10|9|23

Assignment - 1

Part - A

Q1 The walls of a particle in a box are supposed to be infinetely hard and infinitely large. why?

Ans The infinitely hard and infinitely hard walls in a particles in a box scenario are idealization used in Quantum mechanics for mathematical simplicity. They simplify calculation and allow physicist to model particles behaviour within confined spaces, even throught such walls don't exist in reality.

Q2 Calculate the zero point energy for a particle in an infinite potential well for an electron confined to a 1nm atom.

Ans The zero point energy for a particle in an infinite potential well can be calculated using the following formula

$$E_0 = \frac{\pi^2 \hbar^2}{2mL^2}$$

Where

- E_0 is zero point energy
- π is mathematical constant (Pi)
- $\hbar$ is reduced planck's constant with is

approx 1.054×10^{-34}
- m is mass of electron, 9.1×10^{-31}
- L is the width of infinite potential well, which is 1nm

$$E_0 = \frac{(\pi^2 \times (1.05 \times 10^{-34})^2)}{2 \times (9.1 \times 10^{-31}) \times (1 \times 10^{-9})}$$

$$E_0 = 5.9677 \times 10^{-18} \text{ Joules.}$$

Q3 For a particle inside a box of finite potential well, the particle is most stable at what position of x?

Ans In a particle of finite potential well, the particle is most stable at position where it's energy is lowest which corrosponds to the bottom of the well. This position can vary depending on the specific detail of potential well, but generally, it will be at or near center of well.

Q4 The wave function Ψ does not have any physical significance whereas $|\Psi|^2$ does why?

Ans The wave function Ψ ~~d~~ in quantum mechanic does have physical significance, although it might not be as directly observalble as some other quantities. The square of the absolute value of wave function $|\Psi|^2$

often denote as $|\psi|^2$ represent the probability density finding a particle in particular region of space.

Q5 Define the term phase velocity and group velocity.

Ans Phase Velocity:-

Phase velocity refers to the speed at which the phase of a wave propogates through space. It's the rate at which the crists or through of wave move.

Group Velocity:-

Group velocity on the other hand represent the speed at which the envelop or group of wave propogates. It describe how the amplitude and shape of wave packet changes as it moves through space.

Part - B

Q1 The Crompton shift are visible for x-Ray but not visible for light rays? Explain it with numerical result.

Ans The Crompton shift is a phenomenon in which wavelength of x-Rays scatters by electron changes due to their inter-action This shift is not observeable in visible light rays because the energy of visible light photons is much lower compared to x-ray photon

$$\Delta\lambda = \frac{h}{m_e c}(1-\cos\theta)$$

Where
- $\Delta\lambda$ = Change in wavelength
- h = Planck's Constant
- m_e = mass of electron
- c = speed of light
- θ = scattering angle.

Let's consider x-rays with the wavelength of 0.1 nm and visible light with wavelength of 500 nm

For x-rays, let's assume $\theta = 90°$

$$\Delta\lambda = \frac{(6.626 \times 10^{-34}) \times (1-\cos 90)}{(9.1 \times 10^{-31})(3 \times 10^{8})}$$

$$\Delta\lambda = 0.0024 \text{ nm}$$

For visible light, $\theta = 90°$

$$\Delta\lambda = \frac{(6.626 \times 10^{-34})}{(9.1 \times 10^{-31})(3 \times 10^{8})}(1-\cos 90)$$

$$\Delta\lambda = 2.4 \times 10^{11} \text{ m.}$$

Q2 What do you understand with term "Degenerate and Non-Degenerate"? For a motion of a particle in 3-D box. How the degeneracy is effected $n_x = n_y = 2$, $n_z = 3$ when the sides are

1) $a \neq b \neq c$
2) $a \neq b = c$
3) $a = b = c$

Ans

i) Degenerate States:-

Degenerate States are those energy states that have the same energy level. In degenerate system multiple quantum states share the same energy.

ii) Non-Degenerate States

Non-degenerate States are those energy states in quantum system that have distinct and unique energy level. In other ~~words~~ words, each energy level is associated with only one distinct quantum state.

Motion of particle in 3D box.

The motion of a particle in a 3D box is a classic problem in quantum mechanics, often referred to "particle in a box". It describe a particle Confirmed with in three dimentional box.

$$E = \frac{h^2 \times \pi^2}{2m} \times \frac{nx^2}{Lx^2} + \frac{ny^2}{Ly^2} + \frac{nz^2}{Lz^2}$$

Effect of box dimensions.

1) Cube with equal sides ($Lx = Ly = Lz$)
- In this case, all three dimensions have same length, making box a cube
- The energy level depend on quantum number
- If $x = y = z$, then the energy level will be degenerate because they have same energy value.

2) Cuboid with Different sides ($Lx \neq Ly \neq Lz$)
- In this scenario, box has different dimensions along three axis
- The energy level are still determined by quantum number.
- In general, the energy level is not be degenerat because different dimensions introduce different scaling factor to quantum number.

3) Cube with two equal side and one different side ($Lx = Ly \neq Lz$)
- In this case, two dimension are equal, while, third dimension is different

- The energy levels will be degenerate for those quantum states where $nx = ny$ but they will not generates for $nx \neq ny$.

Q3 Qualitatively give a breif quantum mechanics explaination of
1) Alpha particle decay
2) Scanning tunneling microscope

Ans.

→ Alpha particle decay.
Alpha particle decay is quantum mechanics phenomenon observe in decay of certain unstable atomic nuclie, where an alpha particle is emitted from nucleus. An alpha particle is a helium nucleus consisting of two proton and two nuetron.

Quantum mechanics, this process can be explained as follow.

- Nuclear potential well.
The nucleus can be thought of potential well. and the proton and nuetron within it are bound by storage nuclear force

- Energy Conservation
For alpha particle decay to occur, the alpha particle must have sufficient energy to overcome the columb barrier.

- Alpha Decay.
When quantum tunneling allow the alpha particles to pass through coloumb barriers it is emmitted from nucleus as alpha decay event.

→ Scanning Tunneling Microscope.
Scanning Tunneling Microscope is a powerful tool used in nanotechnology to visualize and manipulate individual atom and molecule on a surface. Its operation can be understood using quantum.

- Quantum Tunneling.
The key principle underlaying STM is quantum tunneling, which is a quantum mechanical phenomenon when a sharp metallic tip is brought very close to conducting surface.

- Tunneling Current
The current resulting from Tunneling process is high senstive to the distance between th tip and the surface. As the tip is scanned accross the surface. it maintain a constant

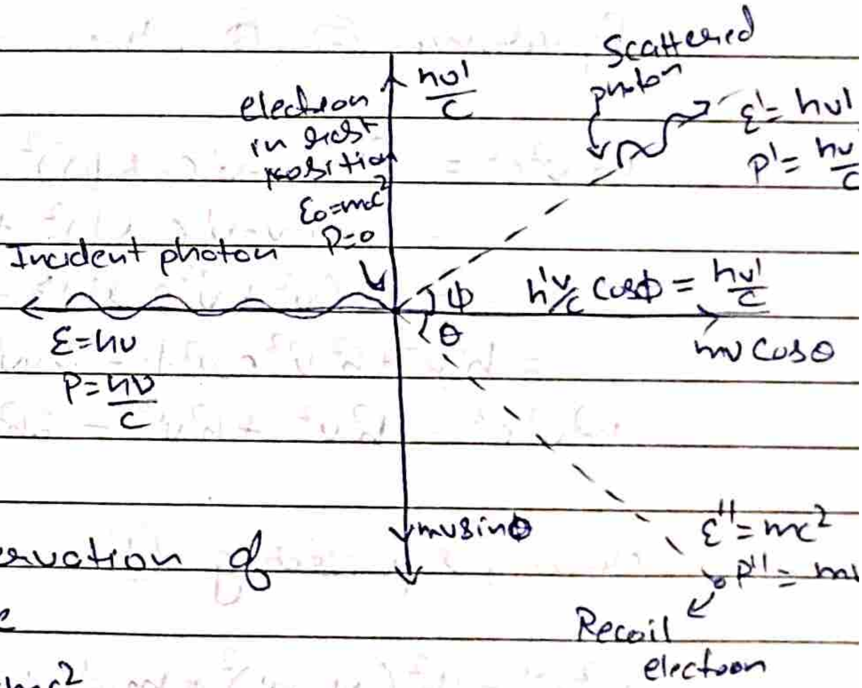
current by adjusting its height to keep the tunneling distance.

- Quantum Mechanical wave function
The electron wave function of the tip and sample play a crucial role in tunneling process. STM used to probe in local density of electron states.

Part - C

Q1 a) Derive an expression for change in the wavelength in Compton Scattering experiment. Draw necessary diagram. Find formula for energy of recoil electron.

Ans



According to conservation of Energy we have

$h\nu + m_0c^2 = h\nu' + mc^2$

$mc^2 = h\nu - h\nu' + m_0c^2$

$mc^2 = h(\nu - \nu') + m_0c^2 \quad -(1)$

Applying the conservation of linear momentum along x-axis

$$\frac{h\nu}{c} + 0 = \frac{h\nu'}{c}\cos\phi + mv\cos\theta$$

$$mv\cos\theta = \frac{h\nu}{c} - \frac{h\nu'}{c}\cos\phi$$

$$mvc\cos\theta = h(\nu - \nu'\cos\phi) \quad -②$$

Applying the conservation of linear momentum along y-axis

$$0 = \frac{h\nu'}{c}\sin\phi - mv\sin\theta$$

$$mvc\sin\theta = h\nu'\sin\phi \quad -③$$

Squaring ②, ③, then adding them

$$m^2v^2c^2 = (h(\nu-\nu'\cos\phi))^2 + (h\nu'\sin\phi)^2$$
$$= h^2(\nu-\nu'\cos\phi)^2 + h^2\nu'^2\sin^2\phi$$
$$= h^2(\nu^2+\nu'^2\cos^2\phi - 2\nu\nu'\cos\phi) + h^2\nu'^2\sin^2\phi$$
$$= h^2\nu^2 + h^2\nu'^2\cos^2\phi - 2\nu\nu'\cos\phi h^2 + h^2\nu'^2\sin^2\phi$$
$$m^2v^2c^2 = h^2\nu^2 + h^2\nu'^2 - 2h^2\nu\nu'\cos\phi \quad -④$$

Now, squaring ①

$$m^2c^4 = h^2(\nu-\nu')^2 + m_0c^4 + 2h(\nu-\nu')m_0c^2$$
$$m^2c^4 = h^2\nu^2 + h^2\nu'^2 - 2h\nu\nu' + m_0c^4 + 2h(\nu-\nu')m_0c^2 \quad -⑤$$

Performing ⑤ − ④

$$m^2c^4 - m^2v^2c^2 = h^2\nu^2 + h^2\nu'^2 - 2h^2\nu\nu' + m_0c^4 + 2h(\nu-\nu')m_0c^2 - h^2\nu^2 - h^2\nu'^2 + 2h^2\nu\nu'\cos\phi$$

$$m^2c^4\left[1-\frac{v^2}{c^2}\right] = -2h^2\nu\nu' + m_oc^4 + 2h(\nu-\nu')m_oc^2 + 2h^2\nu\nu'\cos\phi \quad -(6)$$

We know, $m = \frac{m_o}{\sqrt{1-v^2/c^2}}$, by squaring this eq.

$$m^2\left[1-\frac{v^2}{c^2}\right] = m_o^2$$

Putting this in (6)

$$m_oc^4 = -2h^2\nu\nu' + m_o^2c^4 + 2h(\nu-\nu')m_oc^2 + 2h^2\nu\nu'\cos\phi$$

$$2h^2\nu\nu' - 2h^2\nu\nu'\cos\phi = 2h(\nu-\nu')m_oc^2$$

$$2h^{\cancel{2}}\nu\nu'(1-\cos\phi) = 2h(\nu-\nu')m_oc^2$$

$$\frac{h}{m_oc^2}(1-\cos\phi) = \frac{\nu-\nu'}{\nu\nu'}$$

$$\left[\begin{array}{c} \nu = n\lambda \\ C = \nu\lambda \\ \frac{C}{\nu} = \lambda \end{array}\right]$$

$$\frac{h}{m_oC^2}(1-\cos\phi) = \frac{C}{\nu'} - \frac{C}{\nu'}$$

$$\frac{h}{m_oc}(1-\cos\phi) = \lambda' - \lambda = \Delta\lambda$$

[λ' = Scattered wavelength
λ = Incident wavelength]

- Kinetic Energy of Recoil electron.

K.E = $h\nu - h\nu'$ [Incident Energy − Scattered Energy of photon]

$$K.E = h\nu\left[1-\frac{\nu'}{\nu}\right]$$

$$\frac{\nu'}{\nu} = \frac{1}{1+\frac{h\nu}{m_0c^2}(1-\cos\phi)} \quad \text{[From above]}$$

let $\frac{h\nu}{m_0c^2} = \alpha$

$$K.E = h\nu\left[1 - \frac{1}{1+\alpha(1-\cos\phi)}\right]$$

$$K.E = h\nu\left[\frac{1+\alpha(1-\cos\phi)-1}{1+\alpha(1-\cos\phi)}\right]$$

$$K.E = h\nu\left[\frac{\alpha(1-\cos\phi)}{1+\alpha(1-\cos\phi)}\right]$$

Putting the value of α

$$K.E = h\nu\left[\frac{\frac{h}{m_0c^2}(1-\cos\phi)}{1+\frac{h}{m_0c^2}(1-\cos\phi)}\right]$$

b) X-ray photon of wavelength 0.3 Å is scattered through an angle of 60° by a free electron Find the wavelength of scattered photon and recoil energy of electron.

Ans For Compton scattering, if λ and λ' are the wavelength of the incident photon

$$\Delta\lambda = \lambda - \lambda' = \frac{h}{mc}(1-\cos\phi)$$

$$\Delta\lambda = 0.02425\,(1-\cos 60^\circ)$$
$$\Delta\lambda = 0.01212\ \mathring{A}$$

Therefore :- $\lambda' = \lambda - 0.012$
$$\lambda' = 0.3 - 0.012$$
$$\lambda' = 0.3\ \mathring{A}$$

- Recoil energy of electron.

$$\lambda' = \lambda - 0.012 \Rightarrow 0.3 = \lambda - 0.012$$
$$\lambda = 0.3 + 0.012 \Rightarrow \lambda = 0.312\ \mathring{A}$$

$$K.E = h\nu - h\nu' \Rightarrow \frac{hc}{\lambda} - \frac{hc}{\lambda'} = hc\left[\frac{\lambda'-\lambda}{\lambda\lambda'}\right] = hc\frac{\Delta\lambda}{\lambda\lambda'}$$

$$= \frac{(6.63\times10^{-34})(3\times10^{8})(0.012)}{(0.3\times10^{-10})(1.0486\times10^{-10})} = 0.75\times10^{-6}\ J$$

Q2 What do you mean by quantum tunneling effect?

a) Write the Schrodinger wave equations and solutions for $x \leq 0$, $0 < x < a$, $x \geq 0$ regions. Explain the transmitivity. Write the application of Quantum tunneling effect.

Ans → Quantum tunneling effect is an essential phenomenon for nuclear fusion.

It increases the probability of penetrating Columb barrier and achieve thermonuclear fusion. Though this probability is still low, the extremely large number of nuclei in the core of a star is sufficient to sustain a steady

fusion reaction.
Quantum tunneling is when tiny particles pass through barriers they shouldn't according to classical physics, due to their wave like nature. It's a key phenomenon in quantum mechanics.

→ Schrodinger wave equation and solutions.

The time-independent schroundinger wave equation for 1-D system is given by

$$-\frac{h_0^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi = E\psi$$

The solution to Schrodinger equation in different region are as follows.

• For $0<x<a$:
The general solution is $\psi(x) = Ae^{ik_1x} + Be^{(-ik_1x)}$

where $k_1 = \frac{1}{\sqrt{\frac{1}{2m}(E-V)\left[\frac{1}{h_0^2}\right]}}$

• For $x \geq 0$
The general solution is $\frac{1}{\psi(3x)} = Ee^{(ik_1x)}$

Which represent transmitted wave.

• For $x < 0$

$$\Psi(x,t) = \frac{Ae^{ik-x} - iEt}{h_0 + (e^{-ikx - iEt})}$$

Matching the wave func. and it's derivative at the origin.

→ Transmittivity
It measures how much light electromagnetic waves ~~opacity.~~ can pass through a material, indicating its transparency or opacity. It's a crucial concept in optics and material science

→ Applications of Quantum Tunneling effect.

- Scanning Tunneling Microscopy (STM)
- Quantum Dot Transistors
- Nuclear fusion in Stars
- Flash memory Technology.

Q3 a) For a particle confined to move in 1D box where E is independent of time solve Schrodinger equation. Discuss the probability of finding the particles for first three energy states.

Ans. To solve the time independent schrodinger wave equation for particles confined to move in 1D box, you will need to setup and solve the equation

The Schroundinger equation for this system is:

$$-\frac{h_0^2}{2m} \cdot \frac{d^2\Psi(x)}{dx^2} + V(x)\Psi(x) = E\Psi(x)$$

In this equation
- h_0 is ~~used~~ reduced planck's Constant
- m is mass of particle
- $\Psi(x)$ is wave function describing the particle behaviour.
- $V(x)$ is potential energy function.

Probability of finding of particle is

$$P_1 = \int_0^1 (\Psi_1(x)^2)\, dx$$

$$P_2 = \int_0^1 |\Psi_2(x)|^2\, dx$$

$$P_3 = \int_0^1 |\Psi_3(x)|^2\, dx$$

b) Show that the zero point energy for a particle in one dimensional box have good agreement with uncertainity principle.

Ans The existance of zero point energy of particle in one dimensional box is a Consequence of Heisenberg uncertainity principle.
So, at T=0K, particles are at rest, so energy should be zero, but Quantum mechanics we have finite energy which is also known as zero-point energy.

$$E = \frac{n^2 \pi^2 \hbar^2}{2ma^2}$$

$n = 1$, $\hbar = 1.054 \times 10^{-34}$, $m = 9.1 \times 10^{-31}$, $a \approx 10^{-15}$ m

$$E = \frac{10.96 \times 10^{-68}}{18.2 \times 10^{-61}}$$

$= 6 \times 10^{-8}$ J

$= 3.76 \times 10^{11}$ eV for fixed position

Which is very high for fixed position Hence showed.

54

64