PH24101: Physics (B.Tech. I)

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Section M & N

PH24101: Physics (B.Tech. I)

Module 4

Module -4 : Quantum Mechanics

Planck's theory of black-body radiation, Compton effect, Wave particle duality, De Broglie waves, Davisson and Germer's experiment, Uncertainty principle, Brief idea of Wave Packet, Wave Function and its physical interpretation, Schrodinger equation in one-dimension, free particle, particle in an infinite square well. [9]

Text book: T3: Arthur Beiser (AB), Concept of Modern Physics, 6th edition 2009, Tata McGraw- Hill

Reference book: R1: Fundamentals of Physics, Halliday, Walker and Resnick

Module 4 (Quantum Mechanics)

Introduction

- ☐ Electromagnetic (EM) Wave: Coupled electric and magnetic oscillations that move with the speed of light and exhibit typical wave behavior.
- ☐ We regard EM wave as waves because under suitable circumstances they exhibit *diffraction*, *interference* and *polarization* (wave nature).
- ☐ Similarly, we shall see under other circumstances, EM waves behave as though they consist of streams of particles.
- ☐ It was found that the wave nature of light cannot explain several phenomena like *black body radiation, photoelectric effect, Compton effect*, *etc*.
- ☐ The first sign appeared while trying to understand “black body” radiation.
- ☐ All bodies absorb and emit radiations (may or may not be in the visible range).
- ☐ At thermal equilibrium of a body with its surroundings, must absorb and radiate energy at the same rate, so as to keep the temperature constant.

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Black body radiation

- ❑ A black body absorbs ALL radiations that are incident on it.
- ❑ At thermal equilibrium of a body with its surroundings, it must absorb and emit energy at the same rate.
- ❑ In lab, we can have a hollow object with a very small hole – radiation enters the cavity through the hole – it is trapped by reflection back and forth until it is absorbed – cavity wall is constantly emitting and absorbing radiation. This can be approximated as the black body radiation.

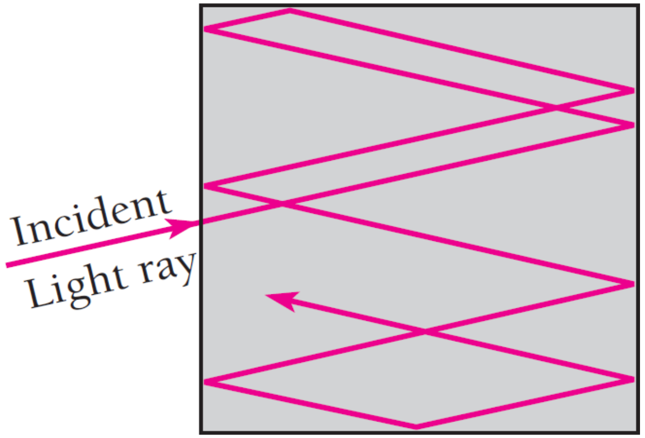
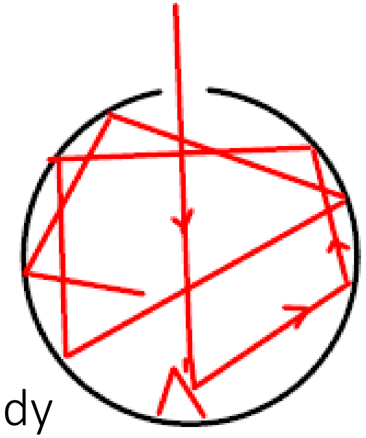


Figure 2.5 A hole in the wall of a hollow object is an excellent approximation of a blackbody.

- ❑ As per classical theory, a blackbody should radiate electromagnetic waves of ALL frequencies, and the energy associated with the radiation INCREASES with increase in frequency.



Ferry's black body

Module 4 (Quantum Mechanics)

Black body radiation

The Ultraviolet Catastrophe – Failure of Classical Physics

- Consider a one-dimensional cavity
- The standing wave must form nodes at two ends: at $x = 0$ and at $x = a$
- Different kinds of oscillations that satisfy this boundary condition are called the different “modes” of the radiation
- Let us calculate the no. of modes having frequencies in the range $\nu, \nu + d\nu \equiv N(\nu)d\nu$
- Now, $\nu = c/\lambda$, where $\lambda = (2a)/n$, where $n = 1,2, \ldots.$ $[a = n\lambda/2]$
- Using $\nu = c/\lambda$ and $\lambda = (2a)/n$, we get, $\nu = \frac{cn}{2a}$, or, $n = \frac{2a}{c}\nu \quad => \quad \Delta n = \frac{2a}{c}\Delta\nu$
- However, a light wave has two polarization directions.
- Hence actual $\Delta n = 2 \times \frac{2a}{c}\Delta\nu = \frac{4a}{c}\Delta\nu$
- So, we get, $dn = N(\nu)d\nu = \frac{4a}{c}d\nu$. (In the limit $\Delta n \to 0\ and\ \Delta\nu \to 0)$ => $N(\nu) = \frac{4a}{c}$

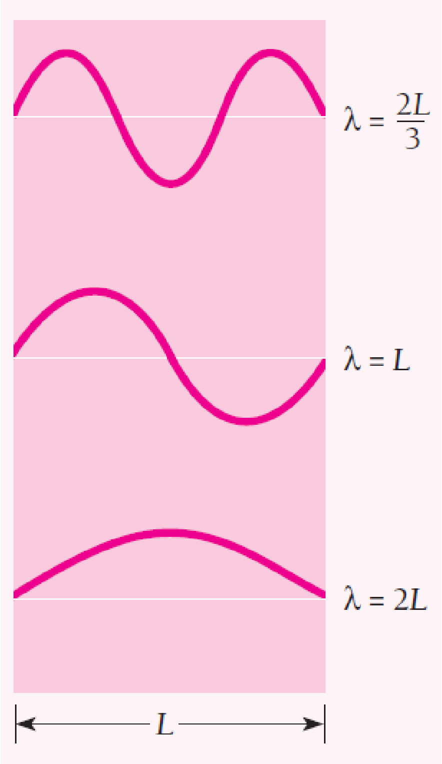


Figure 2.7 Em radiation in a cavity whose walls are perfect reflectors consists of standing waves that have nodes at the walls, which restricts their possible wavelengths. Shown are three possible wavelengths when the distance between opposite walls is L.

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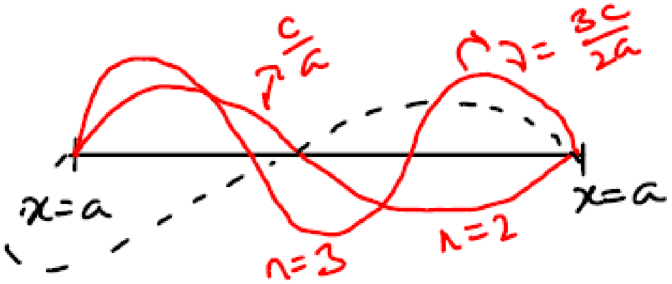
Black body radiation

The Ultraviolet Catastrophe – Failure of Classical Physics

- ❑ No. of modes having frequencies in the range $\nu, \nu + d\nu \equiv N(\nu)d\nu$. Now, $\nu = c/\lambda$, where $\lambda = (2a)/n$, where $n = 1,2, \ldots$. $[a = n\lambda/2]$.
- ❑ Using $\nu = c/\lambda$ and $\lambda = (2a)/n$, we get, $\nu = \frac{cn}{2a}$, or, $n = \frac{2a}{c}\nu$ => $\Delta n = \frac{2a}{c}\Delta\nu$. However, a light wave has two polarization directions. Hence actual $\Delta n = 2 \times \frac{2a}{c}\Delta\nu = \frac{4a}{c}\Delta\nu$. So, we get, $dn = N(\nu)d\nu = \frac{4a}{c}d\nu$. In the limit $\Delta n \to 0\ and\ \Delta\nu \to 0, N(\nu) = \frac{4a}{c}$.

Q.



What is Δn and $\Delta\nu$ in this case.

$\Delta n = 1$.

$\Delta\nu = \frac{3c}{2a} - \frac{c}{a} = \frac{c}{2a}$.

Actual $\Delta n = 2$ due to two modes ⊥ each other.

$\Delta n = \frac{4a}{c}\Delta\nu$ is satisfied.

Module 4 (Quantum Mechanics)

Black body radiation

The Ultraviolet Catastrophe – Failure of Classical Physics

- ☐ Now generalize to three-dimensional cavity:
- ☐ For a cubic cavity of side “a”, $N(\nu)d\nu = \frac{8\pi a^3}{c^3}\nu^2\, d\nu$.
- ☐ Considering the volume, $V\ (=\ a^3)$, we rewrite $N(\nu)d\nu = \frac{8\pi V}{c^3}\nu^2\, d\nu$. This gives the total no. of modes in the cavity.
- ☐ What is the total energy?
- ☐ Average energy per mode can be shown to be $k_B T$, where k_B is the Boltzmann constant = 1.38×10^{-23} J/K and T is the temperature of the cavity (can be derived from the Equipartition Theorem of Statistical Mechanics).
- ☐ Every degree of freedom that appears quadratically in the total energy contributes an average energy of $\frac{1}{2}k_B T$ at equilibrium.
- ☐ For simple harmonic oscillator, $E = \frac{1}{2}kx^2 + \frac{1}{2}mv^2$, So $< E > = \frac{1}{2}k_B T + \frac{1}{2}k_B T = \ k_B T$

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Black body radiation

The Ultraviolet Catastrophe – Failure of Classical Physics

- For a three-dimensional cubic cavity of side “a”, $N(\nu)d\nu = \frac{8\pi a^3}{c^3}\nu^2\, d\nu$. (Solve it!)
- Considering the volume, V (= a^3), we rewrite $N(\nu)d\nu = \frac{8\pi V}{c^3}\nu^2\, d\nu$. This gives the total no. of modes in the cavity.
- What is the total energy?
- Average energy per mode can be shown to be k_BT, where k_B is the Boltzmann constant = 1.38×10^{-23} J/K and T is the temperature of the cavity (can be derived from the Equipartition Theorem of Statistical Mechanics).
- (Considering energy per mode as k_BT), the Total energy (in ν and $\nu+d\nu$) $= k_BT \times N(\nu)d\nu = \frac{8\pi V}{c^3}\nu^2\, k_BT\, d\nu$
- Total energy density, $u(\nu)$ can be calculated by dividing the total energy by volume and $\mathrm{d}\nu$.
- Total energy per unit volume in the frequency range ν, $\nu+d\nu$ is $u(\nu)d\nu = \frac{1}{V} \times \frac{8\pi V}{c^3}\nu^2\, k_BT\, d\nu = (\frac{8\pi k_BT}{c^3})\nu^2 d\nu$,

  or, the energy density per unit frequency range, $u(\nu) = (\frac{8\pi k_BT}{c^3})\nu^2$.

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Black body radiation

The Ultraviolet Catastrophe – Failure of Classical Physics

- ❑ Total energy per unit volume in the frequency range ν, ν+$d\nu$ is $u(\nu)d\nu = \left(\frac{8\pi k_B T}{c^3}\right)\nu^2 d\nu$. This is known as the **Rayleigh-Jeans formula**.
- ❑ $u(\nu)$ is the energy density (total energy per unit volume per unit frequency range) $= \left(\frac{8\pi k_B T}{c^3}\right)\nu^2$.
- ❑ Energy density $u(\nu)$ is therefore **parabolic** in nature.
- ❑ The expression says, as the frequency ν increases toward the ultraviolet end of the spectrum, energy density should increase as ν^2. Hence, $u(\nu) \to \infty$ as $\nu \to \infty$.
- ❑ But, experiments show $u(\nu) \to 0$ as $\nu \to \infty$.
- ❑ This discrepancy is known as **ultraviolet catastrophe** of classical physics.

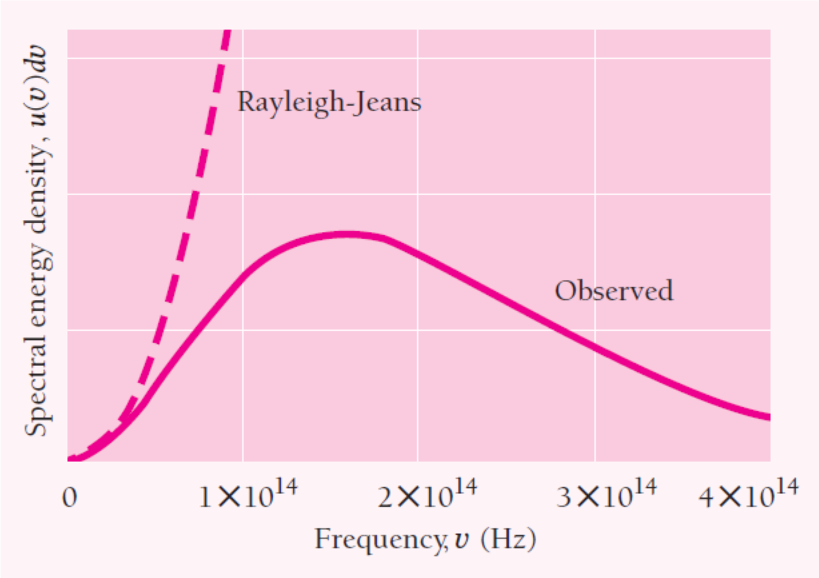

Figure 2.8 Comparison of the Rayleigh-Jeans formula for the spectrum of the radiation from a blackbody at 1500 K with the observed spectrum. The discrepancy is known as the ultraviolet catastrophe because it increases with increasing frequency. This failure of classical physics led Planck to the discovery that radiation is emitted in quanta whose energy is $h\nu$.

Module 4 (Quantum Mechanics)

Black body radiation

Recap

- ☐ Definition of a black body.
- ☐ Mode counting in a cavity: we chose 1D cavity for simplicity.
- ☐ No. of modes present in the 1D cavity in the frequency range ν, ν+$d\nu$ is $N(\nu)d\nu = \frac{4a}{c}d\nu$. An extra factor of 2 is present due to two polarization states of the radiations. (Boundary condition: each mode has nodes at the walls of the cavity).
- ☐ This result can be generalized to 3D cavity: $N(\nu)d\nu = \frac{8\pi V}{c^3}\nu^2\, d\nu$.
- ☐ Energy for each mode is k_BT on average (from Equipartition Theorem).
- ☐ Total energy in the frequency range ν and $\mathrm{d}\nu$, $N(\nu)d\nu \times\ k_BT = \frac{8\pi V}{c^3}\nu^2\, k_BT\, d\nu$
- ☐ Dividing by V, we get total energy per unit volume in the frequency range ν, ν+$d\nu$: $u(\nu)d\nu\ = (\frac{8\pi k_BT}{c^3})\nu^2 d\nu$, or, the energy per unit volume per unit frequency range, $u(\nu) = (\frac{8\pi k_BT}{c^3})\nu^2$, which is parabolic in nature.

Module 4 (Quantum Mechanics)

Black body radiation

The Ultraviolet Catastrophe – Failure of Classical Physics

- ❑ Total energy per unit volume in the frequency range ν, $\nu+d\nu$ is $u(\nu)d\nu = \left(\frac{8\pi k_B T}{c^3}\right)\nu^2 d\nu$. This is known as the **Rayleigh-Jeans formula**.
- ❑ $u(\nu)$ is the energy density (total energy per unit volume per unit frequency range) $= \left(\frac{8\pi k_B T}{c^3}\right)\nu^2$.
- ❑ Energy density $u(\nu)$ is therefore **parabolic** in nature.
- ❑ At short wavelength (high ν), classical theory gives incorrect results. The expression says, as the frequency ν increases toward the ultraviolet end of the spectrum, energy density should increase as ν^2. Hence, $u(\nu) \rightarrow \infty$ as $\nu \rightarrow \infty$.
- ❑ But, experiments show that $u(\nu) \rightarrow 0$ as $\nu \rightarrow \infty$.
- ❑ This discrepancy is known as **ultraviolet catastrophe** of classical physics.

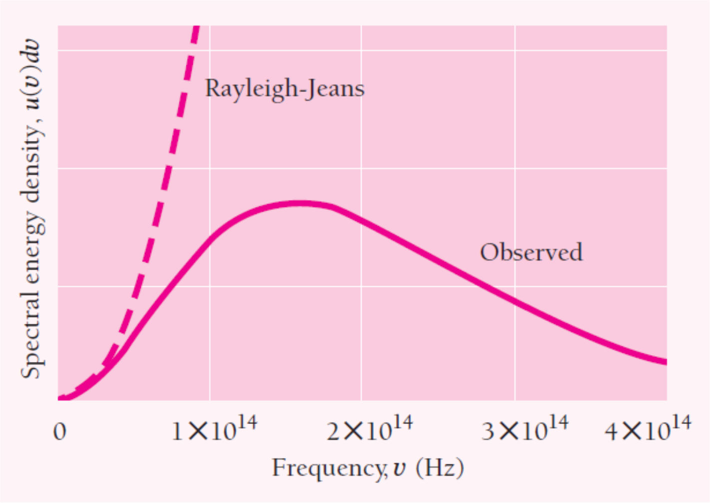

Figure 2.8 Comparison of the Rayleigh-Jeans formula for the spectrum of the radiation from a blackbody at 1500 K with the observed spectrum. The discrepancy is known as the ultraviolet catastrophe because it increases with increasing frequency. This failure of classical physics led Planck to the discovery that radiation is emitted in quanta whose energy is $h\nu$.

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Module 4 (Quantum Mechanics)

Black body radiation

Planck's theory of black body radiation

- ☐ Treated energy as a discrete variable. Planck proposed that the energy can take only certain discrete values: $E = 0, \Delta E,\ 2\Delta E,\ 3\Delta E, \dots\dots\dots.$
- ☐ Planck realized that in order to explain the experimental black body radiation curve, the energy "packets" must be proportional to the frequency of the radiation: $\Delta E \propto \nu$ => $\Delta E = h\nu$, where h is the Planck's constant.
- ☐ He found the average energy per energy packet is $< E(\nu) > = \frac{h\nu}{e^{\frac{h\nu}{k_B T}}-1}$ (instead of $k_B T$).

Planck radiation formula $$u(\nu)\ d\nu = \frac{8\pi h}{c^3}\frac{\nu^3\ d\nu}{e^{h\nu/kT} - 1}$$

Here h is a constant whose value is

Planck's constant $$h = 6.626 \times 10^{-34}\ \mathrm{J \cdot s}$$

Black body radiation

Planck's theory of black body radiation

Derivation

$$< E > = \frac{\sum_{n=0}^{\infty} E_n P(E_n)}{\sum_{n=0}^{\infty} P(E_n)}$$

- Where $E_n = nh\nu = n\,\Delta E$ $(\, n = 0, 1, 2, 3, \ldots..)$
- $P(E_n)$ is the probability of having energy E_n.

$$\sum_{n=0}^{\infty} P(E_n) = 1$$

So, $$< E > = \sum_{n=0}^{\infty} E_n P(E_n)$$

Q. A class has 10 students. 2 students have a height of 6 ft, 5 students have a height of 5.6 ft, and 3 students a height of 5.2 ft. What is the average height?

Soln

$$\frac{2\times 6.0 + 5\times 5.6 + 3\times 5.2}{10}$$

$$= \frac{2}{10}\times 6.0 + \frac{5}{10}\times 5.6 + \frac{3}{10}\times 5.2$$

$$= \sum_{n} h(n)\,P(n).$$

(if the class has a very large no. of students, then P(n) becomes an exact probability of height h(n)).

Black body radiation

Planck's theory of black body radiation

Derivation

$$< E > = \sum_{n=0}^{\infty} E_n P(E_n)$$

- ❑ Where $E_n = nh\nu = n\,\Delta E$ and $P(E_n)$ is the probability of having energy E_n.

- ❑ From Statistical Mechanics, one can show that

$$P(E_n) = \frac{e^{-E_n/k_B T}}{\sum_{n=0}^{\infty} e^{-E_n/k_B T}}$$

(Thermal or Boltzmann probability distribution of energies)

$$\left[\because \text{Check} : \sum_{n=0}^{\infty} P(E_n) = 1 \right]$$

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Black body radiation

Planck's theory of black body radiation

Derivation

$$< E > = \sum_{n=0}^{\infty} E_n P(E_n)$$

$$P(E_n) = \frac{e^{-E_n/k_B T}}{\sum_{n=0}^{\infty} e^{-E_n/k_B T}}$$

- ❑ Where $E_n = nh\nu = n\,\Delta E$ and $P_n(E)$ is the probability of having energy E_n.

- ❑ Therefore $$\langle E \rangle = \sum_{n=0}^{\infty} E_n P(E_n) = \frac{\sum_{n=0}^{\infty} E_n e^{-E_n/k_B T}}{\sum_{n=0} e^{-E_n/k_B T}} = \frac{\sum_{n=0}^{\infty} nh\nu\, e^{-nh\nu/k_B T}}{\sum_{n=0}^{\infty} e^{-nh\nu/k_B T}}$$ (Replacing $E_n = nh\nu$)

In order to do the summation, replace $\alpha = \frac{h\nu}{k_B T}$

Module 4 (Quantum Mechanics)

Black body radiation

Planck's theory of black body radiation

Derivation

$$\langle E \rangle = \frac{\sum_n n\alpha k_B T \, e^{-n\alpha}}{\sum_n e^{-n\alpha}}$$

$$= k_B T \alpha \frac{\sum_n n \, e^{-n\alpha}}{\sum_n e^{-n\alpha}}$$

$$= -k_B T \alpha \frac{\partial}{\partial \alpha} \left[\ln \left\{ \sum_{n=0}^{\infty} e^{-n\alpha} \right\} \right]$$

$$\left[\because \frac{\partial}{\partial x} \ln f(x) = \frac{\frac{\partial f}{\partial x}}{f(x)} \right]$$

$$\langle E \rangle = -k_B T \alpha \frac{\partial}{\partial \alpha} \left[\ln \left\{ \sum_{n=0}^{\infty} e^{-n\alpha} \right\} \right]$$

Module 4 (Quantum Mechanics)

Black body radiation

Planck’s theory of black body radiation

Derivation

$$\langle E \rangle = -k_B T \alpha \frac{\partial}{\partial \alpha}\left[\ln\left\{\sum_{n=0}^{\infty} e^{-n\alpha}\right\}\right]$$

Use

$$\sum_{n=0}^{\infty} e^{-n\alpha} = 1 + e^{-\alpha} + e^{-2\alpha} + \cdots$$

$$= \frac{1}{1-e^{-\alpha}} .$$

So,

$$\ln\left(\sum_{n=0}^{\infty} e^{-n\alpha}\right) = -\ln\left(1-e^{-\alpha}\right).$$

Module 4 (Quantum Mechanics)

Black body radiation

Planck's theory of black body radiation

Derivation

$$< E > = k_B T\alpha \frac{\partial}{\partial \alpha}[\ln(1 - e^{-\alpha})] = k_B T\alpha \left[\frac{e^{-\alpha}}{1 - e^{-\alpha}}\right] = k_B T \left[\frac{\alpha e^{-\alpha}}{1 - e^{-\alpha}}\right]$$

Multiply numerator & denominator by e^{α}:

$$< E > = k_B T \left[\frac{\alpha}{e^{\alpha} - 1}\right]$$

Remember, $\alpha = \frac{h\nu}{k_B T}$. Hence, $< E > = \left(\frac{h\nu}{e^{\frac{h\nu}{k_B T}} - 1}\right)$

Now, the no. of modes in the range ν, ν+$d\nu$ is $N(\nu)d\nu = \frac{8\pi V}{c^3}\nu^2\, d\nu$.

Module 4 (Quantum Mechanics)

Black body radiation

Planck's theory of black body radiation

Derivation

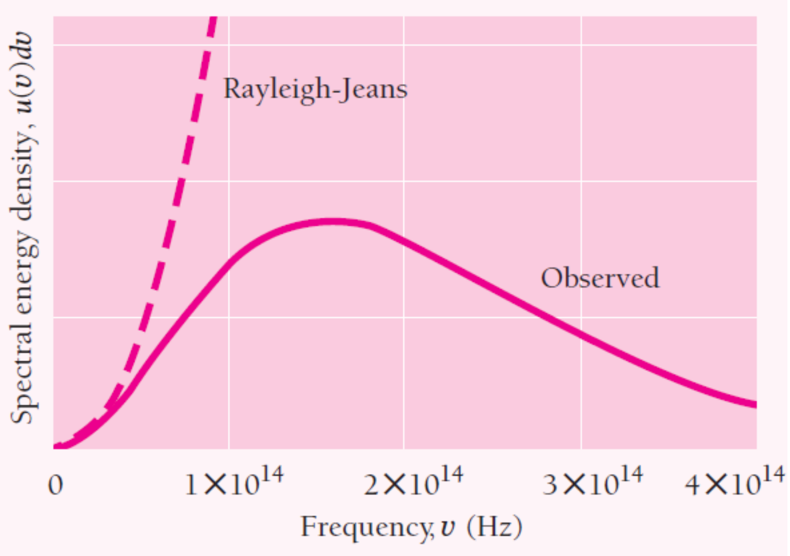
$$< E > = \left(\frac{h\nu}{e^{\frac{h\nu}{k_B T}} - 1}\right)$$

Now, the no. of modes in the range ν, $\nu+d\nu$ is $N(\nu)d\nu = \frac{8\pi V}{c^3}\nu^2\, d\nu.$

Therefore, $u(\nu)d\nu = \frac{1}{V} \times \frac{8\pi V}{c^3}\nu^2\, d\nu \times < E >$

$$= \frac{1}{V} \times \frac{8\pi V}{c^3}\nu^2\, d\nu \times \left(\frac{h\nu}{e^{\frac{h\nu}{k_B T}} - 1}\right)$$

$$= \left(\frac{8\pi h}{c^3}\right)\frac{\nu^3\, d\nu}{e^{h\nu/kBT} - 1}$$



=> Reproduces the experimental curve

Planck radiation formula, $u(\nu)d\nu = \left(\frac{8\pi h}{c^3}\right)\frac{\nu^3\, d\nu}{e^{h\nu/kBT} - 1}$

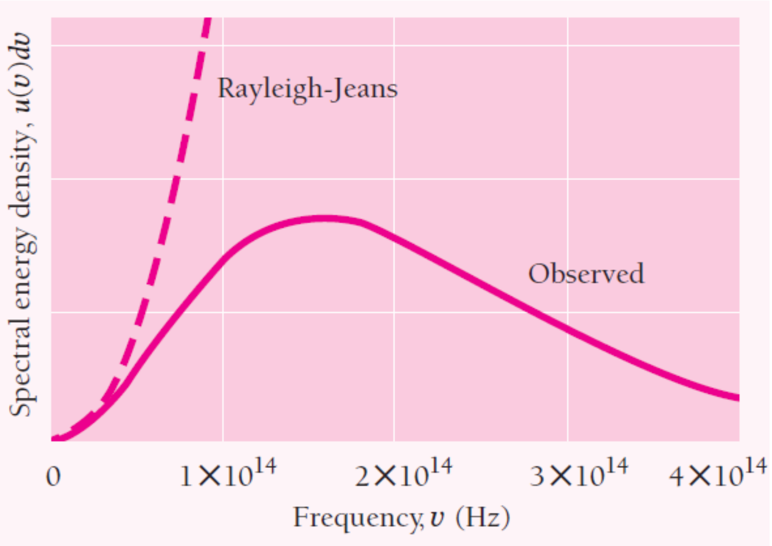
Module 4 (Quantum Mechanics)

Black body radiation

Planck's theory of black body radiation

Derivation

$$u(\nu)d\nu = \left(\frac{8\pi h}{c^3}\right)\frac{\nu^3\, d\nu}{e^{h\nu/kBT} - 1}$$



At high frequencies, $h\nu \gg k_B T$ and $e^{h\nu/k_B T} \to \infty$, which means $u(\nu)d\nu \to 0$.

At low frequencies, $h\nu \ll k_B T$ and $\frac{h\nu}{k_B T} \ll 1$

$$e^x = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \cdots$$

If x is small, $e^x \approx 1 + x$, and so for $h\nu/kT \ll 1$ we have

$$\frac{1}{e^{h\nu/kT} - 1} \approx \frac{1}{1 + \frac{h\nu}{kT} - 1} \approx \frac{kT}{h\nu} \qquad h\nu \ll kT$$

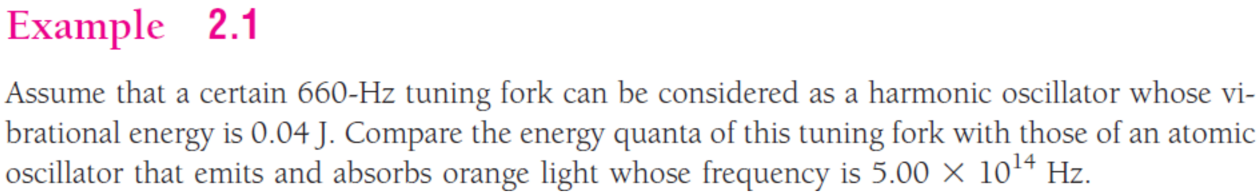
Thus, at low frequencies Planck's formula becomes

$$u(\nu)\, d\nu \approx \frac{8\pi h}{c^3}\nu^3\left(\frac{kT}{h\nu}\right)d\nu \approx \frac{8\pi kT}{c^3}\nu^2\, d\nu$$

Which is Rayleigh-Jeans formula.

Recap so far….

Blackbody radiation – Example Problems

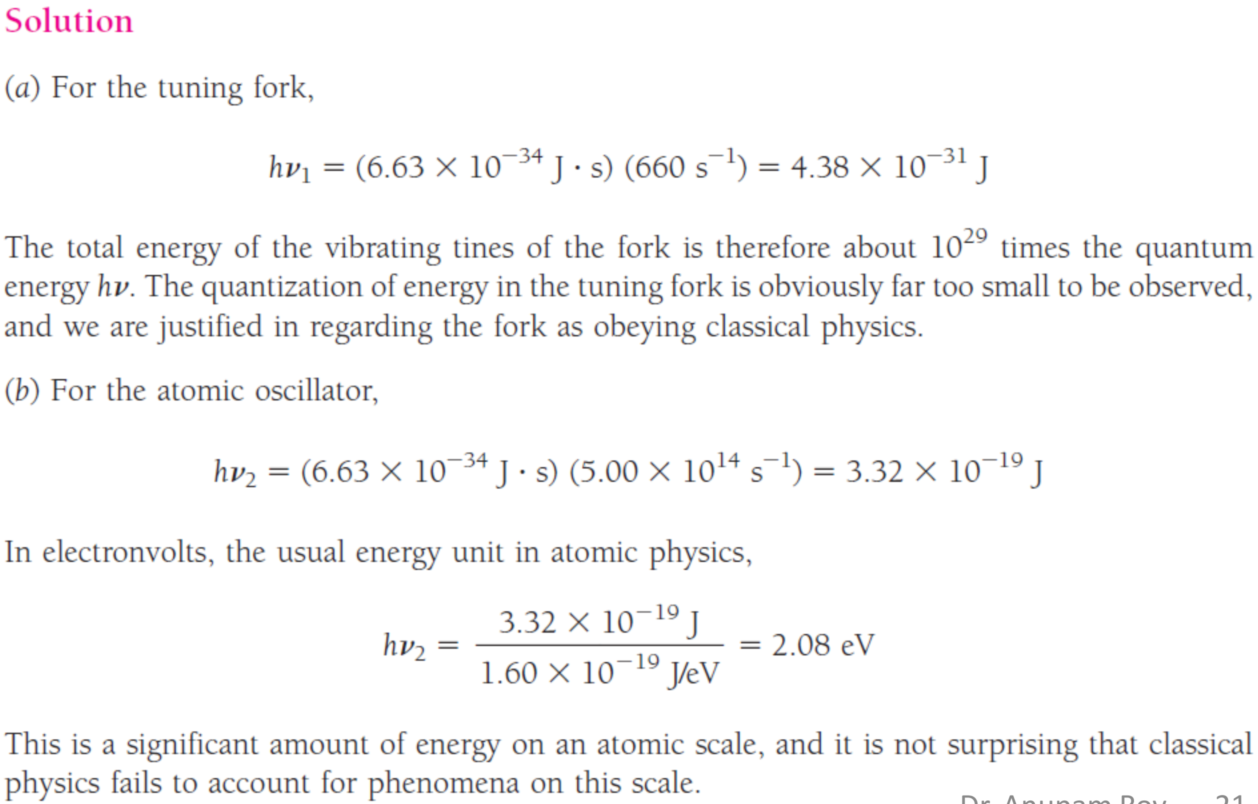


Example 2.1

Assume that a certain 660-Hz tuning fork can be considered as a harmonic oscillator whose vibrational energy is 0.04 J. Compare the energy quanta of this tuning fork with those of an atomic oscillator that emits and absorbs orange light whose frequency is 5.00×10^{14} Hz.

- For the first case, you have $\nu_1 = 660\ Hz = 660\ sec^{-1}$.
- Calculate the corresponding energy $h\nu_1$ in Joule.
- Now compare the value with the vibrational energy $0.04\ J$.

- For the second case, you have $\nu_2 = 5 \times 10^{14}\ \ sec^{-1}$.
- Calculate the corresponding energy $h\nu_2$ in Joule.
- Convert it in electron-volt (eV) unit.
- Now compare.



Solution

(*a*) For the tuning fork,

$$h\nu_1 = (6.63 \times 10^{-34}\ \mathrm{J \cdot s})\ (660\ \mathrm{s}^{-1}) = 4.38 \times 10^{-31}\ \mathrm{J}$$

The total energy of the vibrating tines of the fork is therefore about 10^{29} times the quantum energy $h\nu$. The quantization of energy in the tuning fork is obviously far too small to be observed, and we are justified in regarding the fork as obeying classical physics.

(*b*) For the atomic oscillator,

$$h\nu_2 = (6.63 \times 10^{-34}\ \mathrm{J \cdot s})\ (5.00 \times 10^{14}\ \mathrm{s}^{-1}) = 3.32 \times 10^{-19}\ \mathrm{J}$$

In electronvolts, the usual energy unit in atomic physics,

$$h\nu_2 = \frac{3.32 \times 10^{-19}\ \mathrm{J}}{1.60 \times 10^{-19}\ \mathrm{J/eV}} = 2.08\ \mathrm{eV}$$

This is a significant amount of energy on an atomic scale, and it is not surprising that classical physics fails to account for phenomena on this scale.

Photoelectric Effect (not in syllabus)

Recall Planck's theory of black body radiation

Energy of light is discrete and comes in packets of energy. Such packets represent particles called "*photons*".

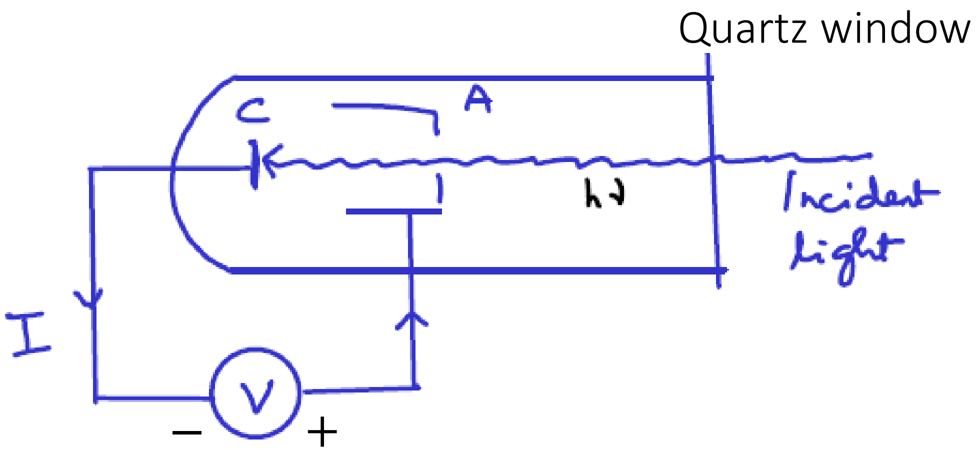
- ☐ **Hertz Experiment** (1886-87): He noticed that sparks occurred more readily in the air gap of his transmitter when ultraviolet light was directed at one of the metal balls.
- ☐ The cause was electrons emitted when the frequency of the light was sufficiently high. This phenomenon is known as the *photoelectric effect* and the emitted electrons are called photoelectrons.
- ☐ *It is one of the ironies that the same work to demonstrate that light consists of electromagnetic waves also gave the first hint that this was not the whole story.*

Module 4 (Quantum Mechanics)

Photoelectric Effect (not in syllabus)

Recall Planck’s theory of black body radiation

Energy of light is discrete and comes in packets of energy. Such packets represent particles called “*photons*”.



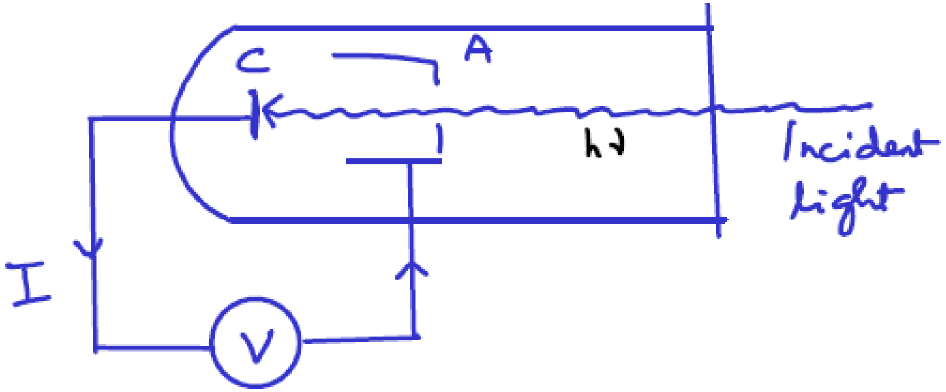
- Experiment:
- An evacuated tube containing two electrodes (cathode and anode) – connected to a source of variable voltage.
- Now, shine the light.
- The incident light knocked out electrons from the cathode in the discharge tube – photoelectrons.
- Now, you have two situations:
- If $V > 0$, the electrons accelerate.
- If $V < 0$, the emitted will decelerate.

Module 4 (Quantum Mechanics)

Photoelectric Effect (not in syllabus)

Recall Planck’s theory of black body radiation

Energy of light is discrete and comes in packets of energy. Such packets represent particles called “*photons*”.



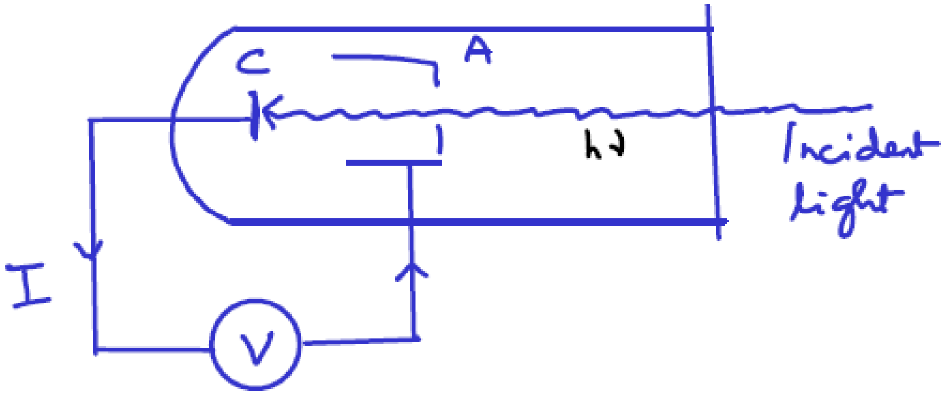
- ❑ If $V > 0$, the electrons accelerate.
- ❑ If $V < 0$, the emitted electrons will decelerate.
- ❑ At a certain value $V = -V_0$, current stops. => V_0 is called the stopping potential.
- ❑ Note: V_0 depends on frequency and not on intensity (not expected classically). Change in intensity DOES NOT change V_0. *Light energy depends on frequency, not on intensity*.

Module 4 (Quantum Mechanics)

Photoelectric Effect (not in syllabus)

Recall Planck's theory of black body radiation

Energy of light is discrete and comes in packets of energy. Such packets represent particles called "*photons*".



- Einstein's explanation:
- Suppose, W_0 is the energy required to knock an electron.
- From the energy conversion, we get, $h\nu = W_0 + \frac{1}{2}m_e v^2$
- At $V = V_0$, Kinetic Energy = 0. So, $\frac{1}{2}m_e v^2 = eV_0$
- From the energy conversion, we get, $h\nu = W_0 + \frac{1}{2}m_e v^2$
- So, we get, $h\nu = W_0 + \frac{1}{2}m_e v^2 = W_0 + eV_0$
- This gives $\nu = \frac{W_0 + eV_0}{h}$ => ν vs. V_0 will give a straight line.

Notice: V_0 depends on frequency and not on intensity.

Module 4 (Quantum Mechanics)

Light – Both wave and particle

- ❑ Recall Planck's theory of black body radiation: Energy of light is discrete and comes in packets of energy. Such packets represent particles called "*photons*".

- ❑ According to the wave theory, light waves leave a source with their energy spread out continuously through the wave pattern. According to the quantum theory, light consists of individual photons, each small enough to be absorbed by a single electron.

- ❑ Yet, despite the particle picture of light it presents, the quantum theory needs the frequency of the light to describe the photon energy.

Light – Both wave and particle

- ☐ So far: the wave theory of light explains diffraction and interference, which the quantum theory cannot account for, and, quantum theory explains the photoelectric effect, which the wave theory cannot account for.
- ☐ The photoelectric effect provides convincing evidence that photons of light can transfer energy to electrons. Is the inverse process also possible? That is, can part or all of the kinetic energy of a moving electron be converted into a photon? The *inverse photoelectric effect*.
- ☐ X-rays (consist of high-energy photons) and X-ray Diffraction
- ☐ Compton Effect (Further confirmation of the photon model)

Compton Effect

- ❑ Recall: According to the quantum theory of light, photons behave like particles except for their lack of rest mass.
- ❑ Compton effect is the scattering of photons by free electrons in the target material.
- ❑ In photoelectric effect, a photon is completely absorbed and an electron is emitted.
- ❑ In Compton effect, the photon is NOT completely absorbed, but scattered by the electron.
- ❑ *Compton allowed X-rays of wavelength λ to fall on a graphite target, and the intensity of the scattered rays were measured as a function of their wavelengths.*
- ❑ An X-ray photon strikes an electron (assumed to be initially at rest in the laboratory coordinate system) and is scattered away from its original direction of motion while the electron receives an impulse and begins to move.
- ❑ We can think of the photon as losing an amount of energy in the collision that is the same as the kinetic energy KE gained by the electron, although actually separate photons are involved.
- ❑ He found peaks in the intensity of scattered rays at two different values of their wavelength: $\lambda_1 = \lambda$ (original X-ray wavelength), and $\lambda_1 = \lambda' > \lambda$.

Compton Effect

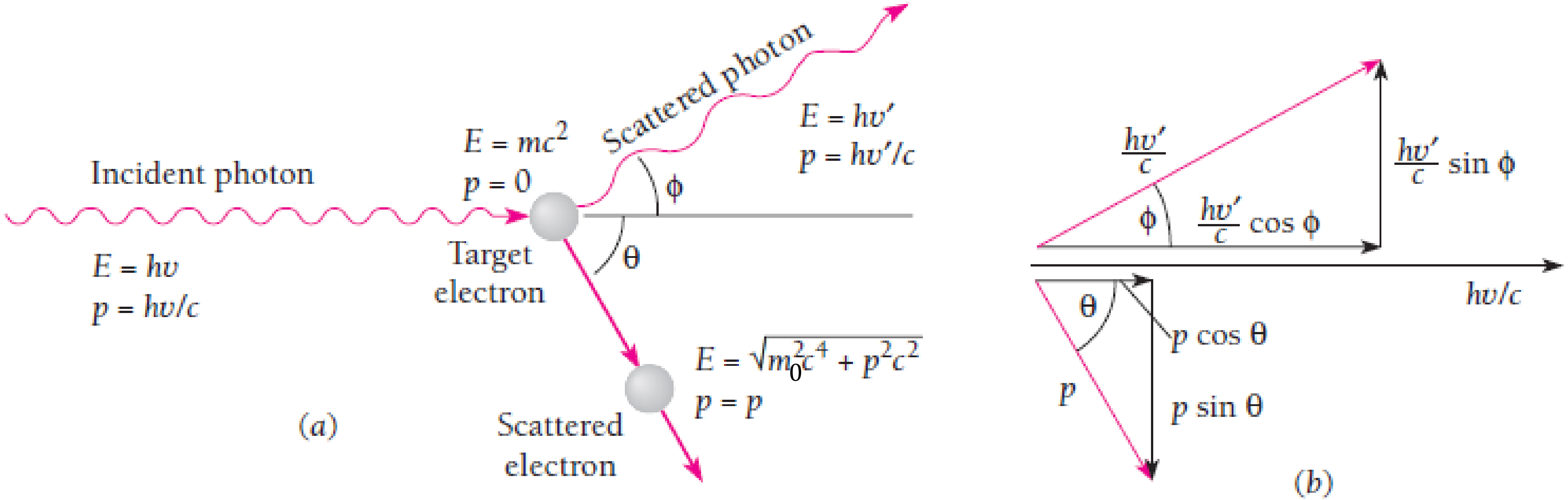
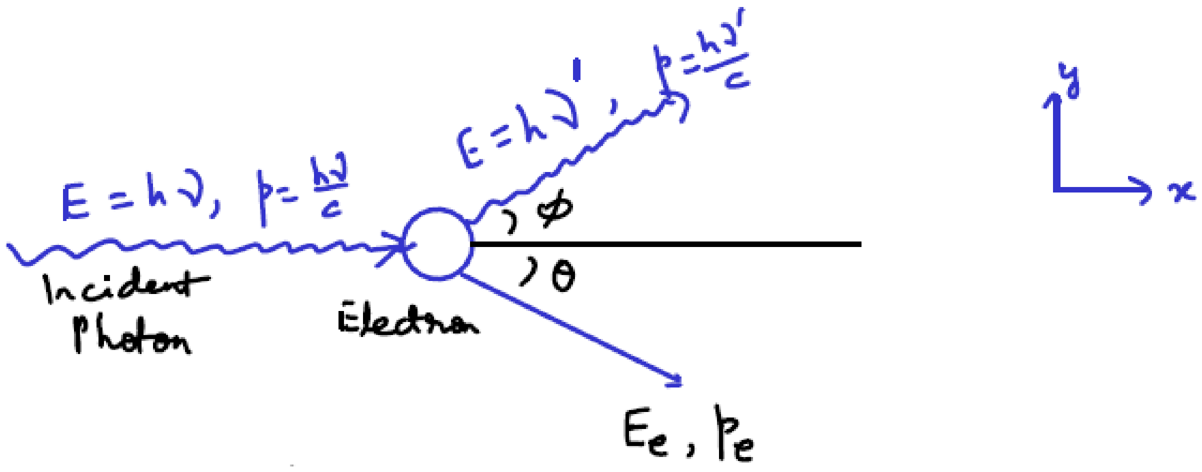


Figure 2.22 (*a*) The scattering of a photon by an electron is called the Compton effect. Energy and momentum are conserved in such an event, and as a result the scattered photon has less energy (longer wavelength) than the incident photon. (*b*) Vector diagram of the momenta and their components of the incident and scattered photons and the scattered electron.

- Momentum of incident photon:
- $E = h\nu = \sqrt{{m_0}^2c^4 + \ p^2c^2}$, where the rest mass of photon, $m_0 = 0$.
- $E = pc \ \ \Longrightarrow \ \ p = \frac{E}{c}$ (momentum).

Compton Effect



- The initial photon momentum is $h\nu/c$, the scattered photon momentum is $h\nu'/c$, and the initial and final electron momenta are respectively 0 and p_e.
- Use the conservation of momentum (Initial momentum = final momentum)

- Conservation of momentum along x-direction (along the direction of the original photon)
- Equation 1: $\frac{h\nu}{c} = \frac{h\nu'}{c} Cos\varphi + p_e Cos\theta \;\; \Longrightarrow p_e c \; Cos\theta = h\nu - h\nu' \; Cos\varphi$

- Conservation of momentum along y-direction (along the direction perpendicular to the original photon)
- Equation 2: $0 = \frac{h\nu'}{c} \; Sin\varphi - p_e \; Sin\theta \;\; \Longrightarrow \; p_e c \; Sin\theta = h\nu' \; Sin\varphi$

Module 4 (Quantum Mechanics)

Compton Effect

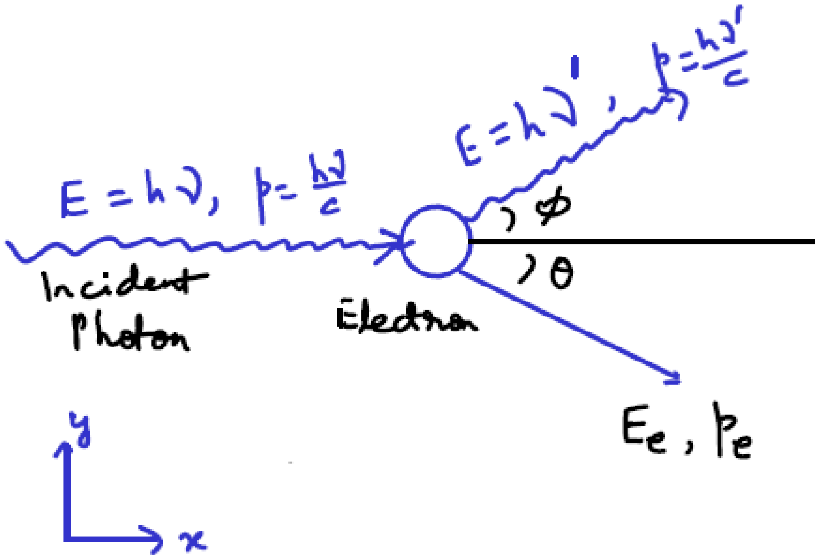
- ☐ Along x-direction: Equation 1: $\frac{h\nu}{c} = \frac{h\nu'}{c} Cos\varphi + p_e Cos\theta \implies p_e c\ Cos\theta = h\nu - h\nu'\ Cos\varphi$
- ☐ Along y-direction: Equation 2: $0 = \frac{h\nu'}{c}\ Sin\varphi - p_e\ Sin\theta \implies p_e c\ Sin\theta = h\nu'\ Sin\varphi$

Squaring and adding, we get :

$$p_e^2 c^2 (\cos^2\theta + \sin^2\theta) = (h\nu - h\nu'\cos\phi)^2 + (h\nu'\sin\phi)^2$$

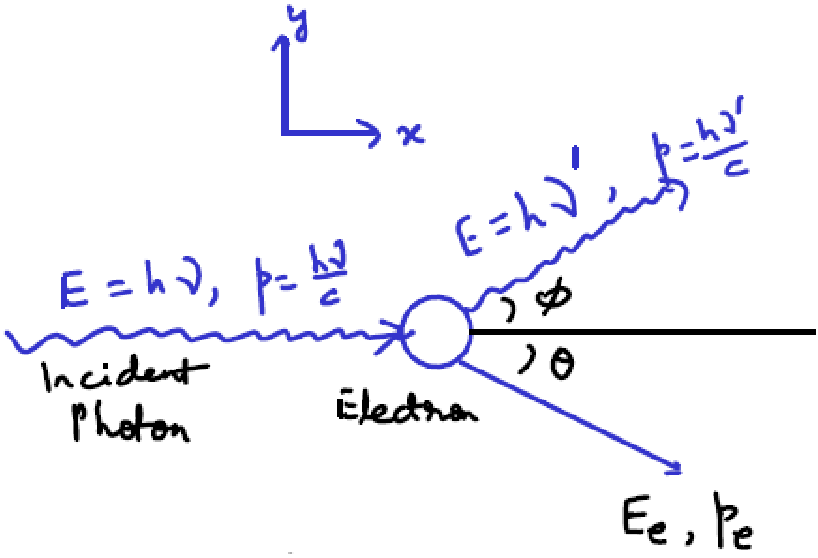
$$\Rightarrow p_e^2 c^2 = (h\nu)^2 + (h\nu')^2\cos^2\phi - 2(h\nu)(h\nu')\cos\phi + (h\nu')^2\sin^2\phi$$

$$\Rightarrow \boxed{p_e^2 c^2 = (h\nu)^2 + (h\nu')^2 - 2(h\nu)(h\nu')\cos\phi} \longrightarrow ③$$



Compton Effect

- ☐ Next, we equate the two expressions for the total energy of a particle.
- ☐ $Initial\ Energy\ = E_{photon}\ +\ E_{electron}\ = h\nu + m_0c^2$ (m_0 = rest mass of electron, electron is at rest initially)
- ☐ $Final\ Energy\ = h\nu' + \sqrt{m_0{}^2c^4 + p_e{}^2c^2}$
- ☐ Using conservation of energy: Initial Energy = Final Energy



$$h\nu + m_0c^2 = h\nu' + \sqrt{m_0^2c^4 + p_e^2c^2}$$

$$(h\nu + m_0c^2 - h\nu')^2 = m_0^2c^4 + p_e^2c^2$$

$$(h\nu - h\nu')^2 + \cancel{m_0^2c^4} + 2m_0c^2(h\nu - h\nu') = \cancel{m_0^2c^4} + p_e^2c^2$$

$$\Rightarrow p_e^2c^2 = (h\nu)^2 + (h\nu')^2 - 2(h\nu)(h\nu') + 2m_0c^2(h\nu - h\nu') \quad \text{④}$$

Module 4 (Quantum Mechanics)

Compton Effect

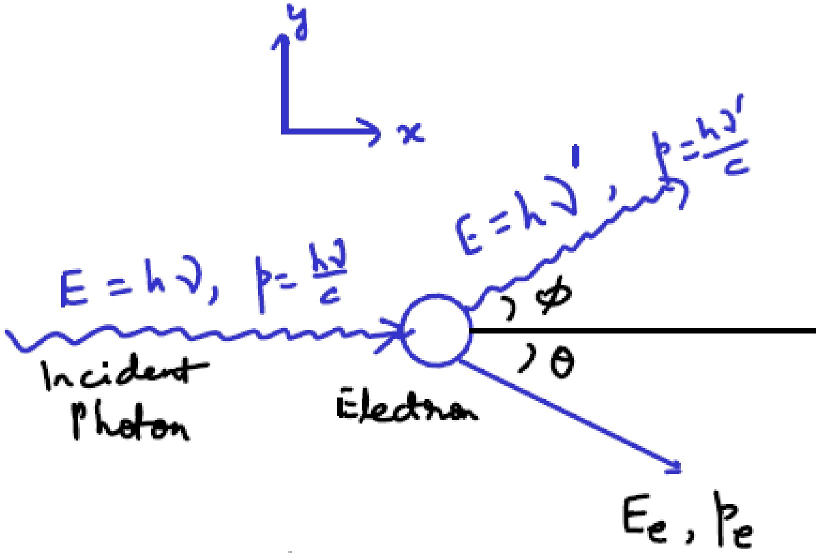
- ☐ Equation **3** (conservation of momentum): ${p_e}^2c^2 = (h\nu)^2 + (h\nu')^2 - 2\,(h\nu)(h\nu')Cos\varphi$
- ☐ Equation **4** (conservation of energy): ${p_e}^2c^2 = (h\nu)^2 + (h\nu')^2 - 2\,(h\nu)(h\nu') + 2m_0c^2(h\nu\ - h\nu')$

Equating RHS of ③ & ④ :

$$\cancel{(h\nu)^2} + \cancel{(h\nu')^2} - \cancel{2}(h\nu)(h\nu')\cos\phi = \cancel{(h\nu)^2} + \cancel{(h\nu')^2} - \cancel{2}(h\nu)(h\nu') + \cancel{2}m_0c^2(h\nu - h\nu')$$

$$\Rightarrow \quad -(h\nu)(h\nu')\cos\phi = -(h\nu)(h\nu') + m_0c^2(h\nu - h\nu')$$

$$\Rightarrow \quad (h\nu)(h\nu')(1-\cos\phi) = m_0c^2(h\nu - h\nu')$$



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Module 4 (Quantum Mechanics)

Compton Effect

$$\Rightarrow \quad (h\nu)(h\nu')(1-\text{Cos}\,\phi) = m_0 c^2 (h\nu - h\nu')$$

Dividing both sides by $h^2 c^2$, we get

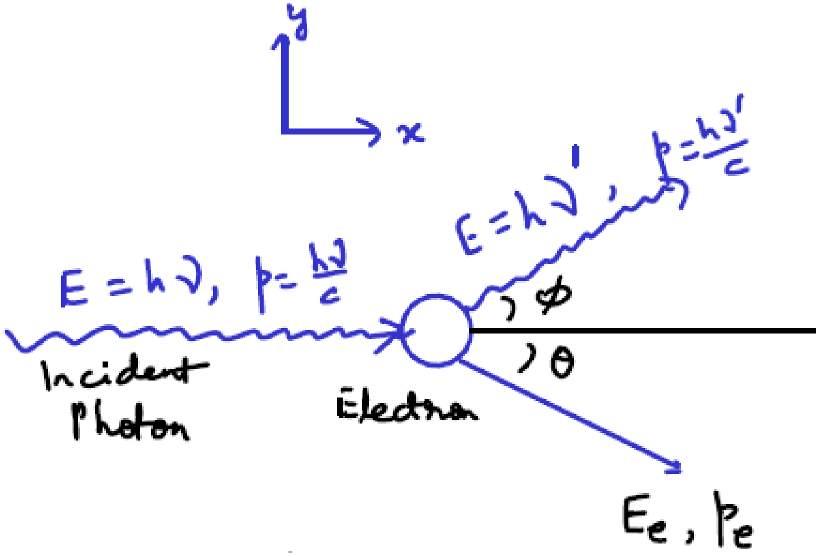
$$\frac{\nu}{c}\cdot\frac{\nu'}{c}(1-\text{Cos}\,\phi) = \frac{m_0}{h}(\nu - \nu')$$

$$\frac{1-\text{Cos}\,\phi}{\lambda\,\lambda'} = \frac{m_0 c}{h}\left(\frac{\nu}{c} - \frac{\nu'}{c}\right) = \frac{m_0 c}{h}\left(\frac{1}{\lambda} - \frac{1}{\lambda'}\right)$$

Multiply by $\lambda\lambda'$ on both sides:

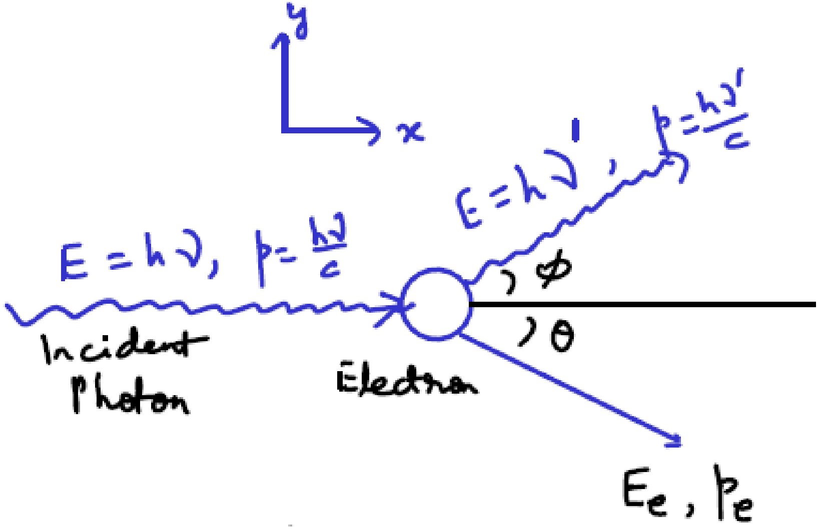
$$1-\text{Cos}\,\phi = \frac{m_0 c}{h}(\lambda' - \lambda)$$

$$\Rightarrow \quad \lambda' - \lambda = \frac{h}{m_0 c}(1-\text{Cos}\,\phi)$$



Module 4 (Quantum Mechanics)

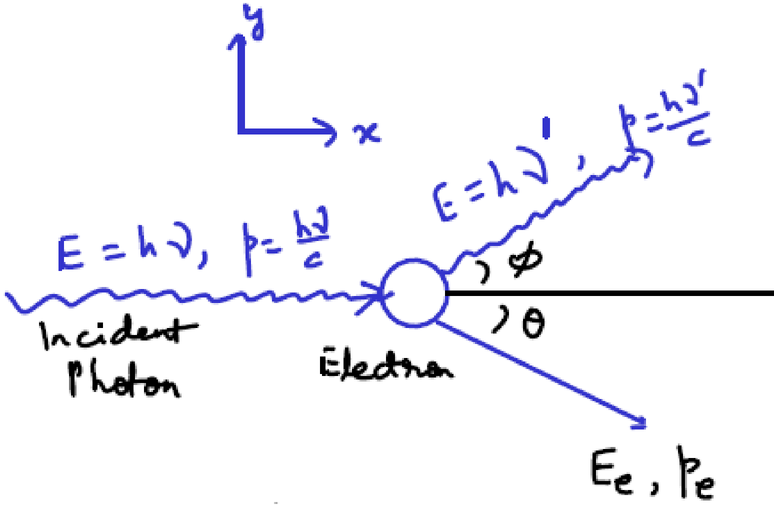
Compton Effect



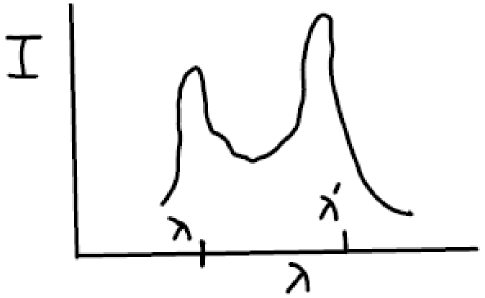
- We have, $\lambda' - \lambda = \frac{h}{m_0 c}(1 - Cos\varphi)$ [φ is the scattering angle]
- It gives change in wavelength due to scattering at an angle ϕ by a particle of rest mass m_0.
- Define the Compton wavelength as: $\lambda_C = \frac{h}{m_0 c}$
- And, we have: $\lambda' - \lambda = \lambda_C(1 - Cos\varphi)$
- The Compton wavelength gives the scale of the wavelength change of the incident photon. The Compton effect is the chief means by which x-rays lose energy when they pass through matter.
- From the equation $\lambda' - \lambda = \lambda_C(1 - Cos\varphi)$, we note that the greatest wavelength change possible corresponds to $\varphi = 180°$, when the wavelength change will be twice the Compton wavelength λ_C.
- For an electron, λ_C =2.426 pm. The maximum wavelength change in the Compton effect is 4.852 pm. Changes of this magnitude or less can be observed using X-rays.

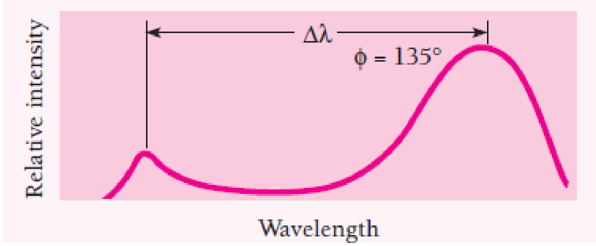
Module 4 (Quantum Mechanics)

Compton Effect



- We have, $\lambda' - \lambda = \frac{h}{m_0 c}(1 - Cos\varphi)$ [φ is the scattering angle]
- Compton wavelength, $\lambda_C = \frac{h}{m_0 c}$ and, we have: $\lambda' - \lambda = \lambda_C(1 - Cos\varphi)$
- So, $\lambda' > \lambda$ (This cannot be explained classically)
- One peak is obtained at $\lambda_1 = \lambda$ (scattered photon has the **same wavelength** as that of the incident photon)
- Other peak is obtained at $\lambda_2 = \lambda' > \lambda$ (scattered photon has **smaller wavelength**)
- Peak at unshifted wavelength λ: Once the outer electron (loosely bound) has been removed from the atom, the remaining electrons remain tightly bound, so the incident X-ray beam cannot remove them easily. In this case, during the collision, the entire atom moves (instead of a single electron). So m_0 becomes very large (~4 orders of magnitude), since rest mass of atom is very large => $\lambda' \simeq \lambda$

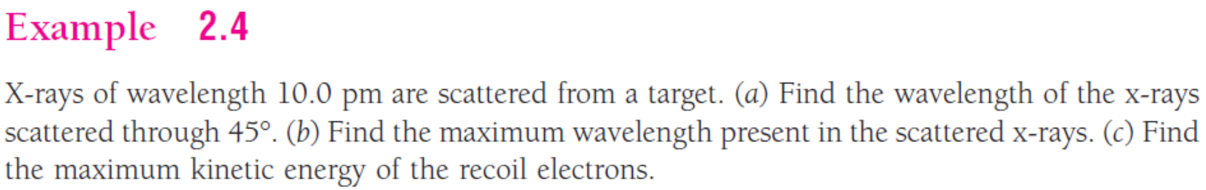




Module 4 (Quantum Mechanics)

Recap so far….

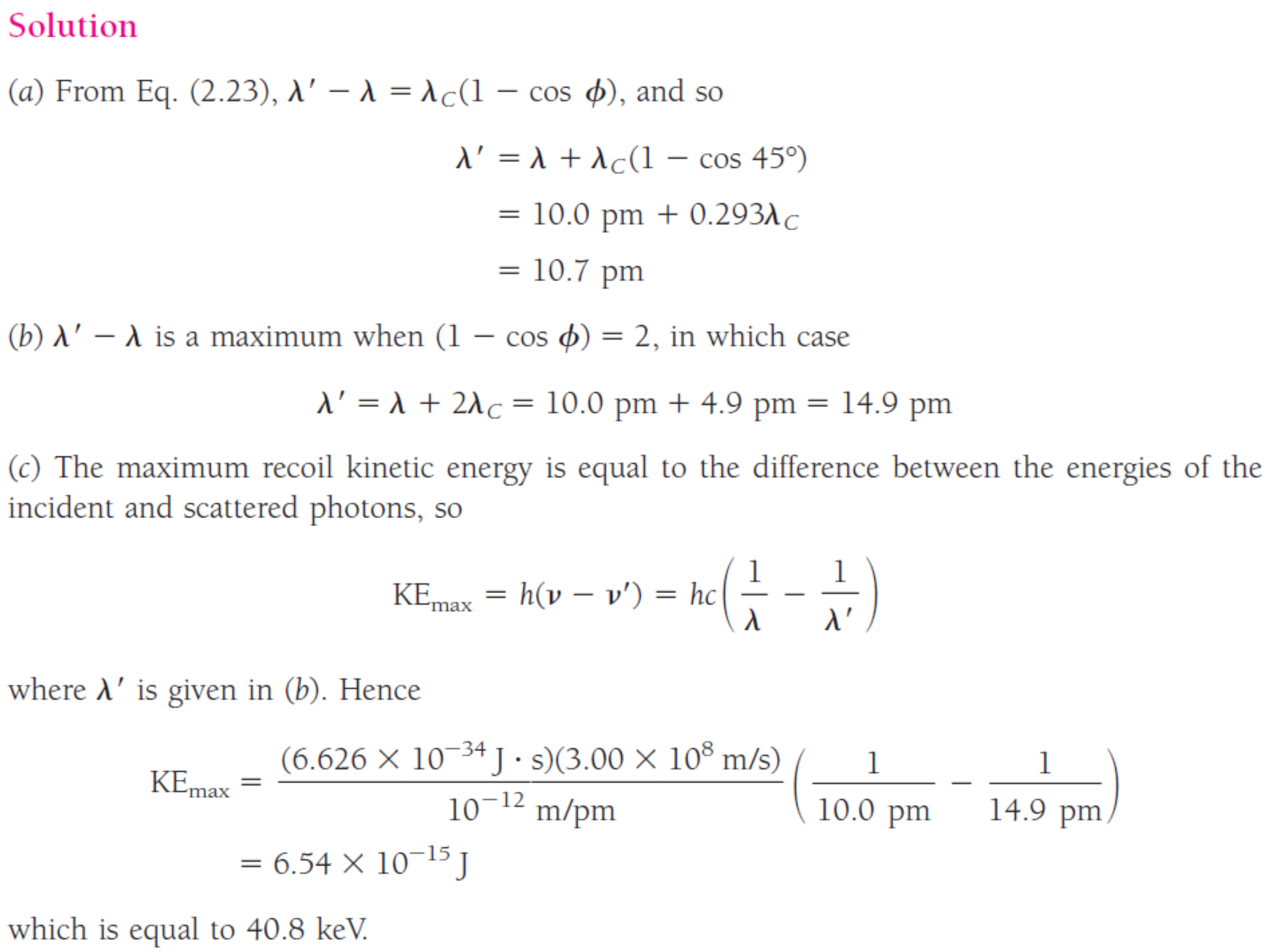
Compton effect – Example Problems



Example 2.4

X-rays of wavelength 10.0 pm are scattered from a target. (*a*) Find the wavelength of the x-rays scattered through 45°. (*b*) Find the maximum wavelength present in the scattered x-rays. (*c*) Find the maximum kinetic energy of the recoil electrons.

- Incident wavelength, $\lambda = 10\ pm$ and scattering angle, $\phi = 45°$.
- Calculate the scattered wavelength, λ'.
- Use the Compton effect expression:
- $\lambda' - \lambda = \frac{h}{m_0 c}(1 - Cos\varphi) = \lambda_C(1 - Cos\varphi)$
- For the second case, $\lambda' - \lambda$ is maximum when $\phi = 180°$.
- For the third case, maximum recoil kinetic energy is $KE_{max} = h\nu - h\nu' = hc\left(\frac{1}{\lambda} - \frac{1}{\lambda'}\right)$



Solution

(*a*) From Eq. (2.23), $\lambda' - \lambda = \lambda_C(1 - \cos\phi)$, and so

$$\begin{aligned}\lambda' &= \lambda + \lambda_C(1 - \cos 45°)\\ &= 10.0\ \text{pm} + 0.293\lambda_C\\ &= 10.7\ \text{pm}\end{aligned}$$

(*b*) $\lambda' - \lambda$ is a maximum when $(1 - \cos\phi) = 2$, in which case

$$\lambda' = \lambda + 2\lambda_C = 10.0\ \text{pm} + 4.9\ \text{pm} = 14.9\ \text{pm}$$

(*c*) The maximum recoil kinetic energy is equal to the difference between the energies of the incident and scattered photons, so

$$\text{KE}_{\max} = h(\nu - \nu') = hc\left(\frac{1}{\lambda} - \frac{1}{\lambda'}\right)$$

where λ' is given in (*b*). Hence

$$\begin{aligned}\text{KE}_{\max} &= \frac{(6.626 \times 10^{-34}\ \text{J}\cdot\text{s})(3.00 \times 10^{8}\ \text{m/s})}{10^{-12}\ \text{m/pm}}\left(\frac{1}{10.0\ \text{pm}} - \frac{1}{14.9\ \text{pm}}\right)\\ &= 6.54 \times 10^{-15}\ \text{J}\end{aligned}$$

which is equal to 40.8 keV.

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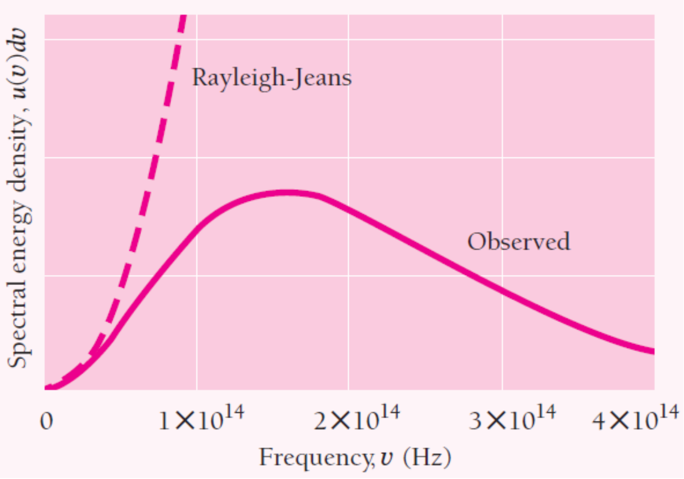
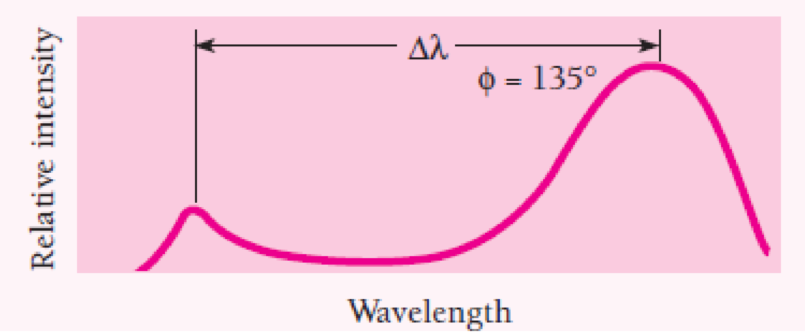
Module 4 (Quantum Mechanics)

Recap so far….

- ☐ Blackbody radiation
  - ☐ Rayleigh-Jeans formula
  - ☐ The ultraviolet catastrophe of classical physics
  - ☐ Planck's theory of blackbody radiation
- ~~☐ Photoelectric effect (not in syllabus)~~
- ☐ Compton effect





Textbook: Arthur Beiser – Concepts of Modern Physics

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Module 4

Module -4 : Quantum Mechanics

Planck's theory of black-body radiation, Compton effect, Wave particle duality, De Broglie waves, Davisson and Germer's experiment, Uncertainty principle, Brief idea of Wave Packet, Wave Function and its physical interpretation, Schrodinger equation in one-dimension, free particle, particle in an infinite square well. [9]

Text book: T3: Arthur Beiser (AB), Concept of Modern Physics, 6th edition 2009, Tata McGraw- Hill

Reference book: R1: Fundamentals of Physics, Halliday, Walker and Resnick

Module 4 (Quantum Mechanics)

Wave particle duality – de Broglie Waves

- ☐ We know about this phenomenon for light (which has both particle-like and wave-like properties).
- ☐ Louis de Broglie suggested in 1924 that any moving objects have both wave as well as particle-like characters [in 1929 de Broglie received the Nobel Prize].
- ☐ For a photon of light of frequency ν has the momentum, $p = \frac{h\nu}{c} = \frac{h}{\lambda}$ [Recall: $\lambda\nu = c$]
- ☐ So, we have $\lambda = \frac{h}{p}$ (where λ = wavelength, p = momentum, h = Planck's constant)
- ☐ Louis de Broglie suggested that this relation is applicable to material particles as well.
- ☐ Consider a particle of mass m_0 moving with velocity v. Momentum of the particle is $p = \gamma m_0 v$ and its de Broglie wavelength is $\lambda = \frac{h}{\gamma m_0 v}$ [Recall: γ is the relativistic factor: $\gamma = \frac{1}{\sqrt{1-v^2/c^2}}$]
- ☐ The greater the particle's momentum, the shorter its wavelength λ.

Wave particle duality – de Broglie Waves

- Example Problem:
- Find the de Broglie wavelengths of a golf ball of mass 46 gm moving with a velocity of 30 m/s.
- Find the same for an electron moving velocity of 10^7 m/s.

- Solution:
- Problem 1: $\gamma \approx 1.$ So, $\lambda = \frac{h}{p} = \frac{h}{m_0 v} = \frac{6.63 \times 10^{-11}}{0.046 \times 30}$ m. $\lambda \approx 4.8 \times 10^{-34}$ m => The wavelength λ of the golf ball is so small compared with its dimension of the ball – so, *it is not possible to detect the wave nature*.
- Problem 2: In case of an electron, $\lambda \approx 7.3 \times 10^{-11}$ m => The wavelength is comparable with the dimensions of atoms (for example, radius of the hydrogen atom is 5.3×10^{-11} m). Thus, *the wave nature is possible to detect*. The wave character of moving electrons is the key to understanding atomic structure and behavior.

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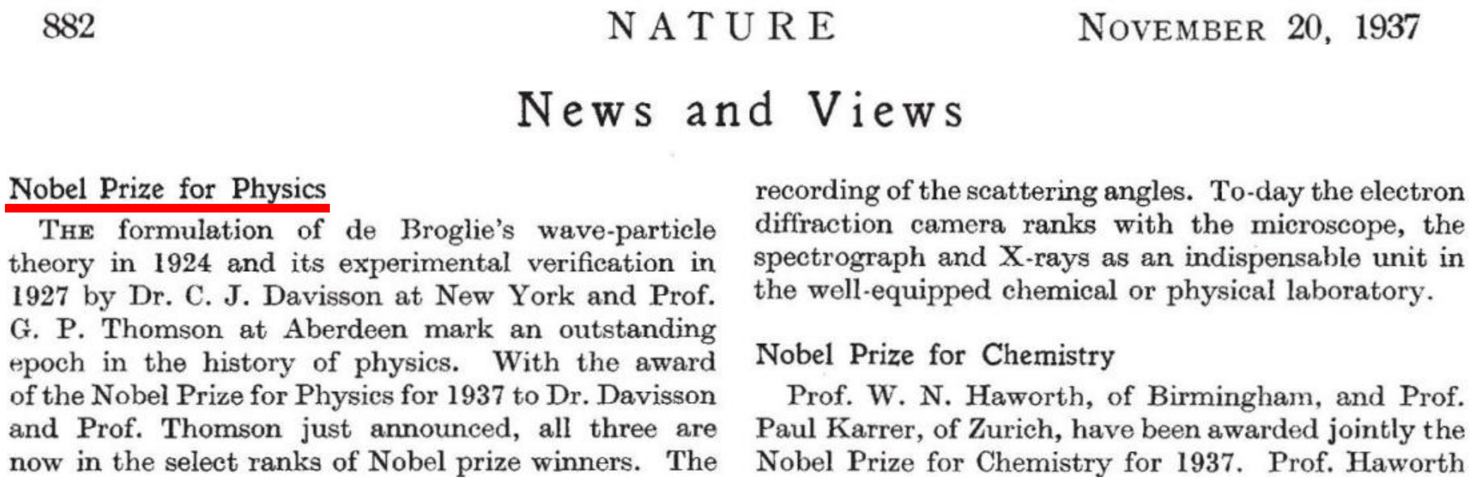
Module 4 (Quantum Mechanics)

Wave particle duality – de Broglie Waves

- Experimental verification of existence of de Broglie waves

- In 1927 Clinton Davisson and Lester Germer in the United States and G. P. Thomson in England independently confirmed de Broglie’s hypothesis.
- *They demonstrated that electron beams are diffracted when they are scattered by the regular atomic arrays of crystals.*



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News and Views

Nobel Prize for Physics

THE formulation of de Broglie’s wave-particle theory in 1924 and its experimental verification in 1927 by Dr. C. J. Davisson at New York and Prof. G. P. Thomson at Aberdeen mark an outstanding epoch in the history of physics. With the award of the Nobel Prize for Physics for 1937 to Dr. Davisson and Prof. Thomson just announced, all three are now in the select ranks of Nobel prize winners. The recording of the scattering angles. To-day the electron diffraction camera ranks with the microscope, the spectrograph and X-rays as an indispensable unit in the well-equipped chemical or physical laboratory.

Nobel Prize for Chemistry

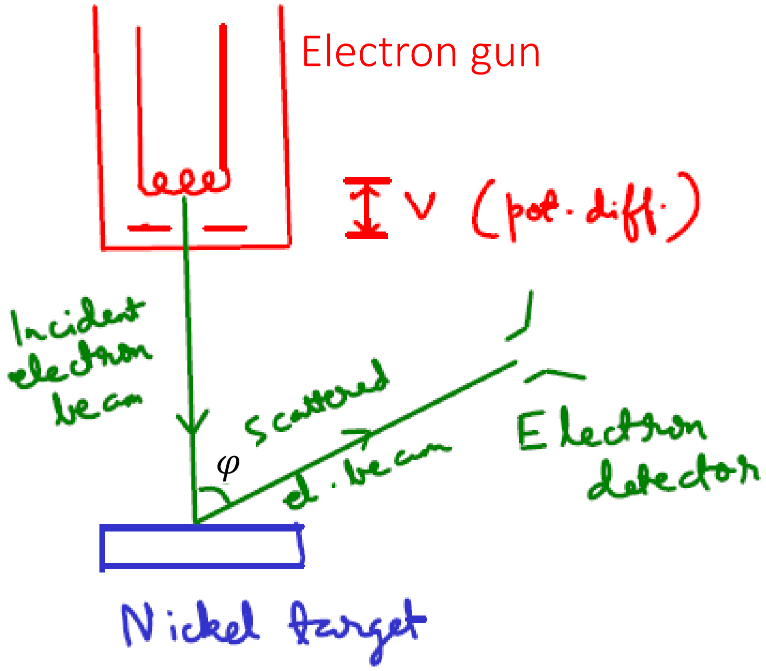
Prof. W. N. Haworth, of Birmingham, and Prof. Paul Karrer, of Zurich, have been awarded jointly the Nobel Prize for Chemistry for 1937. Prof. Haworth

- Let’s look at the experiment of Davisson and Germer (because its interpretation is more direct).

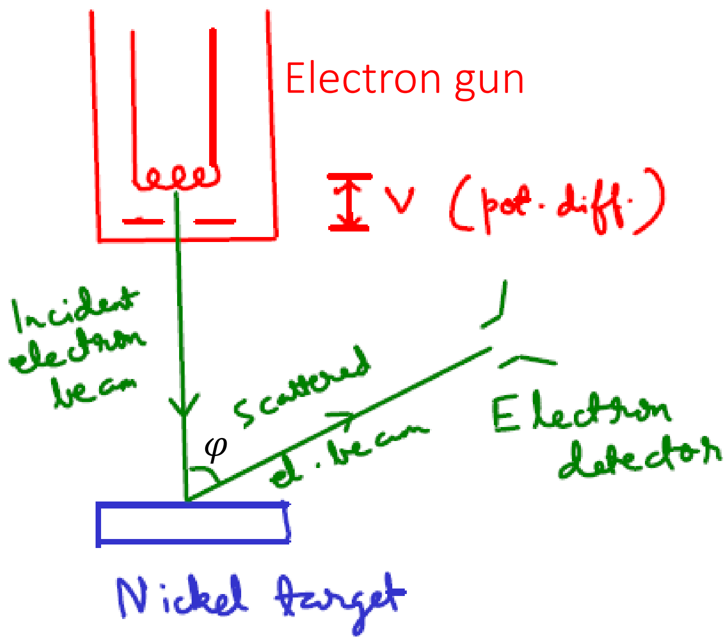
Wave particle duality – de Broglie Waves

- Davisson and Germer Experiment – Confirmation of de Broglie hypothesis

- *They were studying the scattering of electrons from a Nickel target.*
- The electron gun consisted of a heated filament that released electrons. Electrons fell on a nickel crystal, and scattered beam is detected by the electron detector.
- Initially, they found that the *scattered electrons emerge in all directions* and the *intensity depended minimally on* either the scattering angle (φ) or the energy. This is what we should expect from Classical physics.
- During the experiment, an accident occurred that allowed air to enter their apparatus and oxidize the Nickel surface. To remove the oxide to pure nickel, the target was baked (heated at high temperature). After this treatment, they resumed the measurement.
- **Now the results were very different!**



Module 4 (Quantum Mechanics)



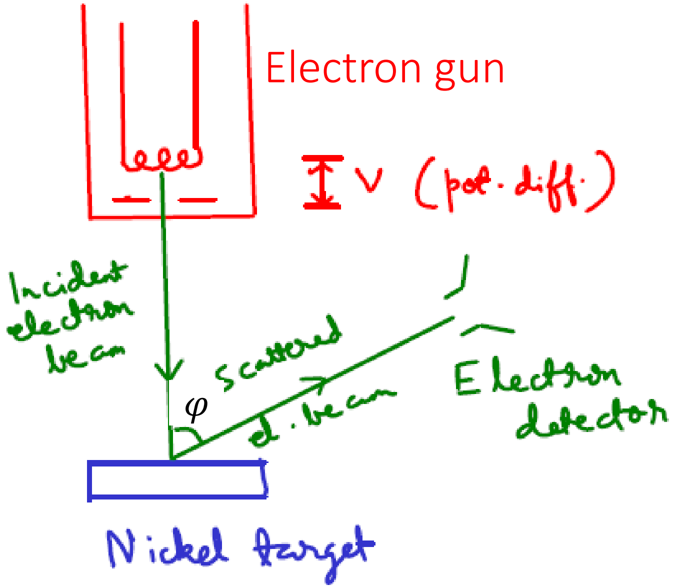
Wave particle duality – de Broglie Waves

- Davisson and Germer Experiment – Confirmation of de Broglie Hypothesis

- *What was the surprising result*?
- After the target sample was baked, there was a strong dependence on both φ and the energy.
- Instead of a continuous variation of scattered electron intensity with angle φ, distinct maxima and minima were observed whose positions depended upon the electron energy (or, the potential difference, V)! (V is the voltage used to accelerate the electrons).

Module 4 (Quantum Mechanics)

Wave particle duality – de Broglie Waves



- Davisson and Germer Experiment – Confirmation of de Broglie Hypothesis

- Scattering of electrons from a Nickel target after baking: *What was the surprise*?
- For different values of V, Davisson and Germer plotted I vs φ graph. The maximum intensity was found for V = 54 volts and φ= 50°.

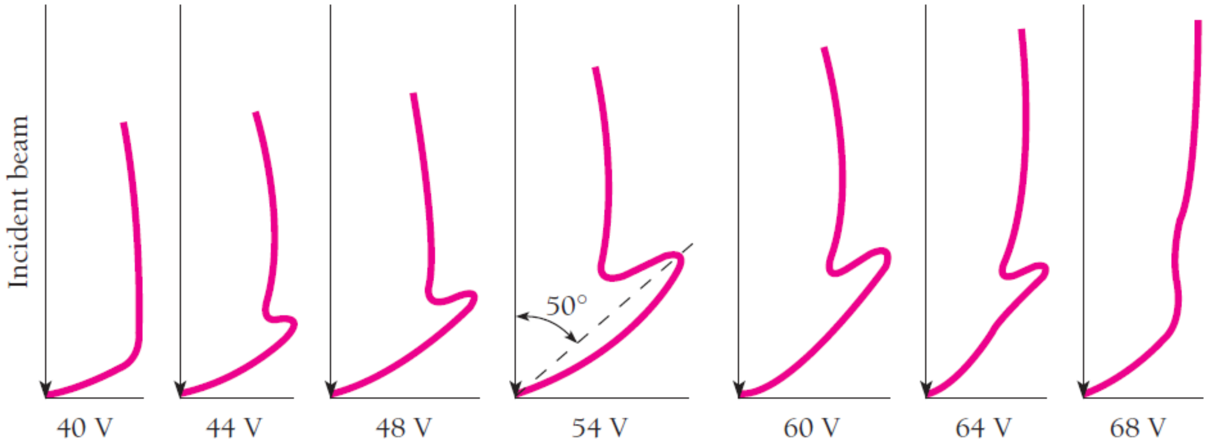


Figure 3.7 Results of the Davisson-Germer experiment, showing how the number of scattered electrons varied with the angle between the incoming beam and the crystal surface. The Bragg planes of atoms in the crystal were not parallel to the crystal surface, so the angles of incidence and scattering relative to one family of these planes were both 65° (see Fig. 3.8).

Module 4 (Quantum Mechanics)

Wave particle duality – de Broglie Waves

- ☐ Davisson and Germer Experiment – Confirmation of de Broglie hypothesis

- ☐ So far……
- ☐ Scattering of electrons from a Nickel target (before baking): They found very little dependence of detector current (I) on either the voltage 'V' or the angle 'φ'. As expected from Classical physics.
- ☐ Scattering of electrons from a Nickel target after baking: Surprising result!!!
- ☐ Instead of a continuous variation of scattered electron intensity with angle φ, distinct maxima and minima were observed whose positions depended upon the electron energy (or, the potential difference, V)!
- ☐ For different values of V, Davisson and Germer plotted I vs φ graph. The maximum intensity was found for V = 54 volts and φ = 50°.
- ☐ Two important questions: *What is the reason for this new effect*? *Why did it not appear until after the nickel target was baked*?

Module 4 (Quantum Mechanics)

Wave particle duality – de Broglie Waves

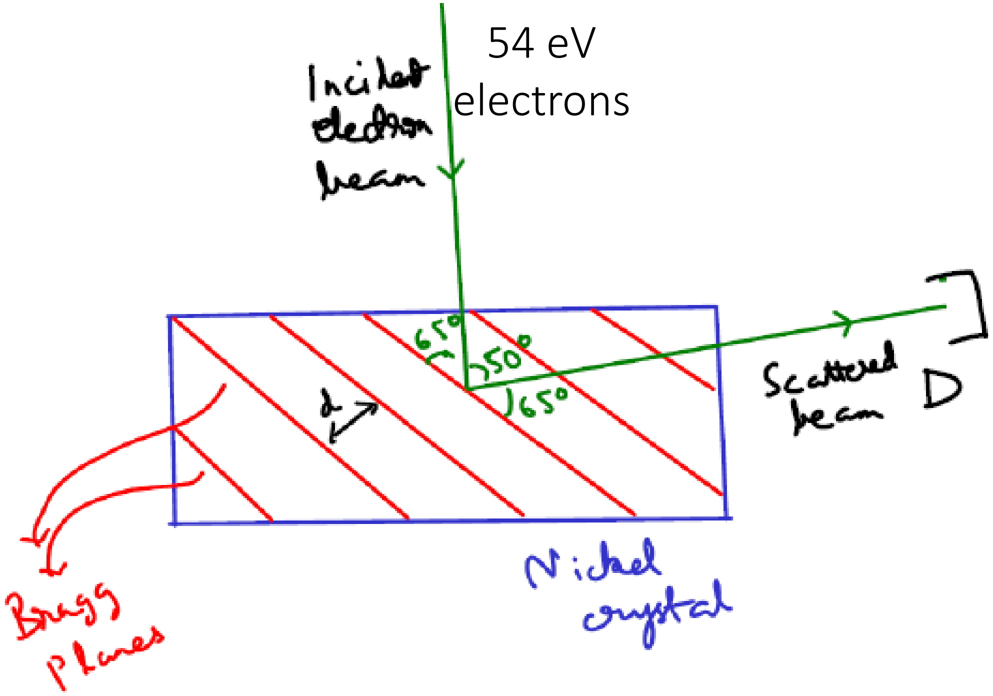
- ☐ Davisson and Germer Experiment – Confirmation of de Broglie hypothesis

- ☐ *What is the reason for this new effect*? *Why did it not appear until after the nickel target was baked*?
- ☐ de Broglie's hypothesis suggested that electron waves were being diffracted by the target, much as x-rays are diffracted by planes of atoms in a crystal.
- ☐ The peaks could only be explained as a constructive interference of waves scattered by the periodically arranged atoms of the crystal.
- ☐ Heating the block of nickel at high temperature causes the many smaller crystal grains to form into a single large crystal, all of whose atoms are arranged in a regular lattice.
- ☐ Any crystal has atoms that are arranged in planes called *Bragg planes*. These planes are all parallel to each other. The scattered beam is said to have undergone Bragg reflections from these planes.
- ☐ Let us see whether we can verify that de Broglie waves are responsible for the findings of Davisson and Germer.

Wave particle duality – de Broglie Waves

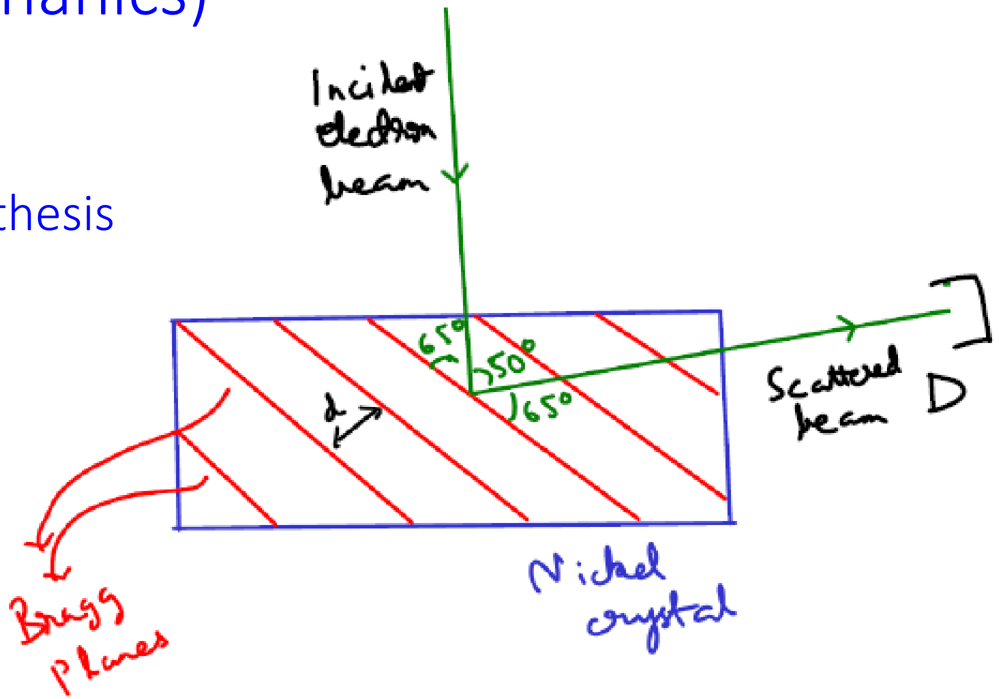
- Davisson and Germer Experiment – Confirmation of de Broglie Hypothesis

- Let us see whether we can verify that de Broglie waves are responsible for the findings of Davisson and Germer.
- In a particular case, a beam of 54 eV electrons was directed perpendicularly at the nickel target and a sharp maximum in the electron distribution occurred at an angle of 50° with the original beam.
- The angles of incidence and scattering relative to the family of Bragg planes shown in Figure are both 65°.
- The distance between two Bragg planes is d = 0.091 nm (This was measured from X-ray diffraction).



Wave particle duality – de Broglie Waves

- Davisson and Germer Experiment – Confirmation of de Broglie Hypothesis
- *Let us see whether we can verify that de Broglie waves are responsible for the findings of Davisson and Germer.*
- The Bragg equation for maxima in the diffraction pattern is $2d\ Sin\theta = n\lambda$
- Here d = 0.091 nm and θ = 65°. For $n = 1$, the de Broglie wavelength λ of the diffracted electrons is $\lambda = 2d\ Sin\theta = 2 \times (0.091\ nm) \times (Sin 65°) = 0.165\ nm$
- Now we use de Broglie's formula $\lambda = \frac{h}{p} = \frac{h}{\gamma m_0 v}$ to find the expected wavelength of the electrons.



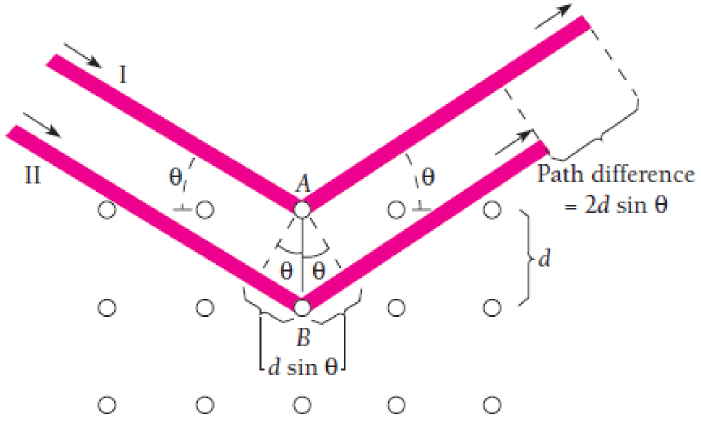
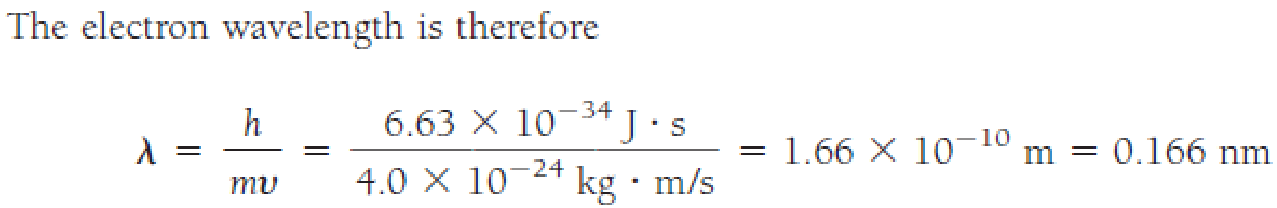


Figure 2.20 X-ray scattering from a cubic crystal.

Wave particle duality – de Broglie Waves

- Davisson and Germer Experiment – Confirmation of de Broglie Hypothesis
- Using the Bragg diffraction, [for d = 0.091 nm, θ = 65°, and $n = 1$], the de Broglie wavelength λ of the diffracted electrons is $\lambda = 2d\ Sin\theta = 2 \times (0.091\ nm) \times (Sin65°) = 0.165$ nm
- Now we use de Broglie's formula $\lambda = \frac{h}{p} = \frac{h}{\gamma m_0 v}$ to find the expected wavelength of the electrons.
- Electron kinetic energy of 54 eV is small compared with its rest energy m_0c^2 of 0.51 MeV, so we consider γ = 1.
- Hence, electron momentum $p = mv = \sqrt{2mE}$ [Recall: Kinetic Energy, $E = \frac{1}{2}mv^2$]
- Use, $E = 54$ eV$= 54 \times 1.6 \times 10^{-19}$ J
- Use, $m = 9.1 \times 10^{-31}$ kg
- Then, $p = \sqrt{2mE} = 4.0 \times 10^{-24}$ kg.m/s



The electron wavelength is therefore

$$\lambda = \frac{h}{mv} = \frac{6.63 \times 10^{-34}\ \text{J} \cdot \text{s}}{4.0 \times 10^{-24}\ \text{kg} \cdot \text{m/s}} = 1.66 \times 10^{-10}\ \text{m} = 0.166\ \text{nm}$$

Module 4 (Quantum Mechanics)

Wave particle duality – de Broglie Waves

- ❑ Davisson and Germer Experiment – Confirmation of de Broglie Hypothesis

- ❑ (Remember the physical phenomena corresponding to waves and particles)

- ❑ Using Bragg diffraction condition, the de Broglie wavelength λ of the diffracted electrons is $\lambda = 2d\ Sin\theta = 2 \times (0.091\ nm) \times (Sin 65°) = 0.165$ nm [In this case, d = 0.091 nm, θ = 65° and $n = 1$.]

- ❑ Using de Broglie's formula, the electron wavelength is $\lambda = \frac{h}{p} = \frac{6.63 \times 10^{-34}\ J.s}{4.0 \times 10^{-24}\ kg.m/s} = 0.166\ nm$

- ❑ de Broglie hypothesis gives the correct value of λ for which constructive interference is obtained at θ = 65° and V = 54 volts. *Davisson-Germer experiment thus directly verifies de Broglie's hypothesis of the wave nature of moving bodies.*

Module 4 (Quantum Mechanics)

Wave particle duality – de Broglie waves

❑ Davisson and Germer Experiment – Confirmation of de Broglie Hypothesis

❑ Problem

An electron has a de Broglie wavelength of λ = 2.0 pm. Find its kinetic energy in keV.

Hint: $p = \frac{h}{\lambda} = \frac{h\nu}{c}$ => $pc = \frac{hc}{\lambda}$ = 6.20 × 10^5 eV [1eV = 1.6 ×10^{-19} J]

$m_0c^2 = 511$ keV

$E = mc^2 = \sqrt{(pc)^2 + (m_0c^2)^2} = ?$

Kinetic Energy, KE = $E - m_0c^2 = 292$ keV.

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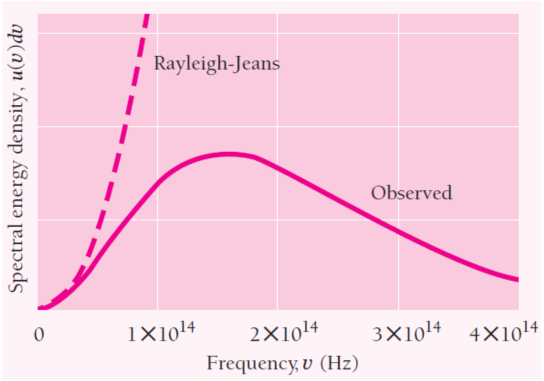
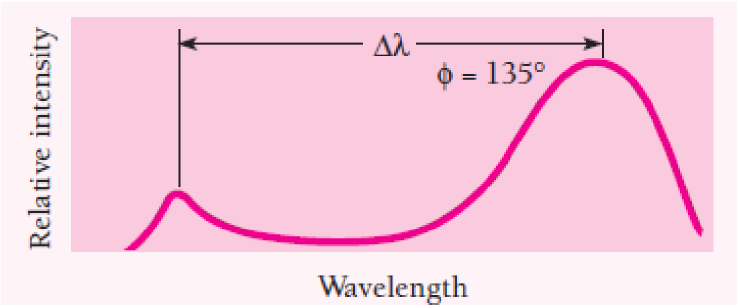
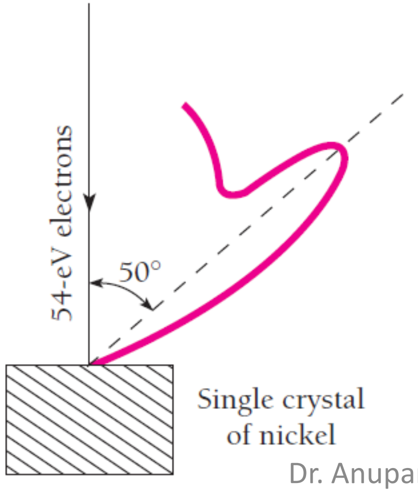
Module 4 (Quantum Mechanics)

Recap so far….

- ☐ Blackbody radiation
  - ☐ Rayleigh-Jeans formula
  - ☐ The ultraviolet catastrophe of classical physics
  - ☐ Planck’s theory of blackbody radiation
- ~~☐ Photoelectric effect (not in syllabus)~~
- ☐ Compton effect
- ☐ Wave particle duality – de Broglie waves
  - ☐ Confirmation of de Broglie hypothesis: Davisson and Germer Experiment







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Module 4

Module -4 : Quantum Mechanics

Planck's theory of black-body radiation, Compton effect, Wave particle duality, De Broglie waves, Davisson and Germer's experiment, Uncertainty principle, Brief idea of Wave Packet, Wave Function and its physical interpretation, Schrodinger equation in one-dimension, free particle, particle in an infinite square well. [9]

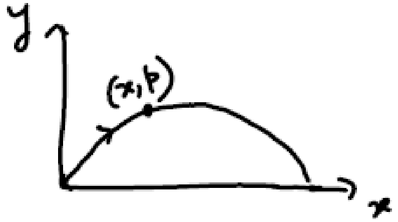
Text book: T3: Arthur Beiser (AB), Concept of Modern Physics, 6th edition 2009, Tata McGraw- Hill

Reference book: R1: Fundamentals of Physics, Halliday, Walker and Resnick

Module 4 (Quantum Mechanics)

Uncertainty Principle

- This principle, discovered by Werner Heisenberg in 1927, is one of the most significant of physical laws
- Classically, we can find the exact trajectory of a particle.
- However, measuring both x and p with infinite precision is impossible in quantum mechanics.



- *It is impossible to know both the exact position and exact momentum of an object at the same time.*
- $\Delta x \, \Delta p_x \geq \frac{\hbar}{2}$ (where, Δx is uncertainty in position and Δp_x is uncertainty in x-component of momentum, $\hbar = h/2\pi$)
- If position is precise, momentum is very imprecise, and vice versa.

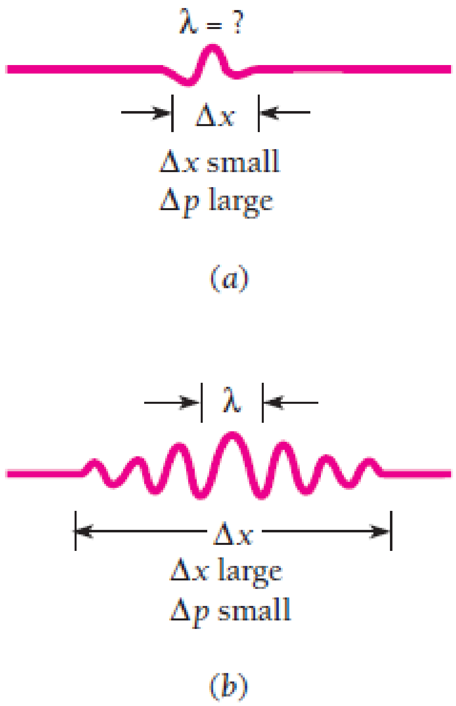
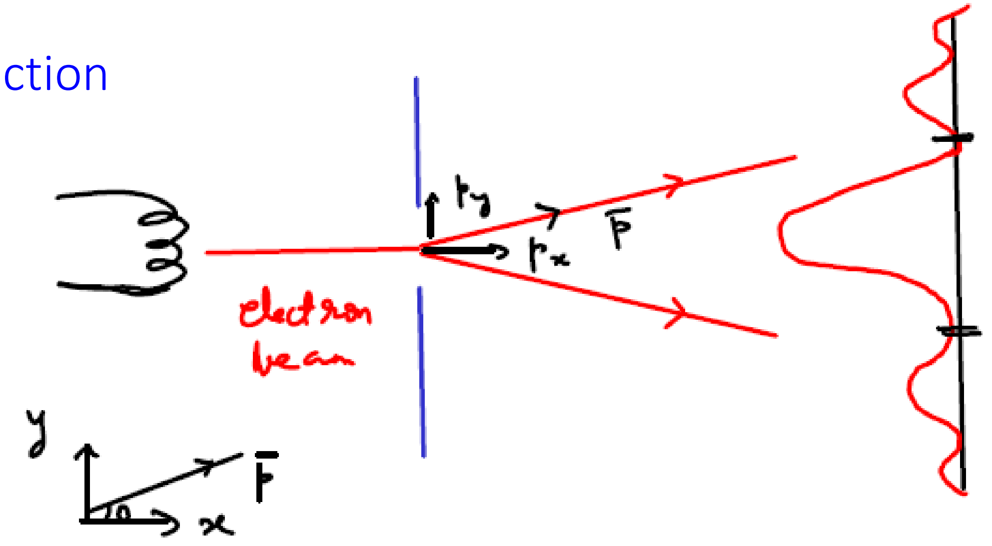


Figure 3.12 (*a*) A narrow de Broglie wave group. The position of the particle can be precisely determined, but the wavelength (and hence the particle's momentum) cannot be established because there are not enough waves to measure accurately. (*b*) A wide wave group. Now the wavelength can be precisely determined but not the position of the particle.

Uncertainty Principle

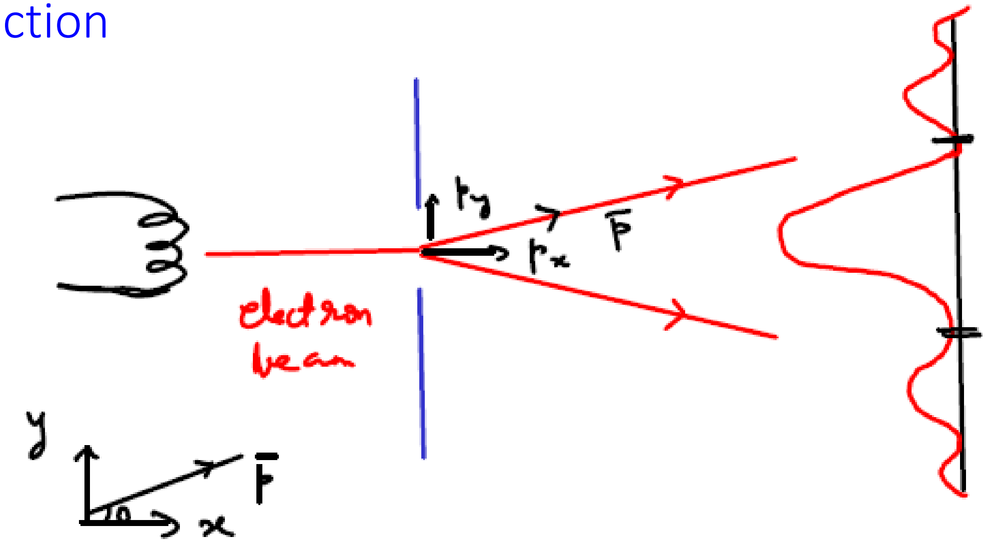
- ❑ This principle, discovered by Werner Heisenberg in 1927, is one of the most significant of physical laws
- ❑ Proof (elementary) of uncertainty principle – Single slit electron diffraction



- ❑ Consider the slit width is ‘a’.
- ❑ Consider electron wavelength to be λ.
- ❑ Most of the electrons strike the screen within the central maximum.
- ❑ A rough estimate of the uncertainty in the electron position in the y-direction, $\Delta y = a$.
- ❑ Let’s estimate (rough) of the uncertainty in the electron momentum Δp_y.
- ❑ For a small diffraction angle (θ), $\frac{p_y}{p_x} = tan\theta \simeq \theta$.
- ❑ So, $p_y \simeq p_x\theta$
- ❑ Now, $-\frac{\lambda}{a} < \theta < +\frac{\lambda}{a}$
- ❑ Using $p_y \simeq p_x\theta$, we can rewrite as $-\frac{\lambda}{a} < \frac{p_y}{p_x} < +\frac{\lambda}{a}$
- ❑ So, uncertainty in p_y is $\Delta p_y \geq p_x \lambda$

Uncertainty Principle

- This principle, discovered by Werner Heisenberg in 1927, is one of the most significant of physical laws
- Proof (elementary) of uncertainty principle – Single slit electron diffraction



- Consider the slit width is ‘a’, so uncertainty in y is $\Delta y = a$.
- We have, $p_y \simeq p_x\theta$
- Uncertainty in p_y is $\Delta p_y \gtrsim p_x\frac{\lambda}{a}$
- Using de Broglie hypothesis, $\lambda = \frac{h}{p} \simeq \frac{h}{p_x}$ (for small θ, $p_y << p_x$)
- Hence, $\Delta p_y \gtrsim p_x \frac{1}{a}\frac{h}{p_x} \gtrsim \frac{h}{a} \gtrsim \frac{h}{\Delta y}$
- Thus, $\Delta y\, \Delta p_y \gtrsim h$
- Similarly, $\Delta x\, \Delta p_x \geq h$

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Module 4 (Quantum Mechanics)

Uncertainty Principle

❑ This principle, discovered by Werner Heisenberg in 1927, is one of the most significant of physical laws

❑ Heisenberg’s uncertainty relations:

- ❑ $\Delta x\, \Delta p_x \geq \frac{\hbar}{2}$
- ❑ $\Delta y\, \Delta p_y \geq \frac{\hbar}{2}$
- ❑ $\Delta z\, \Delta p_z \geq \frac{\hbar}{2}$

- These equations state that the product of the uncertainty Δx in the position of an object at some instant and the uncertainty Δp_x in its momentum component in the x direction at the same instant is equal to or greater than $\frac{\hbar}{2}$.
- If we arrange matters so that Δx is small, corresponding to a narrow wave group, then Δp_x will be large. If we reduce Δp_x in some way, a broad wave group is inevitable and Δx will be large.

❑ Demonstrated this relation using a single slit electron diffraction.

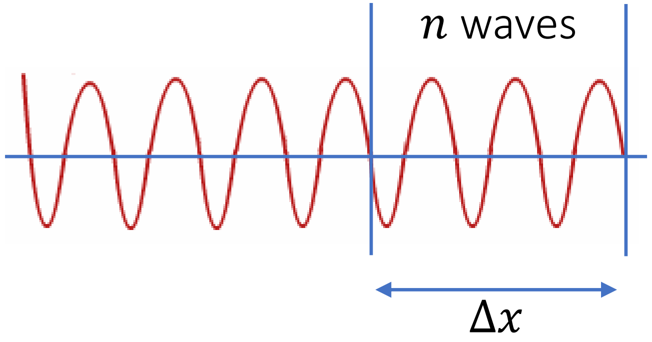
❑ Another uncertainty relation: $\Delta E\, \Delta t \geq \frac{\hbar}{2}$ (ΔE and Δt are the uncertainties in the energy of a particle and in time, respectively.)

Module 4 (Quantum Mechanics)

Uncertainty Principle

- ☐ This principle, discovered by Werner Heisenberg in 1927, is one of the most significant of physical laws

- ☐ Derivation



- ☐ If there are n waves in Δx, then $\Delta x = n\lambda$.
- ☐ For a different wave with wavelength $\lambda + \Delta\lambda$, $\Delta x = (n - \Delta n)\,(\lambda + \Delta\lambda)$.
- ☐ Hence, $(n - \Delta n)\,(\lambda + \Delta\lambda) = n\lambda$

$$\Rightarrow n\lambda - \lambda\Delta n + n\Delta\lambda - \Delta n\Delta\lambda = n\lambda$$

$$\Rightarrow n\Delta\lambda = \lambda\Delta n \qquad \text{(ignoring the term } \Delta n\Delta\lambda\text{)}$$

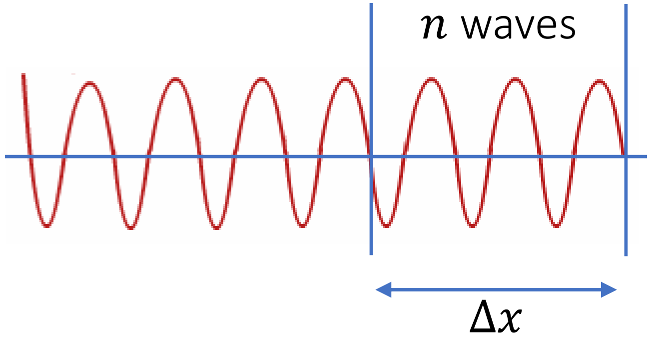
$$\Rightarrow \frac{\Delta\lambda}{\lambda} = \frac{\Delta n}{n}$$

- ☐ Now, $p = \frac{h}{\lambda}$ $\Rightarrow \Delta p = -\frac{h}{\lambda^2}\,\Delta\lambda$ $\Rightarrow \left|\frac{\Delta p}{p}\right| = \left|\frac{\frac{h}{\lambda^2}\Delta\lambda}{\frac{h}{\lambda}}\right| = \left|\frac{\Delta\lambda}{\lambda}\right|$

Module 4 (Quantum Mechanics)

Uncertainty Principle

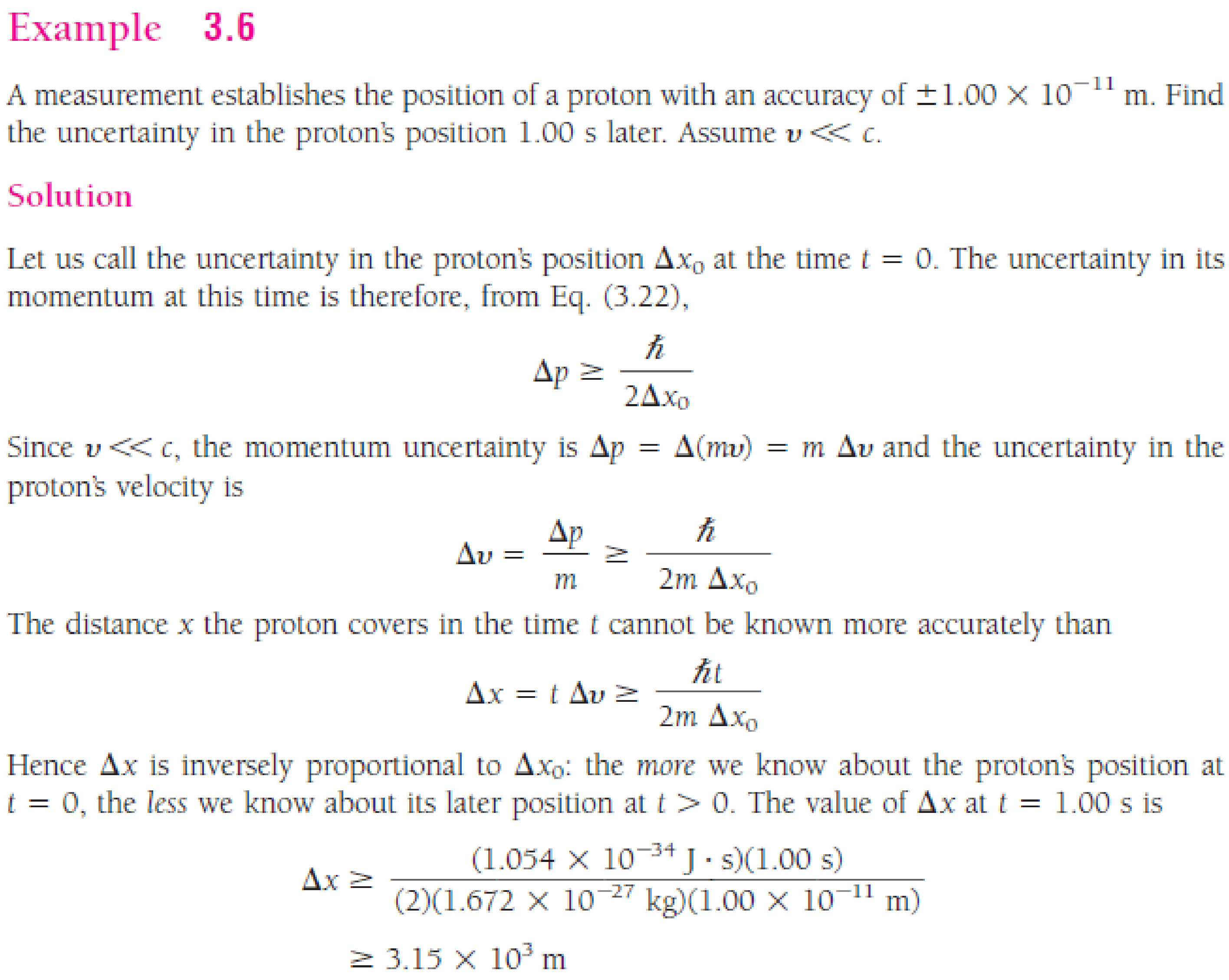
- ❑ This principle, discovered by Werner Heisenberg in 1927, is one of the most significant of physical laws
- ❑ Derivation



- ❑ If there are n waves in Δx, then $\Delta x = n\lambda$.
- ❑ $\frac{\Delta\lambda}{\lambda} = \frac{\Delta n}{n}$
- ❑ Now, $p = \frac{h}{\lambda}$ => $\Delta p = -\frac{h}{\lambda^2}\Delta\lambda$ => $\left|\frac{\Delta p}{p}\right| = \left|\frac{\frac{h}{\lambda^2}\Delta\lambda}{\frac{h}{\lambda}}\right| = \left|\frac{\Delta\lambda}{\lambda}\right|$
- ❑ Now, if uncertainty in the no. of waves in Δx is $\Delta n \geq 1$, then $\frac{\Delta\lambda}{\lambda} \geq \frac{1}{n}$
- ❑ So, $\frac{\Delta p}{p} \geq \frac{1}{n}$
- ❑ So, $\Delta p \geq \frac{p}{n}$
- ❑ From two relations in red, $\Delta x\, \Delta p \geq n\lambda \frac{p}{n} = \lambda p = h$.
- ❑ Hence, $\Delta x\, \Delta p_x \geq h$

Module 4 (Quantum Mechanics)

Uncertainty Principle



Example 3.6

A measurement establishes the position of a proton with an accuracy of $\pm 1.00 \times 10^{-11}$ m. Find the uncertainty in the proton's position 1.00 s later. Assume $v \ll c$.

Solution

Let us call the uncertainty in the proton's position Δx_0 at the time $t = 0$. The uncertainty in its momentum at this time is therefore, from Eq. (3.22),

$$\Delta p \geq \frac{\hbar}{2\Delta x_0}$$

Since $v \ll c$, the momentum uncertainty is $\Delta p = \Delta(mv) = m\,\Delta v$ and the uncertainty in the proton's velocity is

$$\Delta v = \frac{\Delta p}{m} \geq \frac{\hbar}{2m\,\Delta x_0}$$

The distance x the proton covers in the time t cannot be known more accurately than

$$\Delta x = t\,\Delta v \geq \frac{\hbar t}{2m\,\Delta x_0}$$

Hence Δx is inversely proportional to Δx_0: the *more* we know about the proton's position at $t = 0$, the *less* we know about its later position at $t > 0$. The value of Δx at $t = 1.00$ s is

$$\Delta x \geq \frac{(1.054 \times 10^{-34}\ \text{J}\cdot\text{s})(1.00\ \text{s})}{(2)(1.672 \times 10^{-27}\ \text{kg})(1.00 \times 10^{-11}\ \text{m})}$$

$$\geq 3.15 \times 10^{3}\ \text{m}$$

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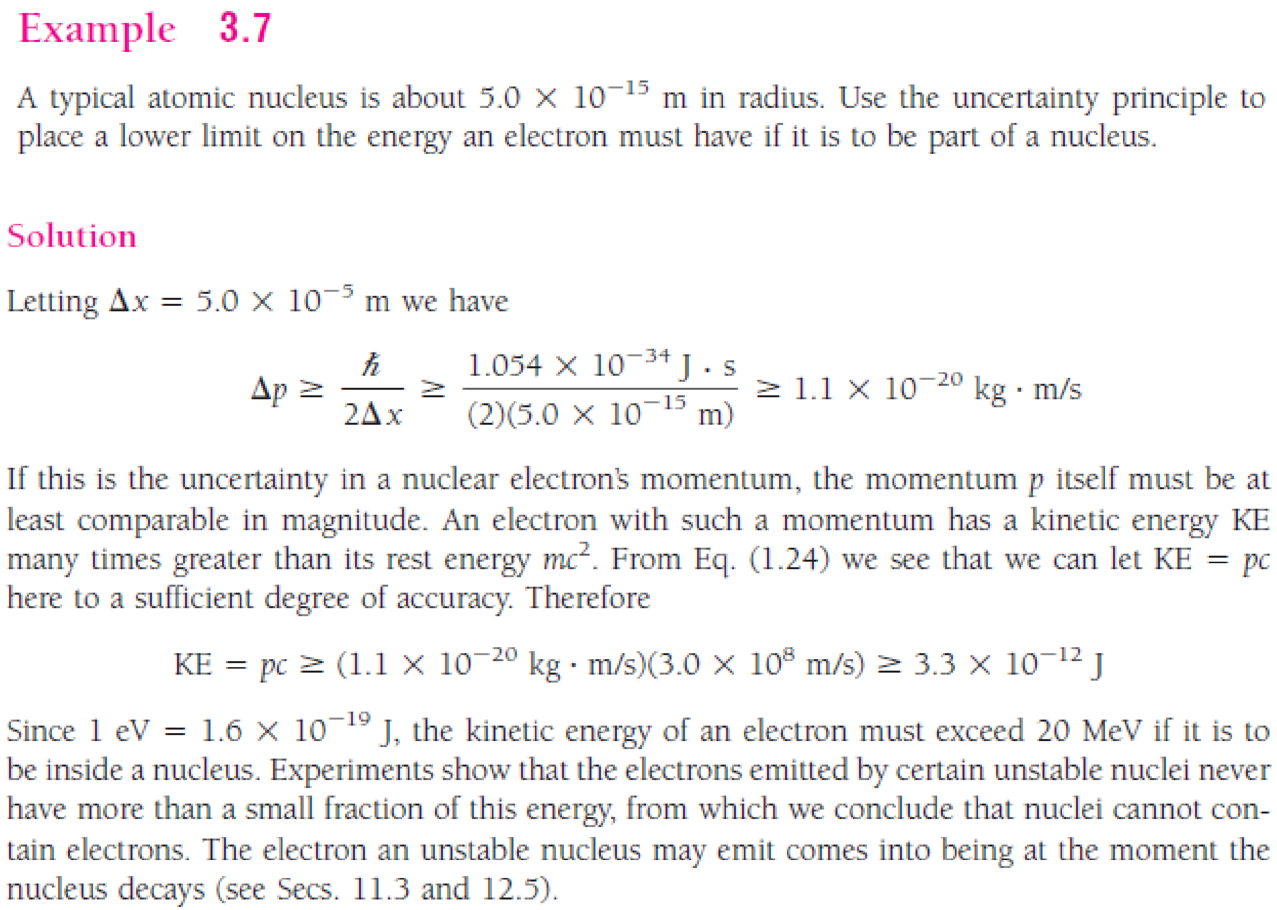
Module 4 (Quantum Mechanics)

Uncertainty Principle

- ☐ This principle, discovered by Werner Heisenberg in 1927, is one of the most significant of physical laws



Example 3.7

A typical atomic nucleus is about 5.0×10^{-15} m in radius. Use the uncertainty principle to place a lower limit on the energy an electron must have if it is to be part of a nucleus.

Solution

Letting $\Delta x = 5.0 \times 10^{-5}$ m we have

$$\Delta p \geq \frac{\hbar}{2\Delta x} \geq \frac{1.054 \times 10^{-34}\ \text{J} \cdot \text{s}}{(2)(5.0 \times 10^{-15}\ \text{m})} \geq 1.1 \times 10^{-20}\ \text{kg} \cdot \text{m/s}$$

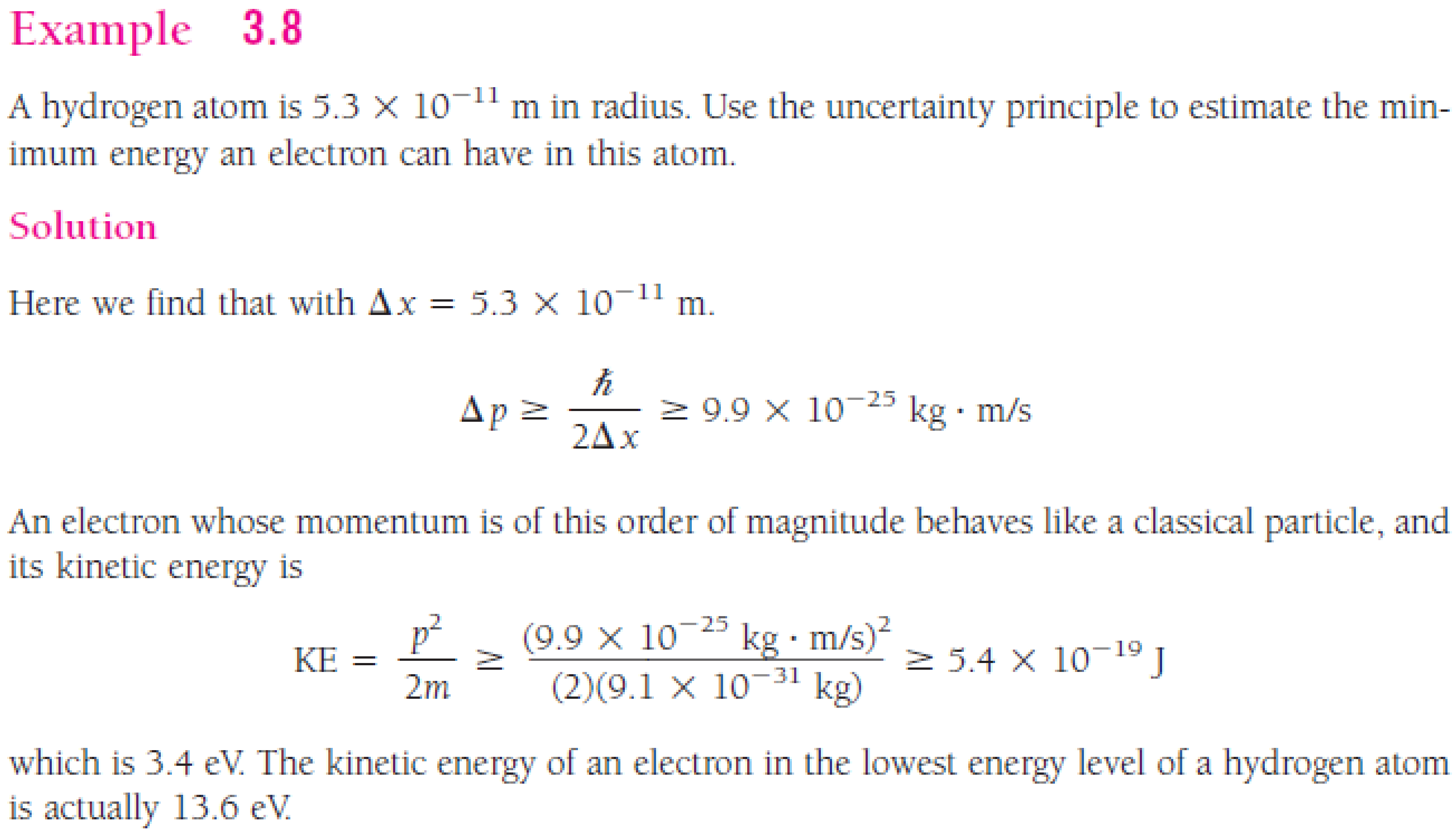
If this is the uncertainty in a nuclear electron's momentum, the momentum p itself must be at least comparable in magnitude. An electron with such a momentum has a kinetic energy KE many times greater than its rest energy mc^2. From Eq. (1.24) we see that we can let $\text{KE} = pc$ here to a sufficient degree of accuracy. Therefore

$$\text{KE} = pc \geq (1.1 \times 10^{-20}\ \text{kg} \cdot \text{m/s})(3.0 \times 10^{8}\ \text{m/s}) \geq 3.3 \times 10^{-12}\ \text{J}$$

Since $1\ \text{eV} = 1.6 \times 10^{-19}$ J, the kinetic energy of an electron must exceed 20 MeV if it is to be inside a nucleus. Experiments show that the electrons emitted by certain unstable nuclei never have more than a small fraction of this energy, from which we conclude that nuclei cannot contain electrons. The electron an unstable nucleus may emit comes into being at the moment the nucleus decays (see Secs. 11.3 and 12.5).

Uncertainty Principle

- ❑ This principle, discovered by Werner Heisenberg in 1927, is one of the most significant of physical laws



Example 3.8

A hydrogen atom is 5.3×10^{-11} m in radius. Use the uncertainty principle to estimate the minimum energy an electron can have in this atom.

Solution

Here we find that with $\Delta x = 5.3 \times 10^{-11}$ m.

$$\Delta p \geq \frac{\hbar}{2\Delta x} \geq 9.9 \times 10^{-25}\ \text{kg} \cdot \text{m/s}$$

An electron whose momentum is of this order of magnitude behaves like a classical particle, and its kinetic energy is

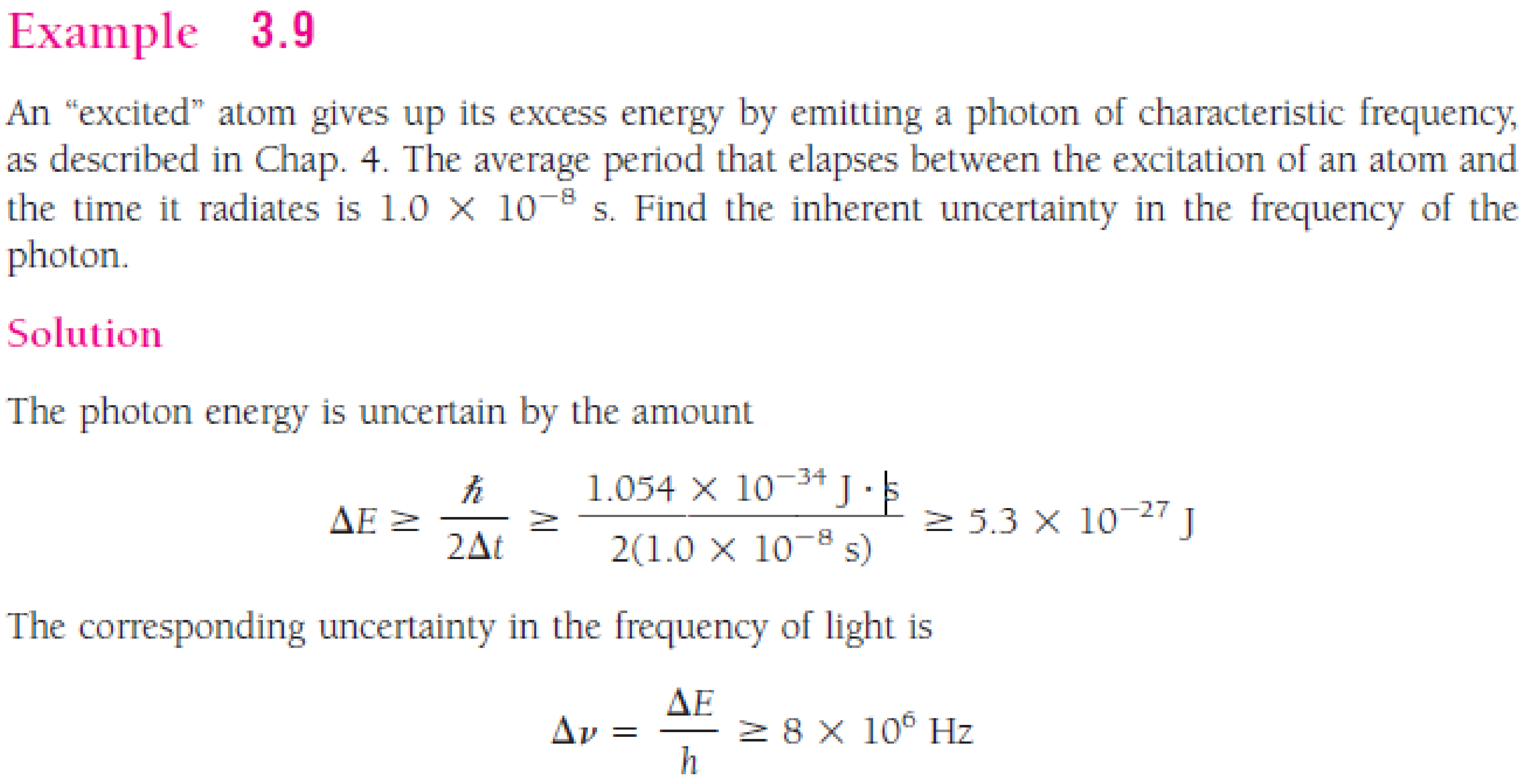
$$\text{KE} = \frac{p^2}{2m} \geq \frac{(9.9 \times 10^{-25}\ \text{kg} \cdot \text{m/s})^2}{(2)(9.1 \times 10^{-31}\ \text{kg})} \geq 5.4 \times 10^{-19}\ \text{J}$$

which is 3.4 eV. The kinetic energy of an electron in the lowest energy level of a hydrogen atom is actually 13.6 eV.

Module 4 (Quantum Mechanics)

Uncertainty Principle

- This principle, discovered by Werner Heisenberg in 1927, is one of the most significant of physical laws



Example 3.9

An "excited" atom gives up its excess energy by emitting a photon of characteristic frequency, as described in Chap. 4. The average period that elapses between the excitation of an atom and the time it radiates is 1.0×10^{-8} s. Find the inherent uncertainty in the frequency of the photon.

Solution

The photon energy is uncertain by the amount

$$\Delta E \geq \frac{\hbar}{2\Delta t} \geq \frac{1.054 \times 10^{-34}\ \text{J}\cdot\text{s}}{2(1.0 \times 10^{-8}\ \text{s})} \geq 5.3 \times 10^{-27}\ \text{J}$$

The corresponding uncertainty in the frequency of light is

$$\Delta\nu = \frac{\Delta E}{h} \geq 8 \times 10^{6}\ \text{Hz}$$

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Module 4

Module -4 : Quantum Mechanics

Planck's theory of black-body radiation, Compton effect, Wave particle duality, De Broglie waves, Davisson and Germer's experiment, Uncertainty principle, Brief idea of Wave Packet, Wave Function and its physical interpretation, Schrodinger equation in one-dimension, free particle, particle in an infinite square well. [9]

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Reference book: R1: Fundamentals of Physics, Halliday, Walker and Resnick

Wavefunction

- ❑ Every object has an associated 'wave'. This wave is described by a function called the 'wavefunction'.

- ❑ In water waves, the quantity that varies periodically is the *height* of the water surface.
- ❑ In sound waves, it is *pressure* that varies.
- ❑ In light waves, *electric* and *magnetic fields* vary.
- ❑ Recall: de Broglie wave is associated with each particle.
- ❑ What is it that varies in the case of matter waves?
- ❑ The quantity whose variations make up matter waves is called the **wavefunction**, denoted as Ψ.
- ❑ Since all matter is made of constituent particles, every object has a corresponding "wavefunction" that is formed due to the superposition of all the waves of its constituent particles.

Wavefunction

- Every object has an associated ‘wave’. This wave is described by a function called the ‘wavefunction’.
- Any object has a large number of constituent particles, each having its own *wave*. They superpose to give to the waveform of the entire object. This *wavefunction* is denoted by Ψ.
- The value of the wavefunction associated with a moving body at the particular point x, y, z in space at the time t is related to the likelihood of finding the body there at the time.
- Consider one-dimension case: The particle can exist only in the region where $\Psi(x)$ is non-zero.
- So, $\Psi(x)$ must be related to the **probability** of finding the particle in a certain region.
- However, the wavefunction Ψ itself has no direct physical significance. Why?

Module 4 (Quantum Mechanics)

Wavefunction

- ☐ Every object has an associated ‘wave’. This wave is described by a function called the ‘wavefunction’.
- ☐ The wavefunction Ψ itself has no *direct* physical significance. Why?
- ☐ The probability that something be in a certain place at a given time must lie between 0 (the object is definitely not there) and 1 (the object is definitely there). An intermediate probability, say 0.2, means that there is a 20% chance of finding the object.
- ☐ But the amplitude of a wave can be negative as well as positive, and a negative probability is meaningless. Hence Ψ by itself cannot be an observable quantity.
- ☐ This objection does not apply to $|\Psi(x)|^2$, the square of the absolute value of the wavefunction, known as **probability density**.
- ☐ $|\Psi(x)|^2$ is known as **probability density**: The probability of experimentally finding the body described by the wave function $\Psi(x)$ at the point x at the time t is proportional to the value of $|\Psi(x)|^2$ there at t.
- ☐ A large value of $|\Psi(x)|^2$ means the strong possibility of the body’s presence, while a small value of $|\Psi(x)|^2$ means the slight possibility of its presence. As long as $|\Psi(x)|^2$ is not actually zero somewhere, there is a definite chance, however small, of detecting it there. *This interpretation was first made by Max Born in 1926*.

Module 4 (Quantum Mechanics)

Wavefunction

- ☐ Every object has an associated 'wave'. This wave is described by a function called the 'wavefunction'.

- ☐ $|\Psi(x)|^2$ is known as **probability density**: The probability of experimentally finding the body described by the wave function $\Psi(x)$ at the point x at the time t is proportional to the value of $|\Psi(x)|^2$ there at t.

- ☐ The probability of finding the particle in the region $(x, x+dx)$ is given by: $P(x, x+dx) \equiv P(x)dx = |\Psi(x)|^2 dx = \Psi^*(x)\,\Psi(x)\,dx$ (where $\Psi^*(x)$ is the complex conjugate)

- ☐ Since wavefunctions are in general complex [i.e., $\Psi(x) = A(x) + iB(x)$], they are not physically measurable objects. (Note: The probability, $|\Psi(x)|^2 = \Psi^*(x)\,\Psi(x)$ is always a positive real quantity, as required). How?

- ☐ As wavefunctions are in general complex, we can write: $\Psi(x) = A(x) + iB(x)$ (where A and B are real functions)

- ☐ So, the complex conjugate, $\Psi^*(x) = A(x) - iB(x)$

- ☐ Hence, $|\Psi(x)|^2 = \Psi^*(x)\Psi(x) = A^2 - i^2B^2 = A^2 + B^2$ (since $i^2 = -1$) $\Rightarrow$ $\Psi^*(x)\,\Psi(x)$ is always a positive real quantity.

- ☐ $\Psi(x)$ is not a measurable quantity, but $P(x) \equiv |\Psi(x)|^2$ is measurable. $\Psi(x)$, however, can be derived analytically by solving the Schrödinger equation.

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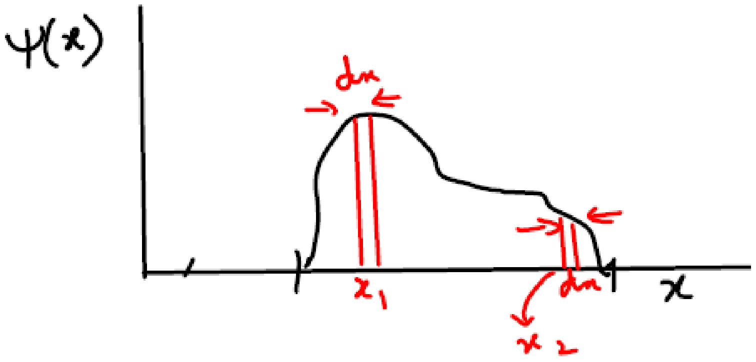
Module 4 (Quantum Mechanics)

Wavefunction

- ❑ Every object has an associated ‘wave’. This wave is described by a function called the ‘wavefunction’.



- ❑ At x_1, $P(x_1, x_1 + dx) \equiv P(x_1)dx = |\Psi(x_1)|^2 dx$
- ❑ At x_2, $P(x_2, x_2 + dx) \equiv P(x_2)dx = |\Psi(x_2)|^2 dx$
- ❑ Since $|\Psi(x_1)|^2 dx > |\Psi(x_2)|^2 dx$, the probability of finding the particle in the range $(x_1, x_1 + dx)$ is larger.

- ❑ Before we start the actual calculation of $\Psi(x)$, we can establish certain requirements it must always fulfill.
- ❑ Since $|\Psi(x)|^2$ is proportional to the probability density $P(x)$ of finding the body described by $\Psi(x)$, the integral of $|\Psi(x)|^2$ over all space must be finite. The body is somewhere, after all.
- ❑ If, $\int_{-\infty}^{\infty} |\Psi(x)|^2 \, dx = 0$ => the particle does not exist, and the integral obviously cannot be ∞ and still mean anything.
- ❑ Furthermore, $|\Psi(x)|^2$ cannot be negative or complex because of the way it is defined.
- ❑ The only possibility left is that the integral be a finite quantity if $\Psi(x)$ is to describe properly a real body.

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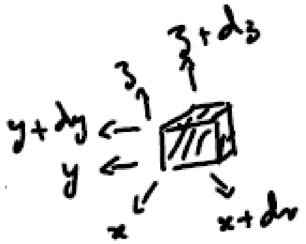
Module 4 (Quantum Mechanics)

Wavefunction

- ❑ Normalization
- ❑ Since $|\Psi(x)|^2$ is proportional to the probability density $P(x)$ of finding the body described by $\Psi(x)$, the integral of $|\Psi(x)|^2$ over all space must be finite. The body is somewhere, after all.
- ❑ $\int_{-\infty}^{\infty}|\Psi(x)|^2\,dx \neq 0$ and $|\Psi(x)|^2$ cannot be negative or complex because of the way it is defined.
- ❑ The only possibility left is that the integral be a finite quantity if $\Psi(x)$ is to describe properly a real body.
- ❑ The total probability of finding a particle in the range $x \in (-\infty, \infty)$ must be 1 (i.e., 100%)
- ❑ $\sum_x P(x, x+dx) = 1 \implies \int_{-\infty}^{\infty} P(x)dx = 1 \implies \int_{-\infty}^{\infty}|\Psi(x)|^2\,dx = 1$ (This is in case of 1-D)

Generalization to 3d:

$$\int_{-\infty}^{\infty} dz \int_{-\infty}^{\infty} dy \int_{-\infty}^{\infty} dx \; |\Psi(x,y,z)|^2 = 1$$



Here, $|\Psi(x,y,z)|^2 dx\,dy\,dz \rightarrow$ Prob of finding the particle in the range $\in (x,y,z)$ and $(x+dx, y+dy, z+dz)$.

Module 4 (Quantum Mechanics)

Wavefunction

- ❑ Normalization

Example :

$$\left.\begin{aligned}\psi_1(x) &= \phi(x)\, e^{i\theta_1} \\ \psi_2(x) &= \phi(x)\, e^{i\theta_2}\end{aligned}\right\} \begin{aligned}&\longrightarrow \text{ⓐ} \\ &\longrightarrow \text{ⓑ}\end{aligned}$$

$|\psi_1(x)|^2$ and $|\psi_2(x)|^2$ are measurable.

$$|\psi_1(x)|^2 \downarrow |\phi(x)|^2 \qquad |\psi_2(x)|^2 \downarrow |\phi(x)|^2$$

Even after measuring $|\psi_1(x)|^2$ and $|\psi_2(x)|^2$, we have no way of finding $\psi_1(x)$ and $\psi_2(x)$ because we have lost the information about θ_1 and θ_2 in the process.

Wavefunction

- ☐ Every object has an associated ‘wave’. This wave is described by a function called the ‘wavefunction’.

- ☐ Any object has a large number of constituent particles, each having its own wave. They *superpose* to give to the waveform of the entire object. This wavefunction is denoted by $\Psi(x)$.

- ☐ The particle can exist only in the region where $\Psi(x)$ is non-zero. So, $\Psi(x)$ must be related to the probability of finding the particle in a certain region.

- ☐ However, $\Psi(x)$ by itself cannot be an observable quantity. (Why? Because the amplitude of a wave can be negative as well as positive, and a negative probability is meaningless.)

- ☐ This objection does not apply to $|\Psi(x)|^2$, the square of the absolute value of the wavefunction, which is known as probability density: The probability of experimentally finding the body described by the wave function $\Psi(x)$ at the point x at the time t is proportional to the value of $|\Psi(x)|^2$ there at t.

- ☐ Since wavefunctions are in general complex [i.e., $\Psi(x) = A(x) + iB(x)$], they are not physically measurable objects. (Note: The probability, $|\Psi(x)|^2 = \Psi^*(x)\,\Psi(x)$ is always a positive real quantity, and is measurable). $\Psi(x)$, however, can be derived analytically by solving the Schrödinger equation.

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Module 4 (Quantum Mechanics)

Wavefunction

❑ Normalization

❑ Before we start the actual calculation of $\Psi(x)$, we can establish certain requirements it must always fulfill.

❑ Since $|\Psi(x)|^2$ is proportional to the probability density $P(x)$ of finding the body described by $\Psi(x)$, the integral of $|\Psi(x)|^2$ over all space must be finite. The body is somewhere, after all.

❑ If, $\int_{-\infty}^{\infty} |\Psi(x)|^2 \, dx = 0$ => the particle does not exist, and the integral obviously cannot be ∞ and still mean anything.

❑ Furthermore, $|\Psi(x)|^2$ cannot be negative or complex because of the way it is defined.

❑ The only possibility left is that the integral be a finite quantity if $\Psi(x)$ is to describe properly a real body.

❑ The total probability of finding a particle in the range $x \in (-\infty, \infty)$ must be 1 (i.e., 100%)

❑ $\sum_x P(x, x + dx) = 1 \implies \int_{-\infty}^{\infty} P(x) dx = 1 \implies \int_{-\infty}^{\infty} |\Psi(x)|^2 \, dx = 1$

❑ In 3-D, $\iiint_{-\infty}^{\infty} |\Psi(x, y, z)|^2 \, dx \, dy \, dz = 1$

Module 4 (Quantum Mechanics)

Wavefunction

- ☐ Linearity and Superposition

- ☐ **Wavefunctions add, but not the Probabilities**

- ☐ Schrödinger's equation is linear in the wave function Ψ.

- ☐ This means – the equation has terms that contain Ψ and its derivatives, but no terms independent of Ψ or that involve higher powers of Ψ or its derivatives.

- ☐ Hence, a linear combination of solutions of Schrödinger's equation for a given system is also itself a solution.

- ☐ If, Ψ_1 and Ψ_2 are two wavefunctions that satisfy the equation (solutions of the equation), then $\Psi = a_1\Psi_1 + a_2\Psi_2$ is also a solution (a_1 and a_2 are constants).

- ☐ This is nothing but the **superposition principle**. The wavefunctions Ψ_1 and Ψ_2 obey the superposition principle (just like other waves do). So, the interference effects can occur for wavefunctions just as they can for light, sound, water, and EM waves.

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Module 4 (Quantum Mechanics)

Wavefunction

- ❑ Linearity and Superposition
- ❑ **Wavefunctions add, but not the Probabilities**

- ❑ The diffraction pattern arises from the superposition of the wavefunctions Ψ_1 and Ψ_2 of the electrons that have passed through slits 1 and 2: $\Psi = \Psi_1 + \Psi_2$.
- ❑ If slit 1 only is open, the intensity varies with the corresponding probability density, $P_1 = |\Psi_1|^2 = \Psi_1{}^* \, \Psi_1$.
- ❑ Similarly, for slit 2, $P_2 = |\Psi_2|^2 = \Psi_2{}^* \, \Psi_2$.
- ❑ We might expect that opening both slits would give an electron intensity variation described by $P_1 + P_2$.
- ❑ However, this is not the case because in quantum mechanics wave functions add, not probabilities.

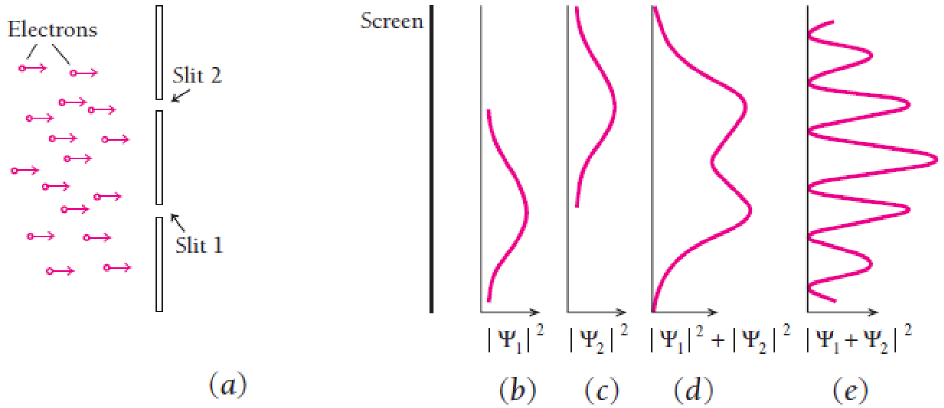

Figure 5.2 (*a*) Arrangement of double-slit experiment. (*b*) The electron intensity at the screen with only slit 1 open. (*c*) The electron intensity at the screen with only slit 2 open. (*d*) The sum of the intensities of (*b*) and (*c*). (*e*) The actual intensity at the screen with slits 1 and 2 both open. The wave functions Ψ_1 and Ψ_2 add to produce the intensity at the screen, not the probability densities $|\Psi_1|^2$ and $|\Psi_2|^2$.

- ❑ The probability density at the screen is therefore:

$$
\begin{aligned}
P = |\Psi|^2 = |\Psi_1 + \Psi_2|^2 &= (\Psi_1^* + \Psi_2^*)(\Psi_1 + \Psi_2) \\
&= \Psi_1^*\Psi_1 + \Psi_2^*\Psi_2 + \Psi_1^*\Psi_2 + \Psi_2^*\Psi_1 \\
&= P_1 + P_2 + \Psi_1^*\Psi_2 + \Psi_2^*\Psi_1
\end{aligned}
$$

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Module 4 (Quantum Mechanics)

Wavefunction

❑ Expectation Values

❑ **How to extract information from a wave function**

❑ Expectation value of the position of the single particle is

$$\langle x \rangle = \frac{\int_{-\infty}^{\infty} x|\Psi|^2\, dx}{\int_{-\infty}^{\infty} |\Psi|^2\, dx} \qquad (5.18)$$

If Ψ is a normalized wave function, the denominator of Eq. (5.18) equals the probability that the particle exists somewhere between $x = -\infty$ and $x = \infty$ and therefore has the value 1. In this case

Expectation value for position

$$\langle x \rangle = \int_{-\infty}^{\infty} x|\Psi|^2\, dx \qquad (5.19)$$

Wavefunction

❑ Well-Behaved Wave Functions

❑ We now know that the **wavefunction (Ψ) must be normalizable**. Every acceptable wave function can be normalized by multiplying it by an appropriate constant (we'll see it later).

❑ Besides being normalizable, **Ψ must be continuous and single-valued**, since the probability, P can have only one value at a particular place and time.

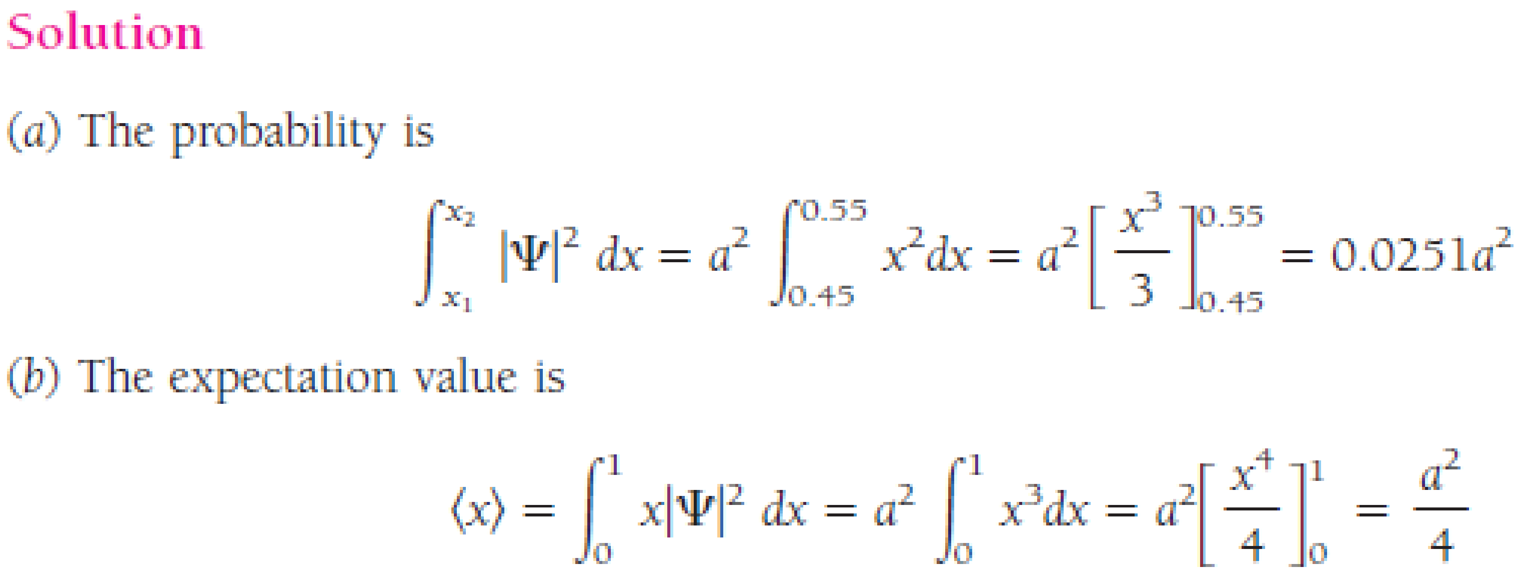
❑ Momentum considerations require that the **partial derivatives** $\frac{\partial \Psi}{\partial x}, \frac{\partial \Psi}{\partial y}, \frac{\partial \Psi}{\partial z}$ be **finite, continuous, and single-valued**.

❑ Only wavefunctions with all these properties can yield physically meaningful results when used in calculations – they are the "*well-behaved*" wavefunctions.

❑ Note: These rules are not always obeyed in model situations where we *approximate* the actual ones. For instance, wavefunctions of a particle in a box with infinitely hard walls do not have continuous derivatives at the walls ($\Psi = 0$ outside the box). But in the real world, walls are never infinitely hard. So, there is no sharp change in Ψ at the walls and the derivatives are continuous.

Wavefunction

- ❑ Probability
- ❑ Solve it
- ❑ A particle limited to the x axis has the wavefunction $\Psi = ax$ between $x = 0$ and $x = 1$; $\Psi = 0$ elsewhere. Find the probability that the particle can be found between $x = 0.45$ and $x = 0.55$.
- ❑ Also find the expectation value $< x >$ of the particle's position.



Solution

(*a*) The probability is

$$\int_{x_1}^{x_2} |\Psi|^2 \, dx = a^2 \int_{0.45}^{0.55} x^2 dx = a^2 \left[\frac{x^3}{3} \right]_{0.45}^{0.55} = 0.0251a^2$$

(*b*) The expectation value is

$$\langle x \rangle = \int_0^1 x|\Psi|^2 \, dx = a^2 \int_0^1 x^3 dx = a^2 \left[\frac{x^4}{4} \right]_0^1 = \frac{a^2}{4}$$

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Module 4

Module -4 : Quantum Mechanics

Planck's theory of black-body radiation, Compton effect, Wave particle duality, De Broglie waves, Davisson and Germer's experiment, Uncertainty principle, Brief idea of Wave Packet, Wave Function and its physical interpretation, Schrodinger equation in one-dimension, free particle, particle in an infinite square well. [9]

Text book: T3: Arthur Beiser (AB), Concept of Modern Physics, 6th edition 2009, Tata McGraw- Hill

Reference book: R1: Fundamentals of Physics, Halliday, Walker and Resnick

Module 4 (Quantum Mechanics)

Schrödinger Equation in one-dimension

- ❑ Schrödinger Equation is a wave equation in the variable Ψ.
- ❑ Fundamental equation of quantum mechanics in the same sense that the second law of motion is the fundamental equation of Newtonian mechanics.
- ❑ For a free particle (no external force), there is a constant momentum p and hence a constant energy E.
- ❑ The wavefunction is of the form of a plane wave: $\Psi(x,t) = A\, e^{i(kx-\omega t)}$
- ❑ Remember: $E = h\nu = \frac{h}{2\pi}(2\pi\nu) = \hbar\omega$
- ❑ Using de Broglie hypothesis: $p = \frac{h}{\lambda} = \frac{h}{2\pi/k} = \frac{h}{2\pi}k = \hbar k$
- ❑ Since, ω and k are constants for $\Psi(x,t)$, so are E and p.
- ❑ Hence, $\Psi(x,t) = A\, e^{i(kx-\omega t)}$ can be written as $\Psi(x,t) = A\, e^{i(px-Et)/\hbar}$

This equation describes the wave equivalent of a free particle of total energy E and momentum p moving in the $+x$ direction.

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Module 4 (Quantum Mechanics)

Schrödinger Equation in one-dimension

- ❑ Schrödinger Equation is a wave equation in the variable Ψ.
- ❑ The wavefunction for a free particle $\Psi(x,t) = A\, e^{i(px-Et)/\hbar}$
- ❑ Now, apply the operator $-i\frac{\partial}{\partial x}$ on $\Psi(x,t)$, we get: $-i\hbar\frac{\partial\Psi}{\partial x} = -i\hbar\,\frac{(ip)}{\hbar}\,Ae^{\frac{i(px-Et)}{\hbar}} = p\Psi$
- ❑ Apply the operator $i\frac{\partial}{\partial t}$ on $\Psi(x,t)$, we get: $i\hbar\frac{\partial\Psi}{\partial t} = E\Psi$
- ❑ Remember: $-i\frac{\partial}{\partial x} \equiv \hat{p}$ (such that $\hat{p}\,\Psi = p\,\Psi$). Momentum operator $\hat{p}$ whose eigen values are p.
- ❑ Remember: $i\frac{\partial}{\partial t} \equiv \widehat{H}$ (such that $\widehat{H}\,\Psi = E\,\Psi$). Hamiltonian or energy operator $\widehat{H}$ whose eigen values are E.
- ❑ For a free particle, $E = \frac{p^2}{2m}$ needs to be imposed.

Schrödinger Equation in one-dimension

- Schrödinger Equation is a wave equation in the variable Ψ.
- Remember: $-i\frac{\partial}{\partial x} \equiv \hat{p}$ (momentum operator) and $i\frac{\partial}{\partial t} \equiv \widehat{H}$ (Hamiltonian or energy operator)
- For a free particle, $E = \frac{p^2}{2m}$ needs to be imposed.
- $-i\hbar\frac{\partial \Psi}{\partial x} = p\Psi \Rightarrow \left(-i\hbar\frac{\partial}{\partial x}\right)^2 \Psi = p^2\Psi \Rightarrow \boxed{-\hbar^2 \frac{\partial^2 \Psi}{\partial x^2} = p^2\Psi}$
- $\boxed{i\hbar\frac{\partial \Psi}{\partial t} = E\Psi}$
- Now $E = \frac{p^2}{2m} \Rightarrow E\Psi = \frac{p^2}{2m}\Psi$ $\Rightarrow$ Now replace the equations encircled: $E\Psi = i\hbar\frac{\partial \Psi}{\partial t}$ and $p^2\Psi = -\hbar^2 \frac{\partial^2 \Psi}{\partial x^2}$
- $i\hbar\frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2}$ This is the Schrödinger Equation for a free particle in one-dimension

Schrödinger Equation in one-dimension

- Schrödinger Equation is a wave equation in the variable Ψ.
- $i\hbar\frac{\partial\Psi}{\partial t}=-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2}$ ⇒ This is the Schrödinger equation for a free particle. This is correct only for freely moving particles.
- However, we are most interested in situations where the motion of a particle is subject to various restrictions. What happens in presence of a potential?
- For a free particle, $E=\frac{p^2}{2m}$, but, in presence of a potential, we have, $E=\frac{p^2}{2m}+V(x,t)$
- $E\Psi=(\frac{p^2}{2m}+V)\Psi$
- $i\hbar\frac{\partial\Psi}{\partial t}=-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2}+V\Psi$
- $i\hbar\frac{\partial\Psi(x,t)}{\partial t}=-\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2}+V(x,t)\Psi(x,t)$

⬅ ⬅ ⬅ ⬅ This is the general form of time-dependent Schrödinger equation for any particle in one-dimension

- Note: Ψ and $\frac{\partial\Psi}{\partial x}$ must be continuous for $\frac{\partial^2\Psi}{\partial x^2}$ to exist.

Module 4 (Quantum Mechanics)

Schrödinger Equation in one-dimension

- Schrödinger Equation is a wave equation in the variable Ψ.
- The Schrödinger equation for a free particle: $i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2}$
- For a free particle, $E = \frac{p^2}{2m}$, but, in presence of a potential, we have, $E = \frac{p^2}{2m} + V(x,t)$
- General form of time-dependent Schrödinger equation for any particle in one-dimension
- $i\hbar\frac{\partial\Psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2} + V(x,t)\Psi(x,t)$
- Note: *Schrödinger's equation cannot be derived from other basic principles of physics; it is a basic principle in itself.*
- In three dimensions the time-dependent form of Schrödinger's equation is
- $i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\left[\frac{\partial^2\Psi}{\partial x^2} + \frac{\partial^2\Psi}{\partial y^2} + \frac{\partial^2\Psi}{\partial z^2}\right] + V\Psi$
- Note: in 3D, particle's potential energy V is some function of $x, y, z,$ and t.

Module 4 (Quantum Mechanics)

Schrödinger Equation

- ☐ Schrödinger Equation is a wave equation in the variable Ψ.
- ☐ In presence of a potential, we have, $E = \frac{p^2}{2m} + V(x,t)$
- ☐ Time-dependent Schrödinger equation in one-dimension: $i\hbar \frac{\partial \Psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi(x,t)}{\partial x^2} + V(x,t)\Psi(x,t)$
- ☐ In three dimensions the time-dependent form of Schrödinger's equation is
- ☐ $i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m}\left[\frac{\partial^2 \Psi}{\partial x^2} + \frac{\partial^2 \Psi}{\partial y^2} + \frac{\partial^2 \Psi}{\partial z^2}\right] + V\Psi$
- ☐ Note: in 3D, particle's potential energy V is some function of x, y, z, and t.
- ☐ Any restrictions that may be present on the particle's motion will affect the potential energy function V.
- ☐ Once V is known, Schrödinger's equation may be solved for the wavefunction Ψ of the particle, from which its probability density $|\Psi|^2$ may be determined for a specified x, y, z, t.

Module 4 (Quantum Mechanics)

Schrödinger Equation in one-dimension

- Schrödinger Equation is a wave equation in the variable Ψ.

- Any restrictions on the particle's motion will affect the potential energy V. Once V is known, Schrödinger's eqn. may be solved for the wavefunction Ψ of the particle, from which its probability density $|\Psi|^2$ may be determined for a specified x, y, z, t.

- In presence of a potential, we have, $E = \frac{p^2}{2m} + V(x,t)$

- Recall: $-i\hbar\frac{\partial\Psi}{\partial x} = p\Psi \quad \Rightarrow \quad -\hbar^2\frac{\partial^2\Psi}{\partial x^2} = p^2\Psi$ and $\boxed{i\hbar\frac{\partial\Psi}{\partial t} = E\Psi}$

- So, time dependent form of Schrödinger equation gives $i\hbar\frac{\partial\Psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2} + V(x,t)\Psi(x,t) = E\Psi(x,t)$

- Rearrange: $\frac{\partial^2\Psi(x,t)}{\partial x^2} + \frac{2m}{\hbar^2}[E - V(x,t)]\Psi(x,t) = 0$

- If $V(x,t) \equiv V(x)$, we get the **time-independent form of Schrödinger equation** in 1D:

- $\frac{\partial^2\Psi(x)}{\partial x^2} + \frac{2m}{\hbar^2}[E - V(x)]\Psi(x) = 0$

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Module 4

Module -4 : Quantum Mechanics

Planck's theory of black-body radiation, Compton effect, Wave particle duality, De Broglie waves, Davisson and Germer's experiment, Uncertainty principle, Brief idea of Wave Packet, Wave Function and its physical interpretation, Schrodinger equation in one-dimension, free particle, particle in an infinite square well. [9]

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Module 4 (Quantum Mechanics)

Schrödinger Equation in one-dimension

- ☐ Schrödinger Equation is a wave equation in the variable Ψ.
- ☐ The wavefunction for a free particle $\Psi(x,t) = A\, e^{i(px-Et)/\hbar}$
- ☐ Apply the momentum operator $-i\frac{\partial}{\partial x}$ on $\Psi(x,t)$, we get: $-i\hbar\frac{\partial\Psi}{\partial x} = -i\hbar\,\frac{(ip)}{\hbar}\,Ae^{\frac{i(px-Et)}{\hbar}} = p\Psi$
- ☐ Apply the energy operator $i\frac{\partial}{\partial t}$ on $\Psi(x,t)$, we get: $i\hbar\frac{\partial\Psi}{\partial t} = E\Psi$
- ☐ $-i\hbar\frac{\partial\Psi}{\partial x} = p\Psi \quad\Rightarrow\quad \left(-i\hbar\frac{\partial}{\partial x}\right)^2\Psi = p^2\Psi \qquad \Rightarrow -\hbar^2\,\frac{\partial^2\Psi}{\partial x^2} = p^2\Psi$
- ☐ $i\hbar\frac{\partial\Psi}{\partial t} = E\Psi$
- ☐ For a free particle, $E = \frac{p^2}{2m}$ needs to be imposed. So, $E = \frac{p^2}{2m} \qquad\Rightarrow\qquad E\Psi = \frac{p^2}{2m}\Psi$
- ☐ $i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2}$ ⮌ This is the Schrödinger Equation for a free particle in 1-D

Module 4 (Quantum Mechanics)

Schrödinger Equation in one-dimension

- ☐ Schrödinger Equation is a wave equation in the variable Ψ.
- ☐ The Schrödinger equation for a free particle: $i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2}$
- ☐ For a free particle, $E = \frac{p^2}{2m}$, but, in presence of a potential, we have, $E = \frac{p^2}{2m} + V(x,t)$
- ☐ Recall: $-i\hbar\frac{\partial\Psi}{\partial x} = p\Psi \quad \Rightarrow \quad -\hbar^2\frac{\partial^2\Psi}{\partial x^2} = p^2\Psi$ and $i\hbar\frac{\partial\Psi}{\partial t} = E\Psi$
- ☐ Time-dependent form of Schrödinger equation gives $i\hbar\frac{\partial\Psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2} + V(x,t)\Psi(x,t) = E\Psi(x,t)$
- ☐ Rearrange: $\frac{\partial^2\Psi(x,t)}{\partial x^2} + \frac{2m}{\hbar^2}[E - V(x,t)]\Psi(x,t) = 0$
- ☐ If $V(x,t) \equiv V(x)$, we get the time-independent form of Schrödinger equation in 1D:
- ☐ $\frac{\partial^2\Psi(x)}{\partial x^2} + \frac{2m}{\hbar^2}[E - V(x)]\Psi(x) = 0$

Module 4 (Quantum Mechanics)

Particle in an infinite square well

- How boundary conditions and normalization determine wavefunctions

- Now we shall see the Schrödinger equation in certain situation: a particle trapped in a box with infinitely hard walls. We'll focus on the one-dimension case.

- Let's consider that the particle's motion is restricted to traveling along the x-axis between $x = 0$ and $x = L$ by infinitely hard walls.

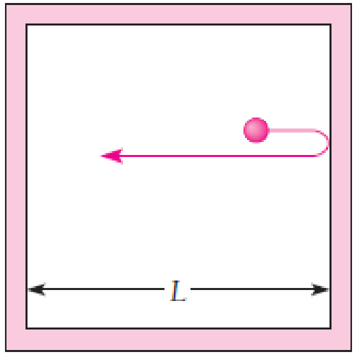
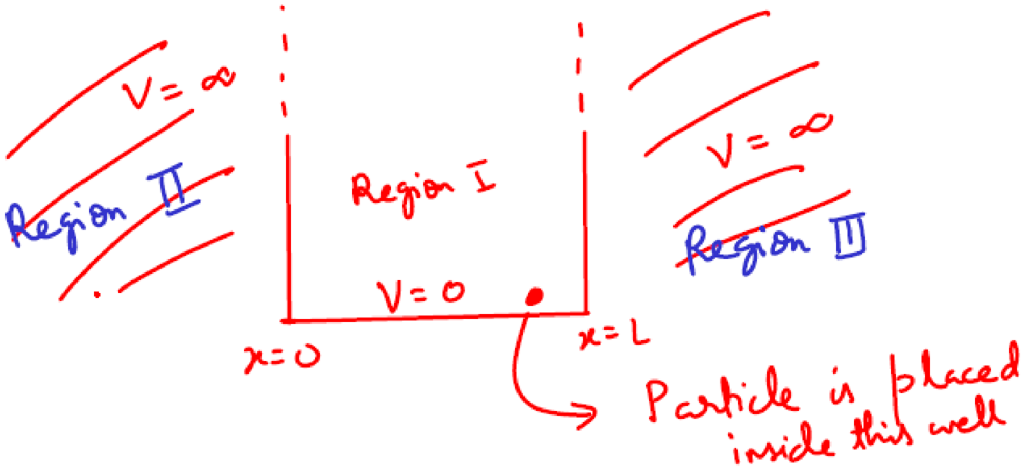


Figure 3.9 A particle confined to a box of width L. The particle is assumed to move back and forth along a straight line between the walls of the box.



$V = 0$ if $0 < x < L$

$V = \infty$ otherwise

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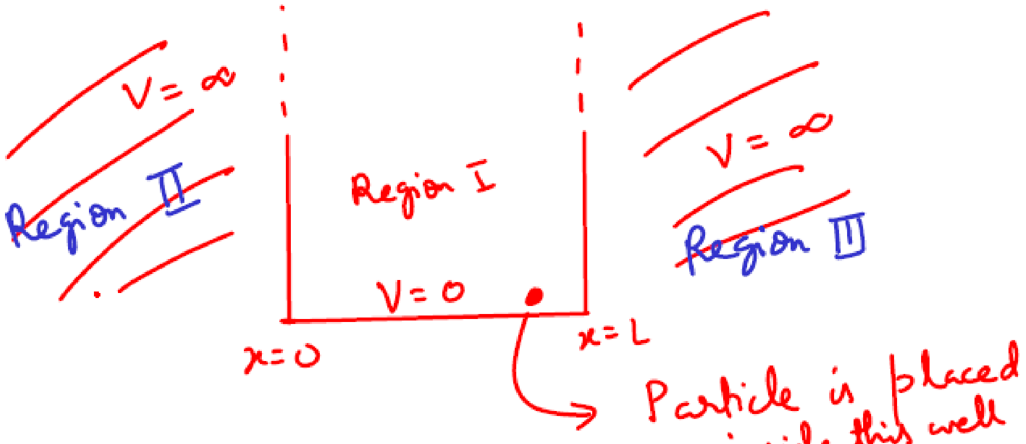
Module 4 (Quantum Mechanics)

Particle in an infinite square well

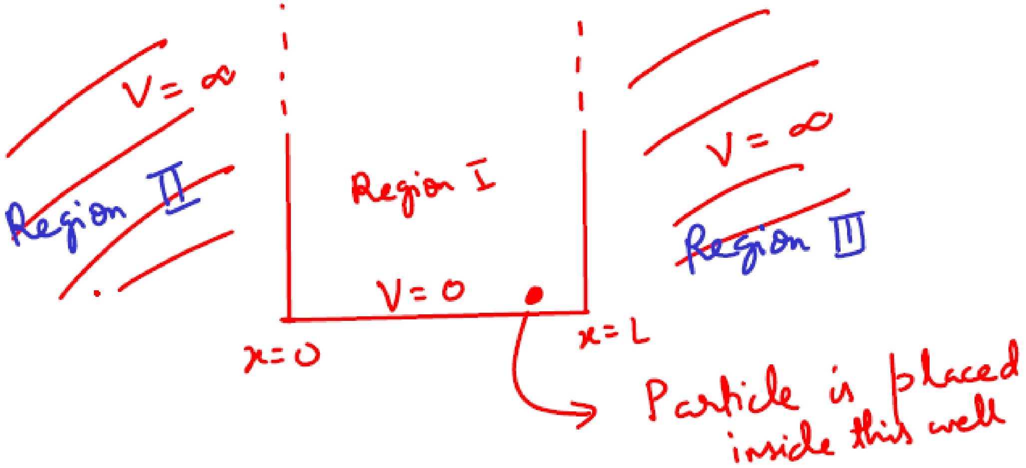
- How boundary conditions and normalization determine wavefunctions
- *Now we shall see the Schrödinger equation in certain situation: a particle in an infinite square well (1-D)*
- Consider that the particle's motion is restricted between $x = 0$ and $x = L$ by infinitely hard walls.
- A particle does not lose energy when it collides with such walls, so that its total energy stays constant.
- The potential energy V of the particle is *infinite* on both sides of the box, while V is a constant inside the box. It is convenient to assume V = 0 in the box.
- Because the particle cannot have an infinite amount of energy, it cannot exist outside the box, and so its wavefunction $\Psi = 0$ for $x \leq 0$ and $x \geq L$.



$V=0$ if $0<x<L$
$V=\infty$ otherwise

Particle in an infinite square well

- ☐ How boundary conditions and normalization determine wavefunctions
- ☐ *Schrödinger eqn. in certain situation: a particle trapped in a box with infinitely hard walls. We'll focus on the 1-D case.*
- ☐ **So we can define three regions** – Region I, Region II and Region III.
- ☐ For an infinite hard wall, $\Psi = 0$ in regions II & III. Probability of detecting the particle is zero in regions II & III.
- ☐ We consider the potential V to be constant in Region I (between $x = 0$ and $x = L$).
- ☐ It is convenient to assume $V = 0$ in Region I.



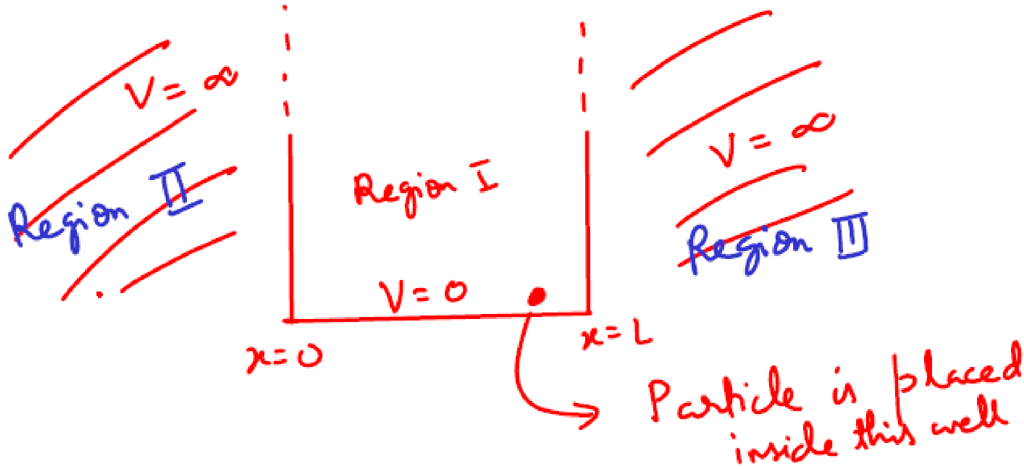
$V = 0$ if $0 < x < L$

$V = \infty$ otherwise

Particle in an infinite square well

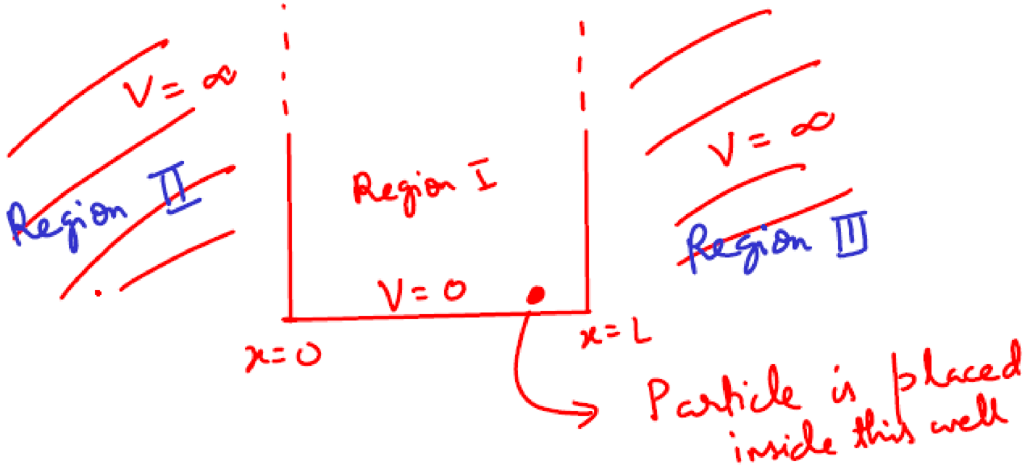
- How boundary conditions and normalization determine wavefunctions
- *Schrödinger eqn. in certain situation: a particle trapped in a box with infinitely hard walls. We'll focus on the 1-D case.*
- Recall the time-independent form of Schrödinger equation in 1D: $\frac{\partial^2\Psi(x)}{\partial x^2} + \frac{2m}{\hbar^2}[E - V(x)]\Psi(x) = 0$
- We consider the potential V to be constant in Region I. It is convenient to assume $V = 0$ in Region I.
- For Region II: $\Psi = 0$.
- For Region III: $\Psi = 0$.
- For Region I: Schrödinger equation in 1D can be expressed as:

$$\frac{\partial^2\Psi(x)}{\partial x^2} + \frac{2mE}{\hbar^2}\Psi(x) = 0$$ ($V = 0$ in this region).



Particle in an infinite square well

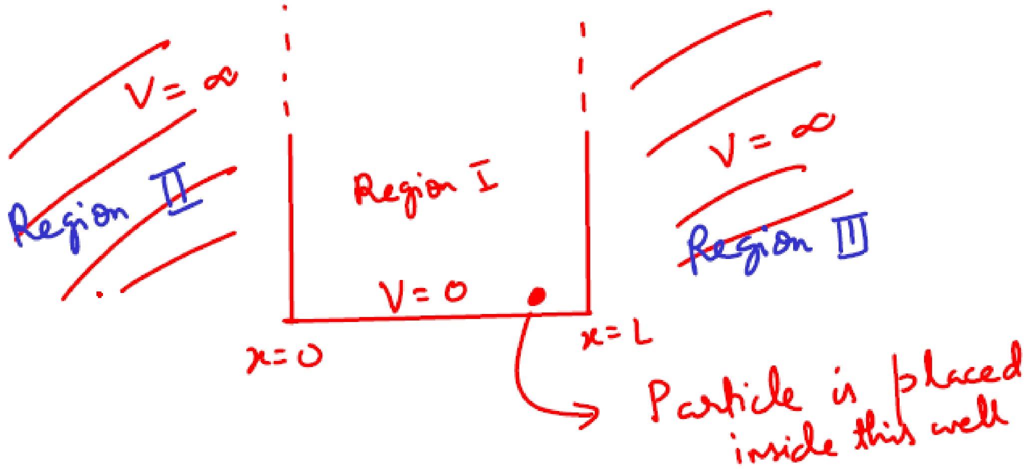
- How boundary conditions and normalization determine wavefunctions
- *Now we shall see the Schrödinger equation in certain situation: a particle in an infinite square well (1-D).*
- For Region II & III: $\Psi = 0$.
- For Region I: Schrödinger equation in 1D can be expressed as: $\frac{\partial^2 \Psi(x)}{\partial x^2} + \frac{2mE}{\hbar^2}\Psi(x) = 0$ ($V = 0$ in this region).
- Let $\alpha^2 = \frac{2mE}{\hbar^2}$, so that $\alpha = \sqrt{\frac{2mE}{\hbar^2}}$
- Schrödinger equation in 1D corresponding to Region I becomes:
- $\frac{d^2\Psi(x)}{dx^2} + \alpha^2\Psi(x) = 0$
- Partial derivative now can be removed, because Ψ is now a function of x only.



Module 4 (Quantum Mechanics)

Particle in an infinite square well

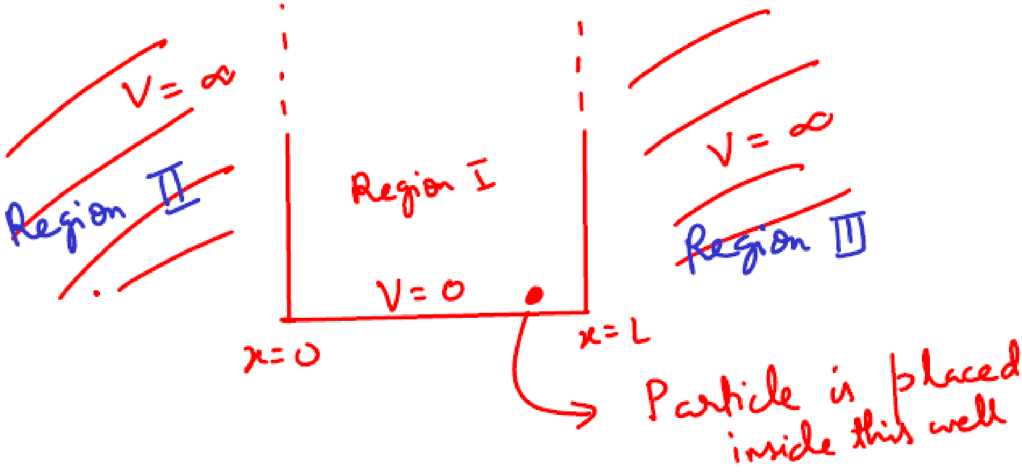
- How boundary conditions and normalization determine wavefunctions
- *Now we shall see the Schrödinger equation in certain situation: a particle in an infinite square well (1-D).*
- $\frac{d^2\Psi(x)}{dx^2} + \alpha^2\Psi(x) = 0$
- This represents the simple harmonic motion. It has the solution of the form:
- $\Psi(x) = A\,Sin(\alpha x) + B\,Cos(\alpha x)$ in Region I.
- A and B are constants to be evaluated. How?
- To evaluate A and B, we use the boundary condition.
- At the boundaries, $\Psi(x) = 0$ at $x = 0$
  at $x = L$



Module 4 (Quantum Mechanics)

Particle in an infinite square well

- How boundary conditions and normalization determine wavefunctions
- Now we shall see the Schrödinger equation in certain situation: a particle in an infinite square well (1-D).
- $\frac{d^2\Psi(x)}{dx^2} + \alpha^2\Psi(x) = 0$ => this represents simple harmonic motion, the solution is of the form:
- $\Psi(x) = A\,Sin(\alpha x) + B\,Cos(\alpha x)$
- To evaluate the constants A and B, we use the boundary condition.
- At the boundaries, $\Psi(x) = 0$ at $x = 0$
  at $x = L$
- $\Psi(x) = 0$ at $x = 0$ gives $0 = A \times 0 + B \times 1 \quad \Rightarrow \quad B = 0$
- $\Psi(x) = 0$ at $x = L$ gives $0 = A\,Sin(\alpha L) \quad \Rightarrow \quad \alpha L = n\pi \quad \Rightarrow \quad \alpha = \frac{n\pi}{L}$



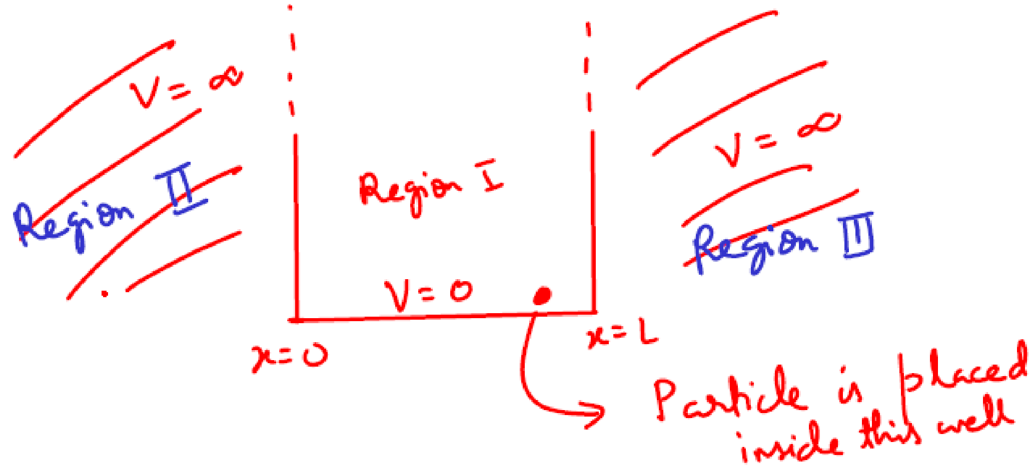
Particle in an infinite square well

☐ How boundary conditions and normalization determine wavefunctions

☐ Now we shall see the Schrödinger equation in certain situation: a particle in an infinite square well (1-D).

☐ $\frac{d^2\Psi(x)}{dx^2} + \alpha^2\Psi(x) = 0$ => this represents simple harmonic motion, the solution is of the form:

☐ $\Psi(x) = A\ Sin(\alpha x) + B\ Cos(\alpha x)$



☐ 1st boundary condition [$\Psi(x) = 0$ at $x = 0$] gives $B = 0$

☐ 2nd boundary condition [$\Psi(x) = 0$ at $x = L$] gives $\alpha = \frac{n\pi}{L}$

☐ Hence, $\Psi(x) = A\ Sin(\alpha x) = A\ Sin(\frac{n\pi x}{L})$

☐ Now, $\alpha = \sqrt{\frac{2mE}{\hbar^2}} \Rightarrow \frac{2mE}{\hbar^2} = \left(\frac{n\pi}{L}\right)^2 \Rightarrow \boxed{E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}} \Rightarrow Discretized\ Energy$

Module 4 (Quantum Mechanics)

Particle in an infinite square well

- ☐ How boundary conditions and normalization determine wavefunctions
- ☐ Now we shall see the Schrödinger equation in certain situation: a particle in an infinite square well (1-D).
- ☐ $\frac{d^2\Psi(x)}{dx^2} + \alpha^2\Psi(x) = 0$ => the solution is of the form: $\Psi(x) = A\,Sin(\alpha x) = A\,Sin\left(\frac{n\pi x}{L}\right)$
- ☐ $E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}$ $\Rightarrow Discretized\ Energy$

✓ From this relation, it is clear that the energy of the particle can have only certain values, which are the **eigenvalues**.

✓ Each permitted energy is called an **energy level**, and the integer n that specifies an energy level E_n is called its quantum number.

- ☐ Remember, $n = 1, 2, 3, \ldots$
- ☐ $E_1 = \frac{\pi^2\hbar^2}{2mL^2}$
- ☐ $E_2 = \frac{4\pi^2\hbar^2}{2mL^2}$ and so on….
- ☐ $E_n = \frac{n^2\pi^2\hbar^2}{2mL^2} = n^2\left(\frac{\pi^2\hbar^2}{2mL^2}\right)$ $\Rightarrow Hence, E_n = n^2E_1$

Module 4 (Quantum Mechanics)

Particle in an infinite square well

- ❑ How boundary conditions and normalization determine wavefunctions
- ❑ *Now we shall see the Schrödinger equation in certain situation: a particle in an infinite square well (1-D).*
- ❑ $E_n = \frac{n^2\pi^2\hbar^2}{2mL^2} = n^2\left(\frac{\pi^2\hbar^2}{2mL^2}\right) \Rightarrow Hence, E_n = n^2 E_1$

- ✓ Unlike a free particle, a particle trapped in a box cannot have an arbitrary energy. It can have only certain specific energies and no others.
- ✓ These energies depends on the mass of the particle and on the details of how it is trapped.
- ✓ Since $n = 1,2,3, \ldots$, particle trapped in a box cannot have zero energy!

Module 4 (Quantum Mechanics)

Particle in an infinite square well

- How boundary conditions and normalization determine wavefunctions
- *Now we shall see the Schrödinger equation in certain situation: a particle in an infinite square well (1-D).*
- $\frac{d^2\Psi(x)}{dx^2} + \alpha^2\Psi(x) = 0$ => the solution is of the form: $\Psi(x) = A\,Sin(\alpha x) = A\,Sin\left(\frac{n\pi x}{L}\right)$
- Now, we need to determine the value of constant A. For this we use the **normalization** method.
- Recall: probability $P\,dx = |\Psi(x)|^2 dx$, probability of finding the particle between x and $x + dx$
- $\int_{-\infty}^{\infty} |\Psi(x)|^2\,dx = 1 \quad \Longrightarrow \quad \underset{\text{Region II}}{\cancelto{0}{\int_{-\infty}^{0} |\Psi(x)|^2\,dx}} + \underset{\text{Region I}}{\boxed{\int_{0}^{L} |\Psi(x)|^2\,dx}} + \underset{\text{Region III}}{\cancelto{0}{\int_{L}^{\infty} |\Psi(x)|^2\,dx}} = 1$

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Module 4 (Quantum Mechanics)

Particle in an infinite square well

- How boundary conditions and normalization determine wavefunctions
- *Now we shall see the Schrödinger equation in certain situation: a particle in an infinite square well (1-D).*
- $\Psi(x) = A\,Sin(\alpha x) = A\,Sin\left(\frac{n\pi x}{L}\right)$
- $\int_{-\infty}^{\infty} |\Psi(x)|^2\,dx = 1 \Rightarrow \int_0^L |\Psi(x)|^2\,dx = 1 \Rightarrow A^2 \int_0^L Sin^2\left(\frac{n\pi x}{L}\right) dx = 1$
- Use the trigonometric identity $Sin^2\theta = \frac{1}{2}(1 - Cos2\theta)$
- $A^2 \int_0^L Sin^2\left(\frac{n\pi x}{L}\right) dx = 1 \Rightarrow \frac{A^2}{2}\left[\int_0^L dx - \int_0^L Cos\left(\frac{2n\pi x}{L}\right) dx\right] = 1 \quad = \frac{A^2}{2}\left[x - \left(\frac{L}{2n\pi}\right)\sin\frac{2n\pi x}{L}\right]_0^L = A^2\left(\frac{L}{2}\right)$
- Solving the above, we find that $A = \sqrt{\frac{2}{L}}$
- Hence, $\Psi(x) = A\,Sin\left(\frac{n\pi x}{L}\right) = \sqrt{\frac{2}{L}}\,Sin\left(\frac{n\pi x}{L}\right)$

Module 4 (Quantum Mechanics)

Particle in an infinite square well

☐ How boundary conditions and normalization determine wavefunctions

☐ *Schrödinger equation in certain situation: a particle in an infinite square well (1-D).*

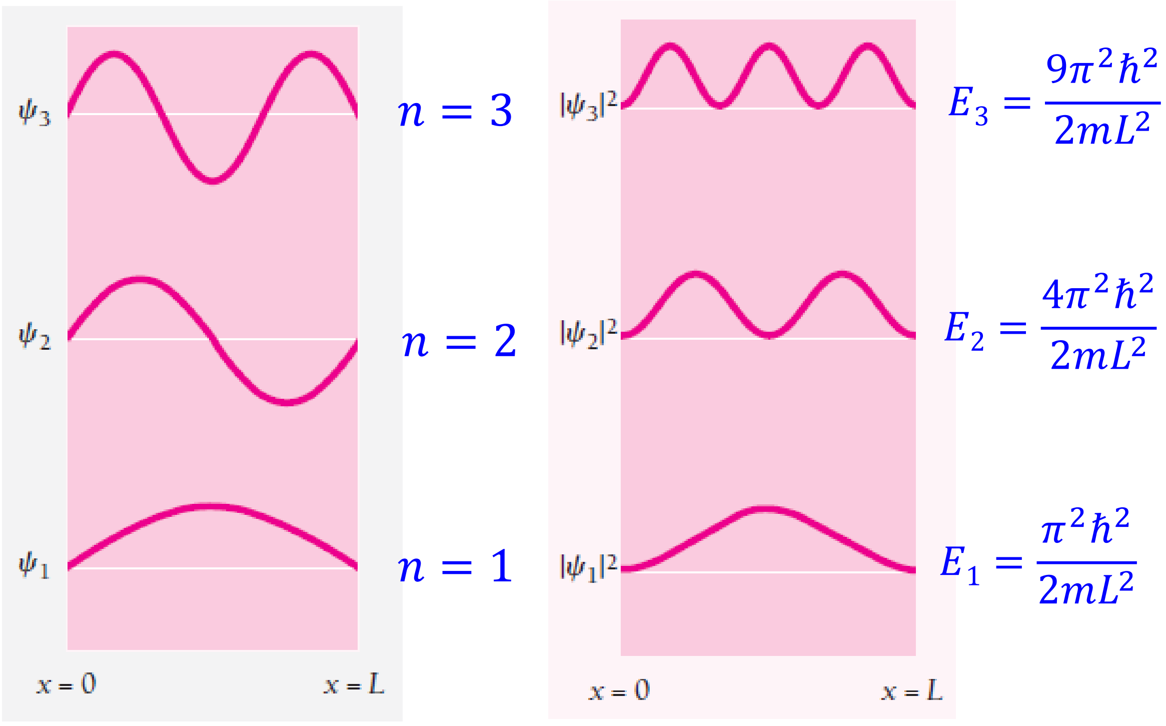
Particle in a box $$\psi_n = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L} \qquad n = 1, 2, 3, \ldots$$

☐ Discretization or Quantization of Energy Levels

☐ Non-zero zero-point energy (Ground State) [$E_n = n^2 E_1$]

☐ Nodes: points (other than two end points) at which the wavefunction vanishes – ZERO probability to find a particle.

☐ Difference between adjacent Energy Levels: $\Delta E = E_{n+1} - E_n = (2n+1)E_1$.



$$E_3 = \frac{9\pi^2\hbar^2}{2mL^2}$$

$$E_2 = \frac{4\pi^2\hbar^2}{2mL^2}$$

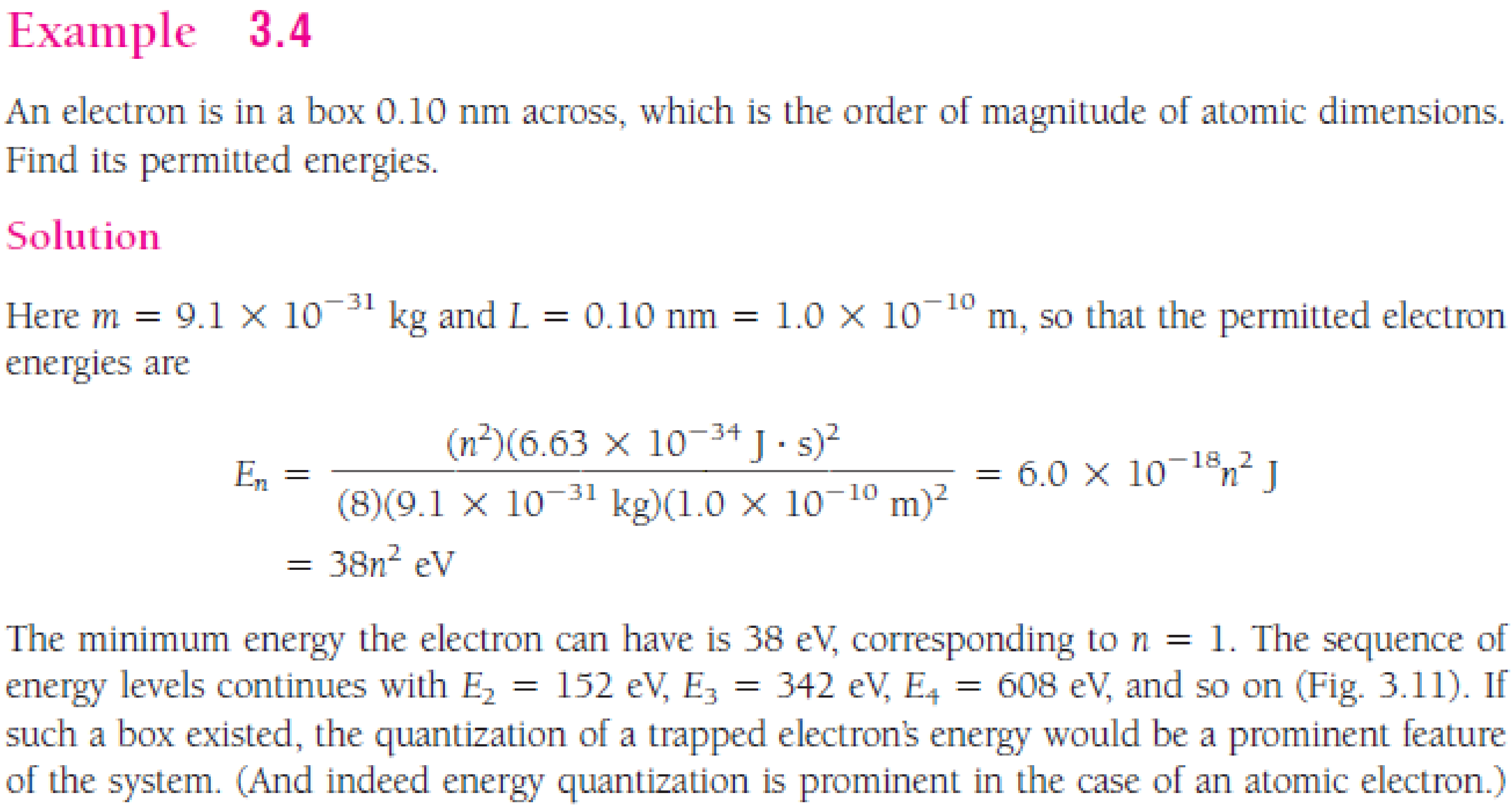
$$E_1 = \frac{\pi^2\hbar^2}{2mL^2}$$

Wave functions and probability densities of a particle confined to a box with rigid walls.

Module 4 (Quantum Mechanics)

Particle in an infinite square well

- ☐ How boundary conditions and normalization determine wavefunctions



Example 3.4

An electron is in a box 0.10 nm across, which is the order of magnitude of atomic dimensions. Find its permitted energies.

Solution

Here $m = 9.1 \times 10^{-31}$ kg and $L = 0.10$ nm $= 1.0 \times 10^{-10}$ m, so that the permitted electron energies are

$$E_n = \frac{(n^2)(6.63 \times 10^{-34}\ \mathrm{J \cdot s})^2}{(8)(9.1 \times 10^{-31}\ \mathrm{kg})(1.0 \times 10^{-10}\ \mathrm{m})^2} = 6.0 \times 10^{-18} n^2\ \mathrm{J}$$
$$= 38 n^2\ \mathrm{eV}$$

The minimum energy the electron can have is 38 eV, corresponding to $n = 1$. The sequence of energy levels continues with $E_2 = 152$ eV, $E_3 = 342$ eV, $E_4 = 608$ eV, and so on (Fig. 3.11). If such a box existed, the quantization of a trapped electron's energy would be a prominent feature of the system. (And indeed energy quantization is prominent in the case of an atomic electron.)

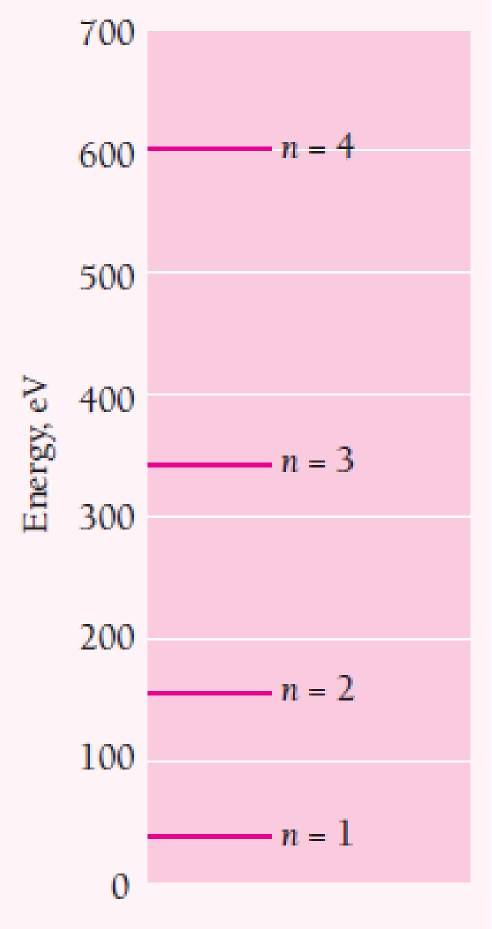
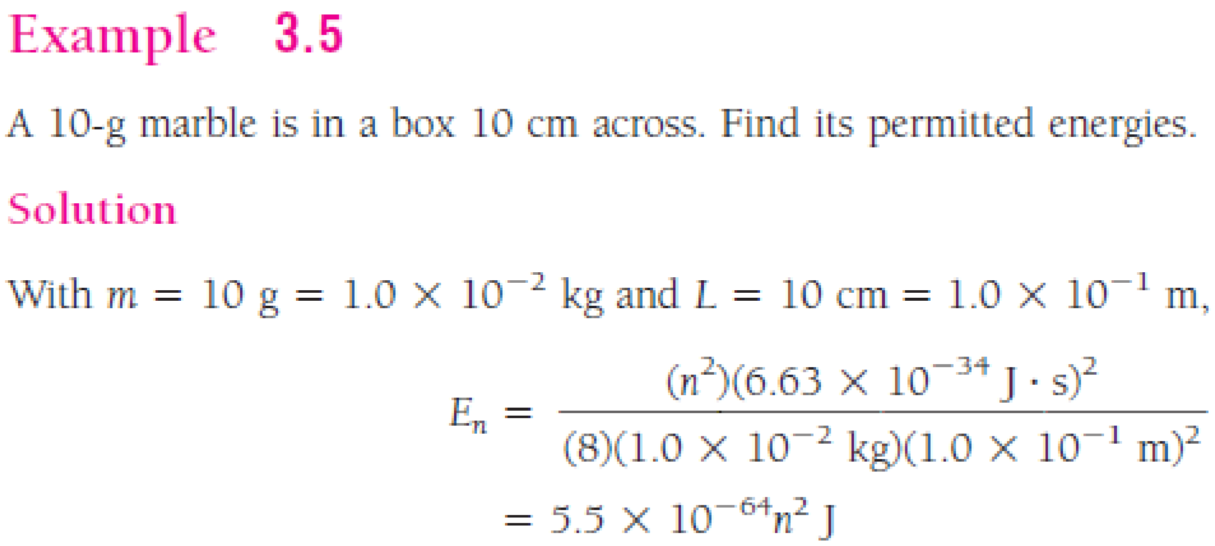


Figure 3.11 Energy levels of an electron confined to a box 0.1 nm wide.

Particle in an infinite square well

- ☐ How boundary conditions and normalization determine wavefunctions



Example 3.5

A 10-g marble is in a box 10 cm across. Find its permitted energies.

Solution

With $m = 10\ \text{g} = 1.0 \times 10^{-2}\ \text{kg}$ and $L = 10\ \text{cm} = 1.0 \times 10^{-1}\ \text{m}$,

$$E_n = \frac{(n^2)(6.63 \times 10^{-34}\ \text{J}\cdot\text{s})^2}{(8)(1.0 \times 10^{-2}\ \text{kg})(1.0 \times 10^{-1}\ \text{m})^2}$$
$$= 5.5 \times 10^{-64} n^2\ \text{J}$$

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Module 4

Module -4 : Quantum Mechanics

Planck's theory of black-body radiation, Compton effect, Wave particle duality, De Broglie waves, Davisson and Germer's experiment, Uncertainty principle, Brief idea of Wave Packet, Wave Function and its physical interpretation, Schrodinger equation in one-dimension, free particle, particle in an infinite square well. [9]

Text book: T3: Arthur Beiser (AB), Concept of Modern Physics, 6th edition 2009, Tata McGraw- Hill

Reference book: R1: Fundamentals of Physics, Halliday, Walker and Resnick