cos\left(\frac{\sqrt{2mE}}{\hbar} x\right) \quad (11)$$

$$E = \frac{\hbar^2 k^2}{2m} \quad (12)$$

Here note that there are no restriction on energy of the particle so no quantisation.

Particle in 1-D Square-Well Potential

Here we restrict the particle by considering the potential distribution that for $x < 0$ and $x > L$ $V(x) = \infty$ otherwise $V(x) = 0$. We can also conclude that for $x < 0$ and $x > L$ ψ has to be zero otherwise normalization condition cannot be satisfied.

Therefore the solution is similar to the free particle case but with some constraints. By applying the constraints (value at $x = 0$ and $x = L$ is zero) we conclude $k = \frac{n\pi}{L}$ $n \in \mathbb{N}$. On solving the equations we get:

$$\psi = \sqrt{\frac{2}{L}} \sin \frac{n\pi}{L} x \quad (13)$$

$$E_n = \frac{n^2 \hbar^2}{8mL^2}, n \in \mathbb{N} \quad (14)$$

$$h\nu = \Delta E = E_f - E_i = (n_f^2 - n_i^2) \frac{\hbar^2}{8mL^2} \quad (15)$$

Particle in 2D Square-Well Potential: Similar idea could be extended in 2D

by considering the hamiltonian operator $\hat{H} = \hat{H}_x + \hat{H}_y$ and $\psi(x, y) = \psi(x) \cdot \psi(y)$ and $E_n = E_{n_x} + E_{n_y}$. We can now similarly derive the equations like 1D case. Similar for 3D case.

Application in chemistry: We then study a few applications of particle in a box.

1. To explain the wavelength of light emitted by hexatriene and other conjugated straight chain compounds.
2. Application of quantum dots in microbiology and solar cells . Quantum dots are extended particles in a box.