

Phase space or μ -space \Rightarrow The six dimensional space which is used to specify the dynamical state of any particle is called phase space. The six coordinates are x, y, z, P_x, P_y, P_z .

Microstate \Rightarrow The microstate of the system at a particular instant be defined when we ~~not~~ specify as to which particular cell each molecule of the system belongs at that instant.

Macrostate \Rightarrow It can be defined by just giving the number of molecules in each cell.

(b) Maxwell-Boltzmann Velocity Distribution Law

Substitute $E = \frac{1}{2}mv^2$ and $dE = mvdv$ in Eq. (3.23).

Then we get

$$\therefore n(v)dv = \frac{\sqrt{2}\pi N m^{3/2}}{(\pi k_B T)^{3/2}} v^2 e^{-mv^2/2k_B T} dv \quad \dots(3.26)$$

Equation (3.26) represents the number of molecules with speed between v and $(v+dv)$ in an assembly of ideal gas containing N molecules at absolute temperature T . This formula is plotted in Fig. 3.3.

Example 3.1 An electron gas obeys the Maxwell-Boltzman statistics. Calculate average thermal energy (in eV) of an electron in the system at 300 K. [GGSIPU, March 2015 (2 marks)]

$$\text{Solution. } E = \frac{3}{2} k_B T = \frac{3}{2} \times 1.38 \times 10^{-23} \times 300 \text{ J} = \frac{3 \times (1.38 \times 10^{-23}) \times 300}{2\pi(1.6 \times 10^{-19})} \text{ eV} = 0.039 \text{ eV}$$

Example 3.2 At what temperature would one in a thousand of atom in a gas of atom hydrogen be in $n=2$ energy level?

$$\text{Solution. For hydrogen } n(E) = -\frac{13.6}{n^2} \text{ eV}$$

$$n(E_1) = n_1 = -13.6 \text{ eV}$$

$$n(E_2) = n_2 = -3.4 \text{ eV}$$

$$g(E) = \text{no. of states formed} = 2n^2$$

$$g(E_1) = g_1 = 2 \text{ and } g(E_2) = g_2 = 8$$

For Maxwell-Boltzmann distribution is

$$\frac{n_2}{n_1} = \frac{g_2}{g_1} \frac{e^{-E_2/k_B T}}{e^{-E_1/k_B T}} = \frac{8}{2} e^{-(E_2-E_1)/k_B T}$$

$$\frac{1}{10^3} = 4e^{-(E_2-E_1)/k_B T} \quad \text{or} \quad e^{(E_2-E_1)/k_B T} = \frac{10^4}{2.5} = 4000$$

Taking logarithms both the sides

$$\frac{E_2 - E_1}{k_B T} = \ln 4000$$

$$k_B T = \frac{(E_2 - E_1)}{\ln 4000} = \frac{10.2 \text{ eV}}{8.29}$$

$$T = \frac{10.2 \times 1.6 \times 10^{-19}}{8.29 \times 1.38 \times 10^{-23}} \text{ K} = 1.43 \times 10^4 \text{ K}$$

$$T = 14300 \text{ K} = 14300 - 273 = 14027^\circ \text{C}$$

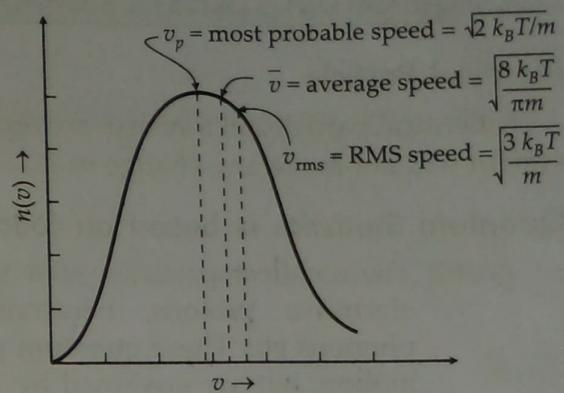


Fig. 3.3

The corresponding Fermi energy is given by

$$E_F = \frac{h^2}{2m} \left(\frac{2N}{8\pi V} \right)^{2/3}$$

$$E_F = \frac{(6.63 \times 10^{-34} \text{ J} \cdot \text{s})^2}{(2 \times 9.11 \times 10^{-31} \text{ kg} / \text{electron})} \left[\frac{3 \times (8.48 \times 10^{28} \text{ electrons} / \text{m}^3)}{8\pi} \right]^{2/3}$$

$$= 1.13 \times 10^{-18} \text{ J} = 7.04 \text{ eV}$$

At absolute zero, $T = 0 \text{ K}$, there should be electrons with energy upto 7.04 eV in copper. By contrast, all the molecules in an ideal gas at 0 K would have zero energy. The electron gas in a metal is said to be 'degenerate'.

Example 3.5 Consider silver in the metallic state with one free electron per atom. Density of silver is 10.5 g/cc and atomic weight is 108. **Find fermi energy?** [GGSIPU, May 2014 reappear (6 marks)]

Solution. Here $\frac{N}{V} = \frac{N}{M/\rho} = \frac{6.02 \times 10^{26}}{108/(10.5 \times 1000)}$

$$= \frac{6.02 \times 10^{26} \times 10.5 \times 1000}{108} = 5.85 \times 10^{28}$$

$$E_F = \frac{h^2}{2m} \left(\frac{3}{8\pi} \frac{N}{V} \right)^{2/3} = \frac{(6.625 \times 10^{-34})^2}{2 \times (9 \times 10^{-31})} \times \left(\frac{3}{8\pi} \times (5.85 \times 10^{28}) \right)^{2/3}$$

$$= 8.92 \times 10^{-19} \text{ J} = 5.57 \text{ eV}$$

(b) Electronic Specific Heat

The specific heat at constant volume of metals (solids) is given as

$$C_V = \left(\frac{\partial E}{\partial T} \right)_V = 3R = 24.9 \text{ J mol}^{-1} \text{ K}^{-1}$$

...(3.90)

The correct explanation of specific heat of metals remained a puzzle for a long time. Of course it should be no surprise to us that classical statistics fails to give the right answer because an assembly of electron (electron gas) obey Fermi-Dirac statistics. We can easily show, using Fermi-Dirac statistics that electronic specific heat varies with temperature. Moreover, heat of a metal at low temperatures is the sum of an electronic contribution which is proportional to T , and the lattice contribution which is proportional to T^3 .

Experiments reveal that the contribution of electronic specific heat is about 1% of the total. To show this we assume that only those electrons which occupy energy states upto $k_B T$ of the Fermi level participate in thermal processes. Hence the fraction of particles thermally excited is proportional to $(k_B T / E_F)$. Since the thermal energy per excited particle is $k_B T$

$$E \sim (k_B T) \frac{k_B T}{E_F} N = \frac{N k_B^2 T^2}{E_F}$$

Hence

$$(C_V)_{El} = \left(\frac{\partial E}{\partial T} \right)_V \frac{N k_B^2 T^2}{E_F} = N k_B \left(\frac{T}{T_F} \right)$$

...(3.91)

That is, for $T \ll T_F$, the electronic specific heat of fermions varies linearly with temperature.

At room temperature

$$\frac{T}{T_F} = \frac{300}{10^4} \sim 0(10^{-2}) \quad \dots(3.92)$$

A more exact, but somewhat difficult, calculation gives the following result :

$$(C_V)_{El} = \frac{Nk_B\pi^2}{2T_F} T = aT \quad \dots(3.93)$$

$$a = \frac{Nk_B\pi^2}{2T_F} = \frac{Nk_B^2\pi^2}{2E_F} \quad \dots(3.94)$$

is known as **Sommerfeld constant**.

The total heat capacity of a metal is made up of two parts. The electronic contribution dominates at low temperatures. But around room temperature, the electronic contribution is a small fraction of total

$$(C_V)_{Total} = aT + bT^3 \quad \dots(3.95)$$

$$\frac{(C_V)_{Total}}{T} = a + bT^2 \quad \dots(3.96)$$

A plot of Eq. (3.96) is visualised in Fig. 3.6 as a function for potassium. The agreement is seen to be excellent. The intercept gives the value of a . For potassium, sodium and copper the typical values are 2.08, 1.38, 0.695 respectively.

3.8 DYING STARS

~~Metals are not the only systems that contain degenerate fermion gases – many dead and dying star fall into this category also.~~

3.8.1 White/Black Dwarfs

A star like our Sun will become a white dwarf when it has exhausted its nuclear fuel. Near the end of its nuclear burning stage, such a star expels most of the outer material (creating a planetary nebula) until only the hot ($T > 100,000$ K) core remains, which then settles down to become a young **white dwarf**. A typical white dwarf is half as massive as Sun, yet only slightly bigger than the earth. This makes white dwarfs one of the densest of matter, surpassed only by neutron stars. White dwarfs have no way to keep themselves hot (unless they accrete matter from other closely starts); therefore, they cool down over the course of many billions of years. Eventually, such stars cool completely and become **black dwarfs**. Black dwarf do not radiate at all.

Many nearby, young white dwarfs have been detected as source of soft X-rays (*i.e.*, lower energy X-rays); soft X-ray and extreme ultraviolet observations enable astronomers to study the composition and structure of the thin atmospheres of these stars.

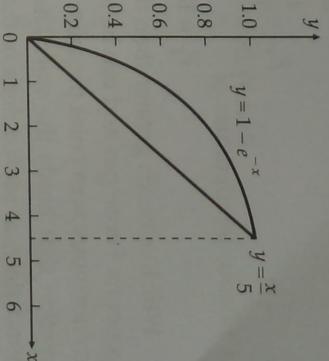


Fig. 3.6 Plot of Eq. (3.6) as a function of T^2 .

free electrons per unit volume at the temperature.

Solution. Given $E_F = 2.1 \text{ eV} = 2.1 \times 1.6 \times 10^{-19} \text{ J}$, $n_c = ?$

$$n_c = \left(\frac{2m}{h^2} E_F \right)^{3/2} \times \frac{8\pi}{3} = \left[\frac{2 \times 9.1 \times 10^{-31} \times 2.1 \times 1.6 \times 10^{-19}}{(6.625 \times 10^{-34})^2} \right]^{3/2} \times \frac{8 \times 3.14}{3}$$

$$= (5.579 \times 10^{18}) \times 1.047 = 1.379 \times 10^{28} \text{ electrons/m}^3$$

Problem 3.6 The density of zinc is $7.13 \times 10^3 \text{ kg/m}^3$ and its atomic weight is 65.4. Calculate the Fermi energy and the mean energy at $T = 0 \text{ K}$.

Solution. Given : $\rho = 7.13 \times 10^3 \text{ kg m}^{-3}$, $M = 65.4$

Since we know that

$$E_F = \frac{h^2}{2m} \left(\frac{3n_c}{8\pi} \right)^{2/3} \quad \text{or} \quad E_F = 3.65 \times 10^{-19} n_c^{2/3} \text{ eV} \quad (\text{On putting the value } h, m, \pi)$$

$$n_c = \frac{2\rho N_A}{M} = \frac{2 \times \text{density} \times \text{Avogadro's number}}{\text{Molecular weight}}$$

$$n_c = \frac{2 \times 7.13 \times 6.023 \times 10^{26}}{65.4} = 1313 \times 10^{26}$$

$$E_F = 3.65 \times 10^{-19} \times (1313 \times 10^{26})^{2/3} = 11.1 \text{ eV}$$

and Mean energy (\bar{E}) = $\frac{3}{5} E_F = \frac{3}{5} \times 11.1 \text{ eV} = 6.66 \text{ eV}$

Problem 3.7 At what temperature can we expect a 10% probability that electrons in a metal will have an energy which is 1% above E_F ? The Fermi energy of the metal is 5.5 eV. [IGGSIPU, May 2014 (4.5 marks)]

Solution. Given : $f(E) = 10\%$, $E = E_F + 1\%$ of E_F , $E_F = 5.5 \text{ eV}$, $T = ?$

$$f(E) = \frac{1}{e^{(E-E_F)/k_B T} + 1}$$

$$E = 5.5 + \frac{5.5}{100} = 5.5 + 0.555; \quad E - E_F = 0.555.$$

$$0.1 = \frac{1}{\exp \left(\frac{0.555 \times 1.6 \times 10^{-19}}{1.38 \times 10^{-23} T} \right) + 1} = \frac{1}{\exp \left(\frac{637.7}{T} \right) + 1} \quad \text{or} \quad T = 290.2 \text{ K}$$

Problem 3.8 Suppose that the maximum temperature in an atomic bomb explosion is 10^7 K . What is the corresponding wavelength of maximum energy?

$$\lambda = 0.289 \text{ cm K}$$

On account of the relativistic increase in the mass of the high velocity electrons, the necessary correction in Eq. (1.7) may be made.

...(1.9)

correction in Eq. (1.7) may be made.

The relativistic mass is given by

$$m = \frac{m_0}{\sqrt{1 - \frac{v^2}{c^2}}}$$

where m_0 is the rest mass of the particle, v is its velocity and c the velocity of light.

Applying relativistic equation for kinetic energy K , viz

$$K = (m - m_0)c^2, \text{ we have}$$

$$(m - m_0)c^2 = Ve$$

$$(m - m_0) = \frac{Ve}{c^2}$$

or

$$m = m_0 + \frac{Ve}{c^2} = m_0 \left(1 + \frac{Ve}{m_0 c^2} \right)$$

or

$$m^{1/2} = m_0^{1/2} \left(1 + \frac{Ve}{m_0 c^2} \right)^{1/2}$$

Substituting the value of $m^{1/2}$ in Eq. (1.7), above, we get

$$\lambda = \frac{h}{\sqrt{2} V e m_0} \left(1 + \frac{Ve}{m_0 c^2} \right)^{-1/2} \quad \dots(1.10)$$

For the wavelength of electrons of known energy,

$$\frac{h}{\sqrt{2} V e m_0} = \frac{12.28}{\sqrt{V}} \text{ Å} \quad \dots(1.11)$$

Substitution in the above gives

$$\lambda = \frac{12.28}{\sqrt{V}} \left(1 + \frac{Ve}{m_0 c^2} \right)^{-1/2} \text{ Å} \quad \dots(1.12)$$


Example 1.1 Calculate the de-Broglie wavelength of

- (i) a particle accelerated by a potential difference of 30,000 V, and
- (ii) an electron moving with a velocity of 0.01 c, where c is the speed of light.

[IGCSEPU, Feb. 2008, Reappear (6 marks)]

Solution. Given : $E = Ve = 1.6 \times 10^{-19}$ V joule

Mass of electron = 9.1×10^{-31} kg

and
Planck's constant (\hbar) = 6.63×10^{-34} Js

(i) The de-Broglie wavelength is given by

$$\lambda = \frac{h}{mv} = \frac{h}{\sqrt{2mE}}$$

$\therefore E = \frac{1}{2}mv^2$ so that $mv = \sqrt{2mE}$

$$\lambda = \frac{6.63 \times 10^{-34}}{\sqrt{2 \times 9.1 \times 10^{-31} \times 1.6 \times 10^{-19} V}} = \frac{12.28 \times 10^{-10}}{\sqrt{V}}$$

$$= \frac{12.28}{\sqrt{V}} \text{ Å} = \frac{12.28}{1732} \times 10^{-10} = 7.09 \times 10^{-12} \text{ m}$$

(ii) The de-Broglie wavelength is given by

$$\lambda = \frac{h}{mv} = \frac{h}{m \times (0.01c)}$$

$$= \frac{6.63 \times 10^{-34}}{9.1 \times 10^{-31} \times 0.01 \times 3 \times 10^8} \text{ m} = \frac{6.63 \times 10^{-11}}{9.1 \times 0.03} \text{ m} = 2.43 \times 10^{-10} \text{ m} = 2.43 \text{ Å}$$

✓ Example 1.2 Calculate the de-Broglie wavelength of virus particle of mass $1.0 \times 10^{-15} \text{ kg}$ moving at a speed of 2.0 mm/s . [IGGSIPU, May 2005 (2.5 marks)]

Solution. Given $m = 1.0 \times 10^{-15} \text{ kg}$, $v = 2.0 \times 10^{-3} \text{ m/s}$

The de-Broglie wavelength is given by

$$\lambda = \frac{h}{mv} = \frac{6.63 \times 10^{-34}}{1.0 \times 10^{-15} \times 2.0 \times 10^{-3}} = 3.315 \times 10^{-16} \text{ m}$$

1.3 CHARACTERISTICS OF MATTER WAVES

(i) The de-Broglie wavelength of a particle of mass m moving with a velocity v is given by

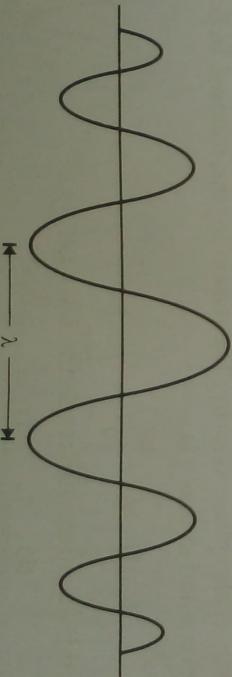
$$\lambda = \frac{h}{\sqrt{2meV}}. \text{ Larger the mass, shorter will be the de-Broglie wavelength.}$$

(ii) The de-Broglie waves are *pilot waves* i.e., these waves guide the particle.

(iii) The de-Broglie waves are not electromagnetic waves.

(iv) Matter waves cannot be observed. It is a wave model to describe and to study matter.

(v) The de-Broglies waves are called *probability waves*. The amplitude of the wave reveals the probability of finding a particle in space at a particular instant. A large wave amplitude means a large probability to find the particle at that position as visualised in Fig. 1.1.



The following conditions must be satisfied :

$$(i) \quad \left(\frac{dE}{da} \right)_{a=\alpha} = 0 \quad \text{and} \quad (ii) \quad \left(\frac{d^2E}{da^2} \right)_{a=\alpha} > 0$$

Applying condition (i), we get

$$\alpha^2 = \frac{\hbar}{2m\omega} \quad \dots (1.93)$$

It can be easily shown that this value satisfies condition (ii).

Substituting $\alpha^2 = \alpha^2 = \frac{\hbar}{2m\omega}$ in Eq. (1.92), the lowest possible value of total energy (E_{\min}) is obtained as

$$E_{\min} = \frac{1}{2} \hbar \omega = \frac{1}{2} \times \frac{\hbar}{2\pi} \times 2\pi v = \frac{1}{2} \hbar v \quad \dots (1.94)$$

Advanced quantum mechanical calculations show that the total energy is given by

$$E_n = \left(n + \frac{1}{2} \right) \hbar v, \quad \text{where } n = 0, 1, 2, 3, \dots \quad \dots (1.95)$$

This is correct expression for the *total energy of a simple harmonic oscillator*.

For $n \neq 0$, the system has the minimum energy, which is $E_0 = \frac{1}{2} \hbar v$. This value is known as the *zero point energy of a simple harmonic oscillator*.

Example 1.5 Find the smallest possible uncertainty in position of the electron moving with velocity 3×10^7 m/s ($Groen h = 6.63 \times 10^{-34}$ Js, $m_0 = 9.1 \times 10^{-31}$ kg) [IGSPU, May 2007 (2.5 marks)]

Solution. Given $v = 3 \times 10^7$ m/s

Let Δx_{\min} be the minimum uncertainty in position of the electron and Δp the maximum uncertainty in the momentum of the electron.

Thus we have, $\Delta x_{\min} \cdot \Delta p_{\max} = \frac{\hbar}{2\pi}$...(i)

or

$$\Delta p_{\max} = p = mv$$

$$\Delta p_{\max} = \frac{m_0 v}{\sqrt{1 - \frac{v^2}{c^2}}} \quad \dots (ii)$$

$$\Delta x_{\min} = \frac{h \sqrt{1 - \frac{v^2}{c^2}}}{2\pi m_0 v} = \frac{6.63 \times 10^{-34} \sqrt{1 - \left(\frac{3 \times 10^7}{3 \times 10^8} \right)^2}}{2 \times 3.14 \times 9.1 \times 10^{-31} \times 3 \times 10^7} \text{ m} \\ = 0.03867 \times 0.9949 \times 10^{-10} \text{ m} = 3.8 \times 10^{-12} \text{ m}$$

Example 1.6 A microscope, using photons, is employed to locate an electron in an atom within a distance of 0.2 \AA . What is the uncertainty in the momentum of the electron located in this way?

Solution. Given $\Delta x = 0.2 \text{ Å} = 2 \times 10^{-11} \text{ m}$; $\Delta p = ?$

Since we know that the uncertainty principle

$$\Delta x \Delta p = \frac{h}{2\pi} \quad \text{or} \quad \Delta p = \frac{h}{2\pi \Delta x}$$

$$\therefore \Delta p = \frac{6.626 \times 10^{-34}}{2 \times 3.14 \times (0.2 \times 10^{-10})} = 5.27 \times 10^{-24} \text{ kg m s}^{-1}$$

Hence uncertainty in momentum (Δp) = $5.27 \times 10^{-24} \text{ kg m s}^{-1}$

Example 1.7 Show that the uncertainty in the location of the particle is equal to de-Broglie wavelength the uncertainty in its velocity is equal to its velocity. [GGSIPU, April 2014 (2 marks)]

Solution. Given $\Delta x = \lambda$,

Since we know that the uncertainty principle

$$\Delta x \Delta p_x = h \quad \text{or} \quad \lambda \Delta p_x = h$$

$$\text{or} \quad \Delta p_x = \frac{h}{\lambda} \quad \text{or} \quad \Delta p_x = p$$

$$\text{or} \quad m \Delta v_x = mv_x \quad \text{or} \quad \Delta v_x = v_x$$

Formulae at a Glance

1.1 Dual Nature of Matter,

The wavelength (λ) = $\frac{h}{p}$ = Planck's constant
momentum

1.2 de-Broglie wavelength of an electron

$$\lambda = \frac{h}{\sqrt{2meV}} = \frac{12.28}{\sqrt{V}} \text{ Å}$$

1.3 Phase Velocity,

$$v_p = \frac{\omega}{k} = \frac{\text{Angular frequency}}{\text{Propagation constant}}$$

1.4 Group Velocity, $v_g = \frac{d\omega}{dk}$

1.5 Relation between v_p and v_g .

$$v_g = v_p - \lambda \frac{dv_p}{dk}$$

1.6 Relation between v_g and particle velocity v_{particle}

$$v_g = v_{\text{particle}} = \frac{dE}{dp}$$

1.7 Relation between velocity of light (c), v_g and v_p

$$v_p v_g = c^2$$

1.8 In Davisson and Germer experiment,

$$(i) \quad 2d \sin \theta = n\lambda$$

$$\Rightarrow \lambda = 1.65 \text{ Å};$$

d = interplanar distance

$$(ii) \quad \lambda_e = \frac{12.28}{\sqrt{V}} \text{ Å} = 1.66 \text{ Å.} \quad (\text{at } V = 54 \text{ V})$$

1.9 Heisenberg's uncertainty principle,

$$(i) \quad \Delta x \Delta p_x \approx \frac{h}{2\pi} = \hbar$$

$$\Delta y \Delta p_y \approx \frac{h}{2\pi} = \hbar \quad \Delta x \Delta p_x \geq \hbar$$

$$\Delta z \Delta p_z \approx \frac{h}{2\pi} = \hbar$$

$$(ii) \quad \Delta E \cdot \Delta t \geq \hbar$$

E = energy

$$(iii) \quad \Delta L \Delta \theta \geq \frac{h}{2\pi} \quad L = \text{angular momentum}$$

$\Delta \theta$ = angular change

- 1.41** Write short notes on (i) Davisson-Germer experiment. (ii) Heisenberg's uncertainty principle.

[GGSIPU, Feb. 2009 [Reappear] (5 marks)]

- 1.42** Give the uncertainty relation among energy and time. Name one phenomenon/experiment that may be considered as the proof of this relation.

[GGSIPU, May 2009 (4.5 marks)]

- 1.43** State Heisenberg's uncertainty principle.

[GGSIPU, Feb. 2010, May 2009 (Reappear) (2 marks)]

- 1.44** Write short note on uncertainty principle.

[GGSIPU, Feb. 2008 (Reappear (4 marks))]

- 1.45** State Heisenberg's uncertainty principle. How does the uncertainty principle account for the absence of electrons in the nucleus.

[GGSIPU, June 2013 (4 marks)]

- 1.46** Show that the de-Broglie wavelength of a particle is approximately the same as that of a photon with the same energy, when the energy of the particle is much greater than its rest energy.

[GGSIPU, Feb. 2013 (2 marks)]

- 1.47** State the uncertainty principle. Apply it to find the minimum energy of particle in box.

[GGSIPU, May 2012 (4.5 marks)]

- 1.48** Explain Heisenberg uncertainty principle with the help of an experiment.

[April 2014 (5 marks)]

- 1.49** State Heisenberg's uncertainty principle and explain its validity by any thought experiment.

[GGSIPU, April 2015 (4 marks)]

- 1.50** State Heisenberg's uncertainty principle by applying uncertainty principle, explain non-existence of electron in atomic nucleus.

Numerical Problems

- 1.1** Find the phase velocity and group velocity of the de-Broglie wave of an electron whose speed is 0.9c.

Hint: $v_p v_g = c^2$ and $v_g = 0.9c$. Then $v_p = 3.33 \times 10^8 \text{ m/s}$.

- 1.2** Calculate the de-Broglie wavelength of (i) a 46 g golf ball moving with velocity 30 m/s and (ii) an electron moving with velocity 10⁷ m/s. Which one is measurable ?

[GGSIPU, May 2010 (2.5 marks)]

Hint : $\lambda = \frac{h}{mv}$

$$(i) \text{ For golf ball : } \lambda = \frac{6.63 \times 10^{-34}}{46 \times 10^{-3} \times 30} = 4.8 \times 10^{-34} \text{ m } [\text{Not measurable}]$$

$$(ii) \text{ For electron : } \lambda = \frac{6.63 \times 10^{-31}}{9.1 \times 10^{-31} \times 10^7} = 72 \text{ nm } [\text{measurable}] .$$

- 1.3.** Give an account of experimental evidence which demonstrates the wave like properties of moving electrons. Calculate the glancing angle at which electrons of energy 100 eV must be incident on the lattice planes of a metal crystal in order to give a strong Bragg reflection in the first order. Use the following data : lattice spacing = 2.15 Å, $m_e = 9.1 \times 10^{-31}$ kg, $e = 1.6 \times 10^{-19}$ C and $\hbar = 6.63 \times 10^{-34}$ Js.

Hint : $n\lambda = 2d \sin \theta$ and $\lambda = \frac{h}{\sqrt{2emV}}$

$$\text{Then, } \sin \theta = \frac{n\lambda}{2d} = \frac{n}{2d} \frac{h}{\sqrt{2emV}} \\ = \frac{6.63 \times 10^{-34}}{2 \times 2.15 \times 10^{-10} \sqrt{2 \times 1.6 \times 10^{-19} \times 9.1 \times 10^{-31} \times 100}} = 0.2847 \text{ or } \theta = 16^\circ 32'$$

1.4 Electrons of 400 eV are diffracted through a crystal and a second order maximum is observed where the angle between the diffracted beam and incident beam is 30° .

Calculate :

- (i) the wavelength of the electron matter wave.
 (ii) the interplanar distance of those lattice planes which are responsible for this maximum.

$$\text{Hint : (i)} \quad \lambda = \frac{h}{(2m_0 E)^{1/2}} = \frac{6.626 \times 10^{-34} \text{ Js}}{(2 \times 9.1 \times 10^{-31} \text{ kg} \times 400 \times 1.6 \times 10^{-19} \text{ J})^{1/2}} = 0.61 \times 10^{-10} \text{ m} = 0.61 \text{ \AA}$$

$$\text{(ii)} \quad n\lambda = 2d \sin \theta, \text{ then } d = \frac{\lambda}{\sin \theta} = \frac{0.61 \times 10^{-10}}{\sin 30^\circ} = 2 \times 0.61 \times 10^{-10} = 1.22 \times 10^{-10} \text{ m} = 1.22 \text{ \AA}$$

1.5 A ball of mass 10^{-3} kg moves with a velocity of 10^{-2} ms^{-1} . What is the de Broglie wavelength of the ball?

$$\text{Hint : } \lambda = \frac{h}{p} = \frac{h}{mv} = \frac{6.626 \times 10^{-34} \text{ Js}}{10^{-3} \text{ kg} \times 10^{-2} \text{ ms}^{-1}} = 6.626 \times 10^{-29} \text{ m}$$

1.6 An electron and a proton have the same de Broglie wavelength. Prove that the energy of electron is greater.

$$\text{Hint : } \lambda = \frac{h}{p} = \frac{h}{mv} = \frac{h}{\sqrt{2mE}} \text{ then } \lambda_e = \lambda_p, \Rightarrow \frac{h}{\sqrt{2m_e E_e}} = \frac{h}{\sqrt{2m_p E_p}}$$

$$m_e E_e = m_p E_p \Rightarrow E_e = \frac{m_p E_p}{m_e} \text{ since } m_e < m_p, \text{ so } E_e = \frac{m_p E_p}{m_e}$$

1.7 An electron and a proton are moving with same velocity. Find the ratio of their (i) de Broglie wavelength, (ii) phase velocity and (iii) group velocity.

[GGSIPU, May 2015 (6 marks)]

$$\text{Hint : (i)} \quad \frac{\lambda_e}{\lambda_p} = \frac{h}{m_p v_p} \times \frac{m_p v_p}{h} = \frac{m_p}{m_e}$$

$$\text{(ii)} \quad \frac{v_{g_e}}{v_{g_p}} = \frac{v_e}{v_p} = 1 \quad \text{and} \quad \text{(iii)} \quad v_p v_g = c^2 \quad \text{so} \quad \frac{v_{p_e}}{v_{p_p}} = \frac{v_e}{v_p} = 1$$

1.8 Calculate the de Broglie wavelength of basket ball of mass 1 kg, moving at a speed of 10 ms^{-1} . Discuss the reason, why we cannot observe its wave nature.

$$\text{Hint : } \lambda = \frac{h}{mv} = \frac{6.63 \times 10^{-34}}{10 \times 10} \text{ m} = 6.63 \times 10^{-36} \text{ m} \text{ which is not measurable.}$$

1.9 Calculate the de-Broglie wavelength of a baseball of mass 1 kg, moving at a speed of 10 m/s. Discuss the reason why we cannot observe its wave nature.

$$\text{Hint : } \lambda = \frac{h}{p} = \frac{h}{mv} = \frac{6.6 \times 10^{-34} \text{ Js}}{1 \text{ kg} \times 10 \text{ m/s}} = 6.6 \times 10^{-35} \text{ m} = 6.6 \times 10^{-25} \text{ \AA}$$

Reason. The wave nature of light is revealed through experiment in optics. To observe diffraction effects, the dimension of the apparatus through which light passes must be comparable with the wavelength. The de-Broglie wavelength of the baseball is so small that we cannot expect to construct an apparatus which is capable of detecting its wave nature by causing the diffraction of its de-Broglie wave.

- 1.10 The energy of a free electron including its rest mass energy is 1 MeV. Calculate the group velocity and the phase velocity of the wave packet associated with the motion of the electron.

Hint : $v_p = \frac{c^2}{v_g}$ and $v_g = \frac{p}{m}$

where $p = (m^2 c^2 - m_0^2 c^2)^{1/2} = (m^2 - m_0^2)^{1/2} c$ and $m = \frac{E}{c^2} = \frac{10^6 \times 16 \times 10^{-19}}{9 \times 10^{16} \text{ m}^2 \text{s}^{-2}} = 1.778 \times 10^{-30} \text{ kg}$

$$\therefore p = [(17.8)^2 - (9.1)^2]^{1/2} \times 10^{-31} \times 3 \times 10^8 \text{ kg ms}^{-1} = 458 \times 10^{-22} \text{ kg ms}^{-1}$$

$$\therefore v_g = \frac{4.58 \times 10^{-22} \text{ kg ms}^{-1}}{1.778 \times 10^{-30} \text{ kg}} = 3.5 \times 10^8 \text{ ms}^{-1} \quad \text{and} \quad v_p = \frac{9}{2.576} \times 10^8 \text{ ms}^{-1} = 3.5 \times 10^8 \text{ ms}^{-1}$$

- 1.11 A certain excited state of hydrogen atom is known to have a life of $2.5 \times 10^{-4} \text{ s}$. What is the minimum error, with which the energy of the excited state can be measured?

Hint : $\Delta E \cdot \Delta t \geq \hbar$

$$\Delta E = \frac{\hbar}{2\pi\Delta t} = \frac{6.62 \times 10^{-34}}{2 \times 3.14 \times 2.5 \times 10^{-14}} \text{ J} = 4.2 \times 10^{-21} \text{ J}$$

or $\Delta E = \frac{4.2 \times 10^{-21}}{16 \times 10^{-19}} = 0.0262 \text{ eV}$

- 1.12 An electron has a speed 500 m/s accurate to 0.01% with what fundamental accuracy can we locate the position of the electron?

Hint : $\Delta v = \frac{0.01}{100} \times 500 = 0.05 \text{ m/s} = 5.0 \times 10^{-2} \text{ m/s}$

Then, $\Delta x \cdot \Delta p_x \geq \frac{\hbar}{2\pi}$

and $\Delta x = \frac{\hbar}{2\pi p_x} = \frac{\hbar}{2\pi m \Delta v} = \frac{6.63 \times 10^{-34}}{2 \times 3.14 \times 9.1 \times 10^{-31} \times 5 \times 10^{-2}} = 2.316 \times 10^{-3} \text{ m}$

- 1.13 Determine the de-Broglie wavelength of an electron having kinetic energy 2.0 eV

[Given : mass of electron = $9.1 \times 10^{-31} \text{ kg}$, $\hbar = 6.63 \times 10^{-34} \text{ J.s}$]

Hint : $\lambda = \frac{\hbar c}{\sqrt{K(K + 2m_0 c^2)}}$

$$= \frac{6.63 \times 10^{-34} \times 3 \times 10^8}{[2.0 \times 1.6 \times 10^{-19} (2.0 \times 1.6 \times 10^{-19} + 2 \times 9.1 \times 10^{-31} \times (3 \times 10^8)^2)]^{1/2}}$$

- 1.14 The phase velocity of a soap bubble is $c\lambda^{-1/2}$. Find group velocity of soap bubble.

Hint : $v_g = v_p - \lambda \frac{dv_p}{dt} = c\lambda^{-1/2} - \lambda \frac{d}{dt}(c\lambda^{-1/2}) = c\lambda^{-1/2} + \frac{\lambda c}{2}\lambda^{-1/2} = \frac{3c\lambda^{-1/2}}{2} = \frac{3}{2}v_p$

- 1.15 Find the group velocity in terms of energy and momentum.

Hint : $v_p = \frac{E}{p}$ and $v_g = v_p - \lambda \frac{dv_p}{d\lambda}$.

So $v_g = \frac{E}{p} - \frac{d(E/p)}{d\lambda}$

1.16 Find the phase and group velocities of an electron whose de-Broglie wavelength is 1.2 \AA .

[GGSIPU, Feb. 2012 (5 marks)]

Hint : $m_0 c^2 = 511 \text{ keV}$, $m_0 = 9.1 \times 10^{-31} \text{ kg}$

$$\frac{p^2}{2m} = \frac{h^2}{2m\lambda^2} \Rightarrow \frac{1}{2}mv^2 = \frac{h^2}{2m\lambda^2}$$

$$\Rightarrow v = \frac{h}{m\lambda} = 6.07 \times 10^6 \text{ m/s}$$

$$v = v_g = 6.07 \times 10^6 \text{ m/s}$$

But

$$v_p v_g = c^2$$

$$\Rightarrow v_p = \frac{c^2}{v_g} = \frac{(3 \times 10^8)^2}{6.07 \times 10^6} = 1.48 \times 10^{10} \text{ m/s.}$$

1.17 Calculate the de-Broglie wavelength of 40 keV electrons used in certain electron microscope.

[GGSIPU, May 2011 (2.5 marks)]

Hint : $E = 40 \text{ keV} = 4.0 \times 10^3 \times 1.6 \times 10^{-16} \text{ J} = 6.4 \times 10^{-15} \text{ J}$

$$E = \frac{1}{2}mv^2 \quad \text{or} \quad v = \sqrt{2E/m}$$

de-Broglie wavelength, $\lambda = \frac{h}{mv} = \frac{h}{\sqrt{2mE}} = 6.15 \times 10^{-15} \text{ m}$

1.18 Calculate the de-Broglie wavelength of an electron accelerated through a potential difference 100 V . [GGSIPU, April 2011 (2 marks)]

Hint : $\lambda = \frac{h}{mv} = \frac{h}{\sqrt{2mE}} = \frac{1.228 \times 10^{-10}}{\sqrt{V}} = 1.228 \times 10^{-10} \text{ m} = 1.228 \text{ \AA}$

1.19 A nuclear particle is confined to a nucleus of diameter $5 \times 10^{-4} \text{ m}$. Calculate the minimum uncertainty in the momentum of the nucleon. Also calculate the minimum kinetic energy of the nucleon.

Hint : The diameter of nucleus (Δx) = $5 \times 10^{-14} \text{ m}$

$$\therefore \Delta p \Delta x = \hbar$$

$$\Rightarrow \Delta p = \frac{\hbar}{\Delta x} = \frac{1.05 \times 10^{-34}}{5 \times 10^{-14}} \text{ kg m s}^{-1} = 2.1 \times 10^{-2} \text{ kg m s}^{-1}$$

and the minimum K.E. of the nucleon = $\frac{p^2}{2m_0} = \frac{2.1 \times 10^{-21}}{2 \times m_0}$ here m_0 = mass of nucleon.

1.20 An electron has a de Broglie wavelength 2 pm . Find its kinetic energy, phase velocity and group velocity of its de Broglie wave. Rest mass energy of electron is 511 keV .

[GGSIPU, Feb. 2017 (3 marks)]

Hint : $m_0 c^2 = 511 \text{ keV} \Rightarrow m_0 = 9.1 \times 10^{-31} \text{ kg}$

$$\text{K.E.} = \frac{p^2}{2m} = \frac{h^2}{2m\lambda^2} = \frac{1}{2}mv_g^2 \Rightarrow v_g = ? \Rightarrow v_p v_g = c^2 = ?$$

- 1.21 Use uncertainty principle to deduce the lowest nature of energy of a particle of mass m enclosed in a box of size a .

Hint : $\Delta x \Delta p \geq h$

$$\Rightarrow \Delta p = \frac{h}{\Delta x} \quad \text{and} \quad E = \frac{(\Delta p)^2}{2m} = \frac{h^2}{2m(\Delta x)^2} \quad \Delta x = a$$

$$\text{Then } E = \frac{h^2}{2ma^2}$$

- 1.22 An electron of energy 200 eV is passed through a circular hole of radius 10^{-6} m. What is the uncertainty introduced in the angle of emergence?

Hint : $\frac{p^2}{2m} = E$

or

$$p = \sqrt{2mE} = \sqrt{(2 \times 9.1 \times 10^{-31} \times 200 \times 1.6 \times 10^{-19})}$$

$$\Delta p_x \approx \frac{h}{\Delta x}$$

$[\Delta x = 2r, \text{ where } r = 10^{-6} \text{ m}]$

$$\Delta p_x = \frac{6.63 \times 10^{-34}}{2 \times 10^{-6}} = 3.316 \times 10^{-28} \text{ kg m / s}$$

$$\Delta \theta = \frac{\Delta p_x}{p} = 5.76 \times 10^{-6} \text{ radian}$$

1.23 A typical atomic nucleus is about 5 Fermi in radius. Use the uncertainty principle to place a lower limit on the energy an electron must have if it is part of nucleus.

Hint : We know that 1 Fermi = 10^{-15} m

The uncertainty principle in electron's position is

$$\Delta x = 5 \times 10^{-15} \text{ m}$$

$$\Delta p \geq \frac{h}{\Delta x} = \frac{6.626 \times 10^{-34} \text{ Js}}{2\pi \times 5 \times 10^{-15} \text{ m}} = 2.11 \times 10^{-20} \text{ kg m/s}$$

The momentum would also be of the same order if this is the uncertainty in it. Thus suggests that the kinetic energy of electron is far greater than its rest energy and it can be written as

$$pc \geq (2.11 \times 10^{-20} \text{ kg m/s}) \times (3 \times 10^8 \text{ m/s}) \geq 6.33 \times 10^{-12} \text{ J} \geq 39 \text{ MeV}$$

Experiments indicate that the electrons in an atom must exceed 39 MeV, for it to be a nucleus constituent. **Q124** An electron has a speed of $2 \times 10^4 \text{ ms}^{-1}$ within the accuracy 0.01%. Calculate the uncertainty in the position of the electron.

Hint : $\Delta x \Delta p_x = \Delta x (m \Delta v_x) = \frac{h}{m}$

$$\Rightarrow \Delta x = \frac{h}{m v_x} = \frac{6.63 \times 10^{-34}}{4\pi \times 9.1 \times 10^{-31} \times (2 \times 10^4 \times 0.0001)} = 29 \mu\text{m}$$

[GGSIPU, May 2017 (2.5 marks)]

$$\text{Similarly, } E_2 = \frac{4 \times (6.63 \times 10^{-34})^2}{8 \times 9.1 \times 10^{-31} \times (2 \times 10^{-10})^2} = 9.093 \times 10^{-19} \text{ J} = 5.68 \text{ eV}$$

$$\Delta E = E_2 - E_1 = (5.68 - 1.42) \text{ eV} = 4.26 \text{ eV}$$

2.5 Normalize the wave function

$$\psi(x) = 0 \text{ outside the box of size } l$$

$$\psi(x) = A \sin kx \quad 0 < x < l$$

where

$$k = \frac{\pi}{l}$$

Hint :

$$\int_{-\infty}^{+\infty} |\psi|^2 dx = 1,$$

Here

$$\psi(x) = A \sin \frac{\pi x}{l} = A \sin \frac{\pi x}{l} = \int_0^l A^2 \sin^2 \frac{\pi x}{l} dx = 1$$

From above expression, $A = \sqrt{\frac{2}{l}}$

Then

$$\Psi_n = \sqrt{\frac{2}{l}} \sin \frac{\pi x}{l}$$

2.6 Obtain the expectation value of x and p_x for the wave function given above numerical problem 2.5.

$$\text{Hint : } \langle x \rangle = \int_{-\infty}^{+\infty} x |\psi|^2 dx = \frac{2}{l} \int_0^l x \sin \frac{\pi x}{l} dx = \frac{a}{l}$$

$$\text{and } \langle p_x \rangle = \int_{-\infty}^{+\infty} \psi^* \left(-ik \frac{\partial}{\partial x} \right) \psi = -\hbar \frac{2\pi}{l^2} \int_0^l \sin \frac{\pi x}{l} \cos \frac{\pi x}{l} dx = 0$$

2.7 An eigen-function of an operator $\frac{d^2}{dx^2}$ is $\psi = e^{\alpha x}$. Find the corresponding eigen value.

[IGGSIPU, May 2016 (2.5 marks)]

$$\text{Hint : } G = \frac{d^2}{dx^2}; \quad G\psi = \frac{d^2}{dx^2}(e^{\alpha x}) = \frac{d}{dx} \left[\frac{d}{dx} e^{\alpha x} \right] = \frac{d}{dx} (\alpha e^{\alpha x}) = a^2 e^{\alpha x}$$

$$\text{But } e^{\alpha x} = \psi \quad \therefore \quad G\psi = a^2 \psi$$

Hence eigen value $G = a^2$.

2.8 An electron is in a box of 0.01 nm. Find its permitted energy.

[IGGSIPU, Feb. 2013, (2 marks); May 2008 (2.5 marks)]

$$\text{Hint : } E_n = \frac{n^2 h^2}{8ml^2} = \frac{n^2 \times (6.626 \times 10^{-34})^2}{8 \times 9.1 \times 10^{-31} \times (0.01 \times 10^{-9})^2}$$

$$= 6 \times 10^{-16} n^2 \text{ J} = \frac{6 \times 10^{-16}}{1.6 \times 10^{-19}} \text{ eV} = \frac{60000}{16} n^2 \text{ eV}$$

For $n = 1, 2, 3, \dots$ the energy eigen value E_1, E_2, E_3, \dots
 $E_1 = 3750 \text{ eV}, \quad E_2 = 15000 \text{ eV}, \quad E_3 = 33750 \text{ eV}, \dots$

- 2.9 Consider a particle confined in one-dimensional box of width l . Find the probability that the particle is found between $x = 0$ and $x = l/n$ when it is in n th state.

[GGSIPU, April 2015 (2 marks)]

Hint : $\psi_n(x) = \sqrt{\frac{2}{l}} \sin \frac{n\pi x}{l}$

$$\begin{aligned} p &= \int_{x_1}^{x_2} |\psi_n(x)|^2 dx = \frac{2}{l} \int_{x_1}^{x_2} \sin^2 \frac{n\pi x}{l} dx \\ &= \left[\frac{x}{l} - \frac{1}{2n\pi} \sin \frac{2n\pi x}{l} \right]_{x_1=0}^{x_2=l/n} = \left[\frac{1}{n} - \frac{1}{2n\pi} \sin \frac{2n\pi l}{nl} \right] = \frac{1}{n}. \end{aligned}$$

- 2.10 An electron is constrained to move in a one dimensional box of length 0.1 nm. Find the first three energy eigen values and the corresponding de Broglie wavelengths.

[GGSIPU, May 2015 (4 marks)]

Hint : $E_n = \frac{n^2 h^2}{8ml^2} \Rightarrow E_n = \frac{n^2 \times (6.623 \times 10^{-34})^2}{8 \times (9.1 \times 10^{-31}) \times (0.1 \times 10^{-9})^2}$

$$E_n = \frac{n^2 \times (6.623 \times 10^{-34})^2}{8 \times (9.1 \times 10^{-31}) \times (0.1 \times 10^{-9})^2 \times (1.6 \times 10^{-19})} \text{ eV} = 37.5 n^2 \text{ eV}$$

Then $E_1 = 37.5 \text{ eV}, E_2 = 150 \text{ eV}, E_3 = 337.5 \text{ eV}$

For de Broglie wavelength $\lambda_n = \frac{h}{\sqrt{2mE_n}}$

- 2.11 Find the probability that a particle trapped in a box 'L' wide can be found between 0.45 L and 0.55 L for the first excited state.

[GGSIPU, May 2015 (4 marks)]

Hint : $\psi_n = \sqrt{\frac{2}{l}} \sin \frac{n\pi x}{l}; P = \int_{x_1}^{x_2} |\psi_n(x)|^2 dx = \frac{2}{l} \int_{x_1}^{x_2} \sin^2 \frac{n\pi x}{l} dx$

$$= \left[\frac{x}{l} - \frac{1}{2n\pi} \sin \frac{2n\pi x}{l} \right]_{x_1}^{x_2}$$

Now $x_1 = 0.45 L$ and $x_2 = 0.55 L$ and $n = 2$ for first excited state, on solving it we get $P = 9.8\%$.

- 2.12 The wave function for a particle in a 1-D box is given by $\psi(x) = \sqrt{\frac{2}{a}} \sin \frac{m\pi x}{a}$. Show that the wave function for two different states are orthonormal.

Hint : For the eigenfunctions in the m th and n th states, $m \neq n$, to be orthogonal, we must have

$$\int_{-\infty}^{\infty} \psi_m^* \psi_n dx = 0$$

For the given wavefunction, $\psi_m(x) = \sqrt{\frac{2}{a}} \sin \frac{m\pi x}{a}$, then $\psi_n(x) = \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a}$

$$\int_{-\infty}^{\infty} \psi_m^* \psi_n dx = \frac{2}{a} \int_0^a \sin \frac{m\pi x}{a} \sin \frac{n\pi x}{a} dx$$

Therefore $= \frac{2}{a} \left[\int_0^a \cos \frac{(m-n)\pi x}{a} dx - \int_0^a \cos \frac{(m+n)\pi x}{a} dx \right]$