Wave Properties of Particles. Schrodinger Equation (Part - 1)

Q.49. Calculate the de Broglie wavelengths of an electron, proton, and uranium atom, all having the same kinetic energy 100 eV.

Ans. The kinetic eneigy is nonrelativistic in all three cases. Now

$$\lambda = \frac{2\pi\hbar}{p} = \frac{2\pi\hbar}{\sqrt{2mT}}$$

using $T = 1{\cdot}602 \times 10^{-17}$ Joules, we get

$\lambda_e = 122.6$ pm

$\lambda_p = 2.86$ pm

$$\lambda_U = \frac{\lambda_p}{\sqrt{238}} = 0{\cdot}185 \text{ pm}$$

(where we have used a mass number of 238 for the U nucleus).

Q.50. What amount of energy should be added to an electron to reduce its de Broglie wavelength from 100 to 50 pm?

Ans. From

$$\lambda = \frac{2\pi\hbar}{p} = \frac{2\pi\hbar}{\sqrt{2mT}}$$

we find $T = \frac{4\pi^2\hbar^2}{2m\lambda^2} = \frac{2\pi^2\hbar^2}{m\lambda^2}$

Thus $T_2 - T_1 = \frac{2\pi^2\hbar^2}{m}\left(\frac{1}{\lambda_2^2} - \frac{1}{\lambda_1^2}\right)$

Substitution gives $\Delta T = 451 \text{ eV} = 0{\cdot}451 \text{ keV}.$

Q.51. A neutron with kinetic energy T = 25 eV strikes a stationary deuteron (heavy hydrogen nucleus). Find the de Broglie wavelengths of both particles in the frame of their centre of inertia.

Ans. We shall use $M_0 = 2M_n$. The CM is moving with velocity

$$V = \frac{\sqrt{2 M_n T}}{3 M_n} = \sqrt{\frac{2T}{9 M_n}}$$

with respect to the Lab frame. In the CM frame the velocity of neutron is

$$v'_n = v_n - V = \sqrt{\frac{2T}{M_n}} - \sqrt{\frac{2T}{9 M_n}} = \sqrt{\frac{2T}{M_n}} \cdot \frac{2}{3}$$

and $$\lambda'_n = \frac{2\pi\hbar}{M_n v'_n} = \frac{3\pi\hbar}{\sqrt{2 M_n T}}$$

Substitution gives $\lambda'_n = 8{\cdot}6 \text{ pm}$
Since the momenta are equal in the CM frame the de Broglie wavelengths will also be

equal. If we do not assume $M_d = 2M_n$ we shall get

$$\lambda'_n = \frac{2\pi\hbar(1 + M_n/M_d)}{\sqrt{2 M_n T}}$$

Q.52. Two identical non-relativistic particles move at right angles to each other, possessing de Broglie wavelengths λ_1 and λ_2. Find the de Broglie wavelength of each particle in the frame of their centre of inertia.

Ans. If $\vec{p_1}, \vec{p_2}$ are the momenta of the two particles then their momenta in the CM frame will be

$\pm(\vec{p_1} - \vec{p_2})/2$ as the particle are identical.

Hence their de Broglie wavelength will be

$$\lambda = \frac{2\pi\hbar}{\frac{1}{2}|\vec{p_1} - \vec{p_2}|} = \frac{4\pi\hbar}{\sqrt{p_1^2 + p_2^2}} \quad (\text{because } \vec{p_1} \perp \vec{p_2})$$

$$= \frac{2}{\sqrt{\frac{1}{\lambda_1^2} + \frac{1}{\lambda_2^2}}} = \frac{2\lambda_1\lambda_2}{\sqrt{\lambda_1^2 + \lambda_2^2}}$$

Q.53. Find the de Broglie wavelength of hydrogen molecules, which corresponds to their most probable velocity at room temperature.

Ans. In thermodynamic equilibrium, Maxwell's velocity distribution law holds :

$$dN(v) = \Phi(v)\,dv = A v^2 e^{-mv^2/2kT}\,dv$$

φ (v) is maximum when

$$\Phi'(v) = \Phi(v)\left[\frac{2}{v} - \frac{mv}{kT}\right] = 0$$

The difines the most probable velocity,

$$v_{pr} = \sqrt{\frac{2kT}{m}}$$

The de Broglie wavelength of H molecules with the most probable velocity is

$$\lambda = \frac{2\pi\hbar}{m v_{pr}} = \frac{2\pi\hbar}{\sqrt{2mkT}}$$

Substituting the appropriate value especially

$m = m_{H_2} = 2m_H,\ T = 300\,K,$ we get

$\lambda = 126$ pm

Q.54. Calculate the most probable de Broglie wavelength of hydrogen molecules being in thermodynamic equilibrium at room temperature.

Ans. To find the most probable de Broglie wavelength of a gas in thermodynamic equilibrium we determine the distribution is λ corresponding to Maxwellian velocity distribution.

It is given by

$$\psi(\lambda)\,d\lambda = -\Phi(v)\,dv$$

(where - sign takes account of the fact that λ decreaes as v increases). Now

$$\lambda = \frac{2\pi\hbar}{mv} \text{ or } v = \frac{2\pi\hbar}{m\lambda}$$

$$dv = -\frac{2\pi\hbar}{m\lambda^2}d\lambda$$

Thus $\Psi(\lambda) = +A v^2 e^{-mv^2/2kT}\left(-\frac{dv}{d\lambda}\right)$

$$= A\left(\frac{2\pi\hbar}{m\lambda}\right)^2\left(\frac{2\pi\hbar}{m\lambda^2}\right)e^{-\frac{m}{2kT}\cdot\left(\frac{2\pi\hbar}{m\lambda}\right)^2}$$

$$= \text{Const}\cdot\lambda^{-4}e^{-a/\lambda^2}$$

where $a = \frac{2\pi^2\hbar^2}{mkT}$

This is maximum when

$$\psi'(\lambda) = 0 = \psi(\lambda)\left[\frac{-4}{\lambda} + \frac{2a}{\lambda^3}\right]$$

or $\lambda_{pr} = \sqrt{a/2} = \pi\hbar/\sqrt{mkT}$

Using the result of the previous problem it is

$$\lambda_{pr} = \frac{126}{\sqrt{2}}\text{ pm} = 89{\cdot}1\text{ pm}.$$

Q.55. Derive the expression for a de Broglie wavelength λ of a relativistic particle moving with kinetic energy T. At what values of T does the error in determining λ using the non-relativistic formula not exceed 1% for an electron and a proton?

Ans. For a relativistic particle

$$T + mc^2 = \text{total energy} = \sqrt{c^2p^2 + m^2c^4}$$

Squaring $\sqrt{T(T+2mc^2)} = cp$

Hence $\lambda = \dfrac{2\pi\hbar c}{\sqrt{T(T+2mc^2)}}$

$$= \frac{2\pi\hbar}{\sqrt{2mT\left(1+\dfrac{T}{2mc^2}\right)}}$$

If we use nonrelativistic formula,

$$\lambda_{NR} = \frac{2\pi\hbar}{\sqrt{2mT}}$$

SO $\dfrac{\Delta\lambda}{\lambda} = \dfrac{\lambda_{NR}-\lambda}{\lambda_{NR}} = \dfrac{T}{4mc^2}$

$$\left(\text{If } T/2mc^2 << 1\text{, we can write } \left(1+\frac{T}{2mc^2}\right)^{-1/2} = 1-\frac{T}{4mc^2}\right)$$

Thus $T \leq \dfrac{4mc^2\Delta\lambda}{\lambda}$ i,f the error is less than Δλ

For electron the error is not more than 1 % if

$$T \leq 4 \times 0{\cdot}511 \times {\cdot}01 \text{ MeV}$$
$$\leq 20{\cdot}4 \text{ keV}$$

For a proton, the error is not more than 1 % if

$T \leq 4$ X 938 X 0.01 MeV

i.e. $T \leq 37.5$ MeV.

Q.56. At what value of kinetic energy is the de Broglie wavelength of an electron equal to its Compton wavelength?

Ans. The de Broglie wavelength is

$$\lambda_{dB} = \frac{\frac{2\pi\hbar}{m_0 v}}{\sqrt{1 - v^2/c^2}} = \frac{2\pi\hbar}{m_0 v}\sqrt{1 - v^2/c^2}$$

and the Compton wavelength is

$$\lambda_c = \frac{2\pi\hbar}{m_0 c}$$

The two are equal if $\beta = \sqrt{1 - \beta^2}$, where $\beta = \frac{v}{c}$

or $\beta = \frac{1}{\sqrt{2}}$

The corresponding kinetic energy is

$$T = \frac{m_0 c^2}{\sqrt{1 - \beta^2}} - m_0 c^2 = \left(\sqrt{2} - 1\right) m_0 c^2$$

Here m_0 is the rest mass of the particle (here an electron).

Q.57. Find the de Broglie wavelength of relativistic electrons reaching the anticathode of an X-ray tube if the short wavelength limit of the continuous X-ray spectrum is equal to λ_{sh}= 10.0 pm?

Ans. For relativistic electrons, the formula for the short wavelength limit of X - rays will be

$$\frac{2\pi\hbar c}{\lambda_{sh}} = m_0 c^2\left(\frac{1}{\sqrt{1 - \beta^2}} - 1\right) = c\sqrt{p^2 + m^2 c^2} - m c^2$$

or $\left(\frac{2\pi\hbar}{\lambda_{sh}} + m c\right)^2 = p^2 + m^2 c^2$

or $\left(\frac{2\pi\hbar}{\lambda_{sh}}\right)\left(\frac{2\pi\hbar}{\lambda_{sh}} + 2 m c\right) = p^2$

or $p = \frac{2\pi\hbar}{\lambda_{sh}}\sqrt{1 + \frac{m c \lambda_{sh}}{\pi\hbar}}$

Hence $\lambda_{dB} = \lambda_{sh} \Big/ \sqrt{1 + \frac{m c \lambda_{sh}}{\pi \hbar}} = 3{\cdot}29 \text{ pm}$

Q.58. A parallel stream of monoenergetic electrons falls normally on a diaphragm with narrow square slit of width b = 1.0 µm. Find the velocity of the electrons if the width of the central diffraction maximum formed on a screen located at a distance l = 50 cm from the slit is equal to Δx = 0.36 mm.

Ans. he first minimum in a Fraunhofer diffraction is given by (b is the width of the slit)

$$b \sin \theta = \lambda$$

Here

$$\sin \theta = \frac{\Delta x/2}{\sqrt{l^2 + \left(\frac{\Delta x}{2}\right)^2}} \approx \frac{\Delta x}{2l}$$

Thus $\lambda = \frac{b \Delta x}{2l} = \frac{2\pi\hbar}{m v}$

so $v = \frac{4\pi\hbar l}{m b \Delta x} = 2{\cdot}02 \times 10^6 \text{ m/s}$

Q.59. A parallel stream of electrons accelerated by a potential difference V = 25 V falls normally on a diaphragm with two narrow slits separated by a distance d = 50µm. Calculate the distance between neighbouring maxima of the diffraction pattern on a screen located at a distance l = 100 cm from the slits.

Ans. From the Young slit foimula

$$\Delta x = \frac{l\lambda}{d} = \frac{l}{d} \cdot \frac{2\pi\hbar}{\sqrt{2meV}}$$

Substitution gives

$$\Delta x = 4{\cdot}90 \ \mu\text{m}.$$

Q.60. A narrow stream of monoenergetic electrons falls at an angle of incidence θ = 30° on the natural facet of an aluminium single crystal. The distance between the neighbouring crystal planes parallel to that facet is equal to d = 0.20 nm. The maximum mirror reflection is observed at a certain accelerating voltage V_0. Find

V_0, if the next maximum mirror reflection is known to be observed when the accelerating voltage is increased η = 2.25 times.

Ans. From Bragg's law, for the first case

$$2d\sin\theta = n_0\lambda = n_0\frac{2\pi\hbar}{\sqrt{2meV_0}}$$

where n_0 is an unknown integer/For the next higher voltage

$$2d\sin\theta = (n_0+1)\frac{2\pi\hbar}{\sqrt{2me\eta V_0}}$$

Thus $$n_0 = \frac{n_0+1}{\sqrt{\eta}}$$

or $$n_0\left(1-\frac{1}{\sqrt{\eta}}\right) = \frac{1}{\sqrt{\eta}} \quad \text{or} \quad n_0 = \frac{1}{\sqrt{\eta}-1}$$

Going back we get

$$V_0 = \frac{\pi^2\hbar^2}{2med^2\sin^2\theta}\frac{1}{\left(\sqrt{\eta}-1\right)^2} = 0{\cdot}150\text{ keV}$$

Note : In the Bragg's formula, θ is the glancing angle and not the angle of incidence. We have obtained correct result by taking θ to be the glancing angle. If θ is the angle of incidence, then the glancing angle will be 90 - θ. Then the final answer will be smaller

by a factor $$\tan^2\theta = \frac{1}{3}.$$

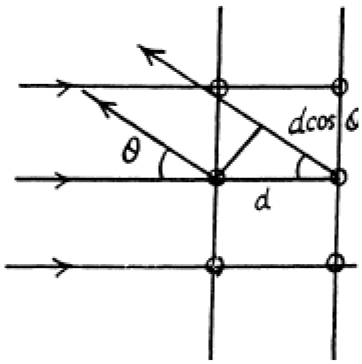
Q.61. A narrow beam of monoenergetic electrons falls normally on the surface of a Ni single crystal. The reflection maximum of fourth order is observed in the direction forming an angle θ = 55° with the normal to the surface at the energy of the electrons equal to T = 180 eV. Calculate the corresponding value of the interplanar distance.

Ans. Path difference is

$$d + d\cos\theta = 2d\cos^2\frac{\theta}{2}.$$

Thus for reflection maximum of the k[th] order

$$2d\cos^2\frac{\theta}{2} = k\lambda = k\frac{2\pi\hbar}{\sqrt{2mT}}$$



Hence $$d = \frac{k\pi\hbar}{\sqrt{2mT}}\,\mathrm{Sec}^2\frac{\theta}{2}.$$

substitution with k = 4gives

d = 0.232

Q.62. A narrow stream of electrons with kinetic energy T = 10 keV passes through a polycrystalline aluminium foil, forming a system of diffraction fringes on a screen. Calculate the interplanar distance corresponding to the reflection of third order from a certain system of crystal planes if it is responsible for a diffraction ring of diameter D = 3.20 cm. The distance between the foil and the screen is l = 10.0 cm.

Ans. See the analogous problem with X - rays (5.156). The glancing angle is obtained from

$$\tan 2\theta = \frac{D}{2l}$$

where D = diameter of the ring, l = distance from the foil to the screen.

Then for the third order Bragg reflection

$$2d\sin\theta = k\lambda = k\frac{2\pi\hbar}{\sqrt{2mT}}, (k = 3)$$

Thus $$d = \frac{\pi\hbar k}{\sqrt{2mT}\sin\theta} = 0{\cdot}232\ \mathrm{nm}$$

Q.63. A stream of electrons accelerated by a potential difference V falls on the surface of a metal whose inner potential is V_1 = 15 V. Find:
(a) the refractive index of the metal for the electrons accelerated by a potential difference V = 150 V;
(b) the values of the ratio V/V_t at which the refractive index differs from unity by not more than η = 1.0%.

Ans. Inside the metal, there is a negative potential energy of - eV_i}. (This potential energy prevents electrons from leaking out and can be measured in photoelectric effect etc.) An electron whose K.E. is eV outside the metal w ill find its K.E. increased to e $(V + V_i)$ in th e metal. Then

(a) de Broglie wavelength in the metal

$$= \lambda_m = \frac{2\pi\hbar}{\sqrt{2me(V+V_i)}}$$

Also de Broglie wavelength in vacuum

$$= \lambda_0 = \frac{2\pi\hbar}{\sqrt{2mVe}}$$

Hence refractive index $n = \frac{\lambda_0}{\lambda_m} = \sqrt{1+\frac{V_i}{V}}$

Substituting we get $n = \sqrt{1+\frac{1}{10}} \simeq 1{\cdot}05$

$$\text{(b)} \quad n - 1 = \sqrt{1+\frac{V_i}{V}} - 1 \le \eta$$

then $1 + \frac{V_i}{V} \le (1+\eta)^2$

or $V_i \le \eta(2+\eta)V$

or $\frac{V}{V_i} \ge \frac{1}{\eta(2+\eta)}$

For $\eta = 1\% = 0{\cdot}01$

we get $\frac{V}{V_i} \geq 50$

Q.64. A particle of mass m is located in a unidimensional square potential well with infinitely high walls. The width of the well is equal to l. Find the permitted values of energy of the particle taking into account that only those states of the particle's motion are realized for which the whole number of de Broglie half-waves are fitted within the given well.

Ans. The energy inside the well is all kinetic if energy is measured from the value inside.

We require

$$l = n\lambda/2 = n\frac{\pi\hbar}{\sqrt{2mE}}$$

or $$E_n = \frac{n^2\pi^2\hbar^2}{2ml^2}, \; n = 1, 2, \ldots$$

Q.65. Describe the Bohr quantum conditions in terms of the wave theory: demonstrate that an electron in a hydrogen atom can move only along those round orbits which accommodate a whole number of de Broglie waves.

Ans. The Bohr condition

$$\oint p\,dx = \oint \frac{2\pi\hbar}{\lambda}\,dx = 2\pi n\hbar$$

For the case when λ is constant (for example in circular orbits) this means

2nr = nλ

Here r is the radius of the circular orbit.

Wave Properties of Particles. Schrodinger Equation (Part - 2)

Q.66. Estimate the minimum errors in determining the velocity of an electron, a proton, and a ball of mass of 1 mg if the coordinates of the particles and of the centre of the ball are known with uncertainly 1µm.

Ans. From the uncertainty principle (Eqn. (6.2b))

$$\Delta x \Delta p_x \gtrsim \hbar$$

Thus $\Delta p_x = m \Delta v_x \gtrsim \dfrac{\hbar}{\Delta x}$

Or $\Delta v_x \gtrsim \dfrac{\hbar}{m \Delta x}$

For an electron this means an uncertainty in velocity of 116 m/s if $\Delta x = 10^{-6} \mathrm{m} = 1 \mu \mathrm{m}$

For a proton $\Delta v_x = 6.3$ cm/s

For a ball $\Delta v_x = 1 \times 10^{-20}$cm/s

Q.67. Employing the uncertainty principle, evaluate the indeterminancy of the velocity of an electron in a hydrogen atom if the size of the atom is assumed to be l = 0.10 nm. Compare the obtained magnitude with the velocity of an electron in the first Bohr orbit of the given atom.

Ans. As in the previous problem

$$\Delta v \lesssim \frac{\hbar}{m l} = 1{\cdot}16 \times 10^6 \mathrm{m/s}$$

The actual velocity v_1 has been calculated in problem 6.21. It is

$v_1 = 2.21 \times 10^6$ m/s

Thus $\Delta v \sim v_1$ (They are of the same order of magnitude)

Q.68. Show that for the particle whose coordinate uncertainty is Δx = λ/2π, where λ is its de Broglie wavelength, the velocity uncertainty is of the same order of magnitude as the particle's velocity itself.

Ans. If $\Delta x = \lambda/2\pi = \frac{2\pi\hbar}{p} \cdot \frac{1}{2\pi} = \frac{\hbar}{p} = \frac{\hbar}{m v}$

Thus $\Delta v \gtrsim \frac{\hbar}{m \Delta x} = v$

Thus Δv is of the same order as v.

Q.69. A free electron was initially confined within a region with linear dimensions l = 0.10 nm. Using the uncertainty principle, evaluate the time over which the width of the corresponding train of waves becomes η = 10 times as large.

Ans. Initial uncertainty $\Delta v \lesssim \frac{\hbar}{m l}$. With this incertainty the wave train will spread out to a distance **ηl**long in time

$$t_0 \approx \eta l \Big/ \frac{\hbar}{m l} \approx \frac{\eta m l^2}{\hbar} \text{sec.} = 8{\cdot}6 \times 10^{16} \text{ sec.} \sim 10^{-15} \text{ sec.}$$

Q.70. Employing the uncertainty principle, estimate the minimum kinetic energy of an electron confined within a region whose size is l = 0.20 nm.

Ans. Clearly $\Delta x \leq l$ so $\Delta p_x \geq \frac{\hbar}{l}$

Now $p_x \geq \Delta p_x$ and so

$$T = \frac{p_x^2}{2m} \geq \frac{\hbar^2}{2 m l^2}$$

Thus $T_{\min} = \frac{\hbar^2}{2 m l^2} \simeq 0{\cdot}95 \text{ eV}.$

Q.71. An electron with kinetic energy T ≈ 4 eV is confined within a region whose linear dimension is l = 1 µm. Using the uncertainty principle, evaluate the relative uncertainty of its velocity.

Ans. The momentum the electron is $\Delta p_x = \sqrt{2 m T}$

Uncertainty in its momentum is

$$\Delta p_x \geq \hbar / \Delta x = \hbar / l$$

Hence relative uncertainty

$$\frac{\Delta p_x}{p_x} = \frac{\hbar}{l\sqrt{2mT}} = \sqrt{\frac{\hbar^2}{2ml^2} \Big/ T} = \frac{\Delta v}{v}$$

Substitution gives

$$\frac{\Delta v}{v} = \frac{\Delta p}{p} = 9{\cdot}75 \times 10^{-5} \approx 10^{-4}$$

Q.72. An electron is located in a unidimensional square potential well with infinitely high walls. The width of the well is l. From the uncertainty principle estimate the force with which the electron possessing the minimum permitted energy acts on the walls of the well.

Ans. By uncertainty principle, the uncertainty in momentum

$$\Delta p \geq \frac{\hbar}{l}$$

For the ground state, we expect $\Delta p \sim p$ so

$$E \sim \frac{\hbar^2}{2ml^2}$$

The force excerted on the wall can be obtained most simply from

$$F = -\frac{\partial U}{\partial l} = \frac{\hbar^2}{ml^3}.$$

Q.73. A particle of mass m moves in a unidimensional potential field U = $kx^2/2$ (harmonic oscillator). Using the uncertainty principle, evaluate the minimum permitted energy of the particle in that field.

Ans. We write

$$p \sim \Delta p \sim \frac{\hbar}{\Delta x} \sim \frac{\hbar}{x}$$

i.e. all four quantities are of the same order of magnitude. Then

$$E \approx \frac{\hbar^2}{2mx^2} + \frac{1}{2}kx^2 = \frac{1}{2m}\left(\frac{\hbar}{x} - \sqrt{mk}\,x\right)^2 + \hbar\sqrt{\frac{k}{m}}$$

Thus we get an equilibrium situation (E = minimum) when

$$x = x_0 = \sqrt{\frac{\hbar}{\sqrt{mk}}}$$

and then $E = E_0 \sim \hbar\sqrt{\frac{k}{m}} = \hbar\omega$

Quantum mechanics gives

$$E_0 = \hbar\omega/2$$

Q.74. Making use of the uncertainty principle, evaluate the minimum permitted energy of an electron in a hydrogen atom and its corresponding apparent distance from the nucleus.

Ans. Hence we write

$$r \sim \Delta r,\ p \sim \Delta p \sim \hbar/\Delta r$$

Then

$$E = \frac{\hbar^2}{2mr^2} - \frac{e^2}{r}$$

$$= \frac{1}{2m}\left(\frac{\hbar}{r} - \frac{me^2}{\hbar}\right)^2 - \frac{me^4}{2\hbar^2}$$

Hence $r_{eff} = \frac{\hbar^2}{me^2} = 53\ \text{pm}$ for the equilibrium state.

and then $E = -\frac{me^4}{2\hbar^2} = -13{\cdot}6\ \text{eV}.$

Q.75. A parallel stream of hydrogen atoms with velocity v = 600 m/s falls normally on a diaphragm with a narrow slit behind which a screen is placed at a distance l = 1.0 m. Using the uncertainty principle, evaluate the width of the slit S at which the width of its image on the screen is minimum.

Ans. Suppose the width of the slit (its extension along they - axis) is δ. Then each electron has an uncertainty $\Delta y \sim \delta.$ This translates to an uncertainty

$\Delta p_y \sim \hbar/\delta.$ We must therefore have

$$p_y \gtrsim \hbar/\delta .$$

For the image, hrodening has two sources.
We write

$$\Delta(\delta) = \delta + \Delta'(\delta)$$

where **Δ**' is the width caused by the spreading of electrons due to their transverse momentum.

We have

$$\Delta' = v_y \frac{l}{v_x} = p_y \frac{l}{p} = \frac{l\hbar}{m v \delta}$$

Thus

$$\Delta(\delta) = \delta + \frac{l\hbar}{m v \delta}$$

For large $\delta, \Delta(\delta) \sim \delta$ and quantum effect is unimportant. For small δ, quantum effects are large. But A (δ) is minimum when

$$\delta = \sqrt{\frac{l\hbar}{m v}}$$

as we see by completing the square. Substitution gives
$\delta = 1{\cdot}025 \times 10^{-5}\,\mathrm{m} = 0{\cdot}01\,\mathrm{mm}$

Q.76. Find a particular solution of the time-dependent Schrodinger equation for a freely moving particle of mass m.

Ans. The Schrodinger equation in one dimension for a free particle is

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2}$$

we write $\psi(x,t) = \varphi(x)\,\chi(t)$. Then

$$\frac{i\hbar}{\chi} \frac{d\chi}{dt} = -\frac{\hbar^2}{2m} \frac{1}{\varphi} \frac{d^2 \varphi}{dx^2} = E\text{, say}$$

Then $\chi(t) \sim \exp\left(-\frac{iEt}{h}\right)$

$$\varphi(x) \sim \exp\left(i\frac{\sqrt{2mE}}{\hbar}x\right)$$

E must be real and positive if φ(x) is to be bounded everywhere. Then

$$\psi(x,t) = \text{Const } \exp\left(\frac{i}{\hbar}\left(\sqrt{2mE}\,x - Et\right)\right)$$

This particular solution describes plane waves.

Q.77. A particle in the ground state is located in a unidimensional square potential well of length 1 with absolutely impenetrable walls (0 < x < l). Find the probability of the particle staying within a region $\frac{1}{3}l \leqslant x \leqslant \frac{2}{3}l.$

Ans. We look for the solution of Schrodinger eqn. with

$$-\frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2} = E\psi,\ 0 \le x \le l \qquad (1)$$

The boundary condition of impenetrable walls means

$$\psi(x) = 0 \text{ for } x = 0 \text{ and } x = l$$
$$(\text{as } \psi(x) = 0 \text{ for } x < 0 \text{ and } x > l,)$$

The solution of (1) is

$$\psi(x) = A \sin \frac{\sqrt{2mE}}{\hbar} x + B \cos \frac{\sqrt{2mE}}{\hbar} \cdot x$$

Then $\psi(0) = 0 \Rightarrow B = 0$

$$\psi(l) = 0 \Rightarrow A \sin \frac{\sqrt{2mE}}{\hbar} l = 0$$

A = 0 so

$$\frac{\sqrt{2mE}}{\hbar} l = n\pi$$

Hence $E_n = \dfrac{n^2 \pi^2 \hbar^2}{2ml^2}$, $n = 1, 2, 3, \ldots$

Thus the ground state wave function is

$$\psi(x) = A \sin \frac{\pi x}{l}.$$

We evaluate A by nomalization

$$1 = A^2 \int_0^l \sin^2 \frac{\pi x}{l} \, dx = A^2 \frac{l}{\pi} \int_0^\pi \sin^2 \theta \, d\theta = A^2 \frac{l}{\pi} \cdot \frac{\pi}{2}$$

Thus $A = \sqrt{\dfrac{2}{l}}$

Finally, the probability P for the particle to lie in $\dfrac{l}{2} \le x \le \dfrac{2l}{3}$ is

$$P = P\left(\frac{l}{3} \le x \le \frac{2l}{3}\right) = \frac{2}{l} \int_{\frac{l}{3}}^{2l/3} \sin^2 \frac{\pi x}{l} \, dx$$

$$= \frac{2}{\pi} \int_{\pi/3}^{2\pi/3} \sin^2 \theta \, d\theta = \frac{1}{\pi} \int_{\pi/3}^{2\pi/3} (1 - \cos 2\theta) \, d\theta$$

$$= \frac{1}{\pi} \left(\theta - \frac{1}{2} \sin 2\theta\right)_{\pi/3}^{2\pi/3}$$

$$= \frac{1}{\pi}\left(\frac{2\pi}{3} - \frac{\pi}{3} - \frac{1}{2}\sin\frac{4\pi}{3} + \frac{1}{2}\sin\frac{2\pi}{3}\right)$$

$$= \frac{1}{\pi}\left(\frac{\pi}{3} + \frac{1}{2}\frac{\sqrt{3}}{2} + \frac{1}{2}\frac{\sqrt{3}}{2}\right) = \frac{1}{3} + \frac{\sqrt{3}}{2\pi} = 0{\cdot}609$$

Q.78. A particle is located in a unidimensional square potential well with infinitely high walls. The width of the well is 1. Find the normalized wave functions of the stationary states of the particle, taking the midpoint of the well for the origin of the x coordinate.

Ans.

Here $-\frac{l}{2} \le x \le \frac{l}{2}$. Again wc have

$$\psi(x) = B\cos\frac{\sqrt{2mE}\,x}{\hbar} + A\sin\frac{\sqrt{2mE}\,x}{\hbar}$$

Then the boundary condition $\psi\left(\pm\frac{l}{2}\right) = 0$

gives $B\cos\frac{\sqrt{2mE}\,l}{2\hbar} \pm A\sin\frac{\sqrt{2mE}\,l}{2\hbar} = 0$

There are two cases.

(1) $A = 0,\ \frac{\sqrt{2mE}\,l}{2\hbar} = n\pi + \frac{\pi}{2}$

gives even solution. Here

$$\sqrt{2mE} = (2n+1)\frac{\pi\hbar}{l}$$

and $E_n = (2n+1)^2\frac{\pi^2\hbar^2}{2ml^2}$

$$\psi_n^e(x) = \sqrt{\frac{2}{l}}\cos(2n+1)\frac{\pi x}{l}$$

n = 0 , 1 , 2 , 3 , . . .

This solution is even under x → - x .

(2) B = 0, $\frac{\sqrt{2mE}\, l}{2\hbar} = n\pi, \; n = 1, 2, \ldots$

$$E_n = (2n\pi)^2 \frac{\hbar^2}{2ml^2}$$

$\psi_n^0 = \sqrt{\frac{2}{l}} \sin\frac{2n\pi x}{l}, \; n = 1, 2, \ldots$ This solution is odd.

Q.79. Demonstrate that the wave functions of the stationary states of a particle confined in a unidimensional potential well with infinitely high walls are orthogonal, i.e. they satisfy the condition

$$\int_0^l \psi_n \psi_{n'}\, dx = 0 \text{ if } n' \neq n.$$

Here l is the width of the well, n are integers.

Ans. The wave function is given in 6.77. We see that

$$\int_0^l \psi_n(x)\, \psi_{n'}(x)\, dx$$

$$= \frac{2}{l}\int_0^l \sin\frac{n\pi x}{l} \sin\frac{n'\pi x}{l}\, dx$$

$$= \frac{1}{l}\int_0^l \left[\cos(n-n')\frac{\pi x}{l} - \cos(n+n')\frac{\pi x}{l}\right] dx$$

$$= \frac{1}{l}\left[\frac{\sin(n-n')\pi x/l}{(n-n')\frac{\pi}{l}} - \frac{\sin(n+n')\frac{\pi x}{l}}{(n+n')\frac{\pi x}{l}}\right]_0^l e.$$

If n = n', this is zero as n and n' are integers.

Q.80. An electron is located in a unidimensional square potential well with infinitely high walls. The width of the well equal to 1 is such that the energy levels are very dense. Find the density of energy levels dN/dE, i.e. their number per unit energy interval, as a function of E. Calculate dN/dE for E = 1.0 eV if l = 1.0 cm.

Ans.

We have found that $E_n = \frac{n^2 \pi^2 \hbar^2}{2 m l^2}$

Let N (E) = number of states upto E. This number is n. The number of states upto E +

dE is N(E + dE) = N(E) + d N (E) . Then dN (E) - 1 and

$$\frac{dN(E)}{dE} = \frac{1}{\Delta E}$$

where ΔE = difference in energies between the n^{th} & $(n + 1)^{th}$ level

$$= \frac{(n+1)^2 - n^2}{2 m l^2} \pi^2 \hbar^2 = \frac{2n+1}{2 m l^2} \pi^2 \hbar^2$$

$$= \frac{\pi^2 \hbar^2}{2 m l^2} 2n, \quad \text{(neglecting } 1 << n\text{)}$$

$$= \frac{\pi^2 \hbar^2}{2 m l^2} \times \sqrt{\frac{2 m l^2}{\pi^2 \hbar^2}} \sqrt{E} \times 2$$

$$= \frac{\pi \hbar}{l} \sqrt{\frac{2}{m}} \sqrt{E}$$

Thus

$$\frac{dN(E)}{dE} = \frac{l}{\pi \hbar} \sqrt{\frac{m}{2E}}.$$

\For the given case this gives $\frac{dN(E)}{dE} = 0{\cdot}816 \times 10^7$ levels per eV

Q.81. A particle of mass m is located in a two-dimensional square potential well with absolutely impenetrable walls. Find:
(a) the particle's permitted energy values if the sides of the well are l_1, and l_2;
(b) the energy values of the particle at the first four levels if the well has the shape of a square with side l.

Ans.

(a) Here the schroditiger equation is

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

we take the origin at one of the comers of the rectangle where the particle can lie. Then the wave function must vanish for

$$x = 0 \quad \text{or} \quad x = l_1$$

or $\quad y = 0$ or $y = l_2$.

we look for a solution in the form

$$\psi = A \sin k_1 x \sin k_2 y$$

cosines are not permitted by the boundary condition. Then

$$k_1 = \frac{n_i \pi}{l_1}, \quad k_2 = n_2 \frac{\pi}{l_2}$$

and
$$E = \frac{k_1^2 + k_2^2}{2m}\hbar^2 = \frac{\pi^2 \hbar^2}{2m}\left(\frac{n_1^2}{l_1^2}+\frac{n_2^2}{l_2^2}\right)$$

Here n_1, n_2 are nonzero integers,

(b) If $l_1 = l_2 = l$ then

$$\frac{E}{\hbar^2/m l^2} = \frac{n_1^2 + n_2^2}{2}\pi^2$$

1^{st} level : $n_1 = n_2 = 1 \rightarrow \pi^2 = 9{\cdot}87$

2nd level : $\left.\begin{matrix} n_1 = 1,\ n_2 = 2 \\ \text{or} \quad n_1 = 2,\ n_2 = 1 \end{matrix}\right\} \rightarrow \frac{5}{2}\pi^2 = 24{\cdot}7$

3rd level : $n_1 = 2, = n_2 = 2 \rightarrow 4\pi^2 = 39{\cdot}5$

4th level : $\left.\begin{matrix} n_1 = 1,\ n_2 = 3 \\ n_1 = 3,\ n_2 = 1 \end{matrix}\right\} \rightarrow 5\pi^2 = 49{\cdot}3$

Q.82. A particle is located in a two-dimensional square potential well with absolutely impenetrable walls (0 < x < a, 0 < y < b).
Find the probability of the particle with the lowest energy to be located within a region 0 < x < a/3.

Ans. The wave function for the ground state is

$$\psi_{11}(x, y) = A \sin\frac{\pi x}{a} \sin\frac{\pi y}{b}$$

we find A by normalization

$$1 = A^2 \int_0^a dx \int_0^d dy \sin^2\frac{\pi x}{a} \sin^2\frac{\pi y}{b} = A^2 \frac{ab}{4}$$

Thus $A = \frac{2}{\sqrt{ab}}$.

Then the requisite probability is

$$P = \int_0^{a/3} dx \int_0^b dy \frac{4}{ab} \sin^2\frac{\pi x}{a} \sin^2\frac{\pi y}{b}$$

$$= \frac{2}{a} \int_0^{a/3} dx \sin^2\frac{\pi x}{a}$$ on doing the y integral

$$= \frac{1}{a} \int_0^{a/3} d\left(1 - \cos\frac{2\pi x}{a}\right) = \frac{1}{a}\left(\frac{a}{3} - \frac{\sin\frac{2\pi}{3}}{2\pi/a}\right) = \frac{1}{3} - \frac{\sqrt{3}}{4\pi} = 0{\cdot}196 = 19{\cdot}6\,\%.$$

Wave Properties of Particles. Schrodinger Equation (Part - 3)

Q.83. A particle of mass m is located in a three-dimensional cubic potential well with absolutely impenetrable walls. The side of the cube is equal to a. Find:
(a) the proper values of energy of the particle;
(b) the energy difference between the third and fourth levels;
(c) the energy of the sixth level and the number of states (the degree of degeneracy) corresponding to that level.

Ans. We proceed axactly as in (6.81). The wave function is chosen in the form
$\psi(x, y, z)$ = A sin k_1x sin k_2 y sin k_3 z .

(The origin is at one comer of the box and the axes of coordinates are along the edges.)
The boundary conditions are that $\psi = 0$ for
x = 0, x = a, y = 0, y = a, z = 0, z = a

This gives

$$k_1 = \frac{n_1 \pi}{a},\ k_2 = \frac{n_2 \pi}{a},\ k_3 = \frac{n_3 \pi}{a}$$

The energy eigenvalues are

$$E(n_1,\ n_2,\ n_3) = \frac{\pi_2 \hbar^2}{2\, m\, a^2}\,(n_1^2 + n_2^2 + n_3)$$

The first level is (1, 1, 1). The second has (1, 1, 2), (1, 2, 1) & (2, 1, 1). The third level is (1, 2, 2) or (2, 1, 2) or (2, 2, 1). Its eneigy is

$$\frac{9\, \pi^2 \hbar^2}{2\, m\, a^2}$$

The fourth energy level is (1, 1, 3) or (1, 3, 1) or (3, 1, 1)

Its eneigy is $E = \frac{11\ \pi^2 \hbar^2}{2\, m\, a^2}$.

(b) Thus $\Delta = E_4 - E_3 = \frac{\hbar^2 \pi^2}{m a^2}$.

(c) The fifth level is (2, 2, 2). The sixth level is (1, 2, 3), (1, 3, 2), (2, 1, 3), (2, 3, 1), (3, 1, 2), (3, 2, 1)

Its eneigy is

$$\frac{7\hbar^2 \pi^2}{m a^2}$$

and its degree of degeneracy is 6 (six).

Q.84. Using the Schrodinger equation, demonstrate that at the point where the potential energy U (x) of a particle has a finite discontinuity, the wave function remains smooth, i.e. its first derivative with respect to the coordinate is continuous.

Ans. We can for definiteness assume that the discontinuity occurs at the point x = 0. Now the schrodinger equation is

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

We integrate this equation around x = 0 i.e., from $x = -\varepsilon_1$ to $x = +\varepsilon_2$ where $\varepsilon_1, \varepsilon_2$ are small positive numbers. Then

$$-\frac{\hbar^2}{2m}\int_{-\varepsilon_1}^{+\varepsilon_2} \frac{d^2\psi}{dx^2}\, dx = \int_{-\varepsilon_1}^{+\varepsilon_2} (E - U(x)\psi(x)\, dx$$

or $$\left(\frac{d\psi}{dx}\right)_{+\varepsilon_2} - \left(\frac{d\psi}{dx}\right)_{-\varepsilon_1} = -\frac{2m}{\hbar^2}\int_{-\varepsilon_1}^{\varepsilon_2} (E - U(x))_{dx}\ \psi(x)$$

Since the potential and the energy E are finite and ψ(x) is bounded by assumption, the integral on the right exists and $\rightarrow 0$ as $\varepsilon_1, \varepsilon_2 \rightarrow 0$

Thus $\left(\frac{d\psi}{dx}\right)_{+\varepsilon_2} = \left(\frac{d\psi}{dx}\right)_{-\varepsilon_1}$ as $\varepsilon_1, \varepsilon_2 \to 0$

So $\left(\frac{d\psi}{dx}\right)$ is continuous at x = 0 (the point where U (x) has a finite jump discontinuity.)

Q.85. A particle of mass m is located in a unidimensional potential field U (x) whose shape is shown in Fig. 6.2, where U (0) = ∞ . Find:

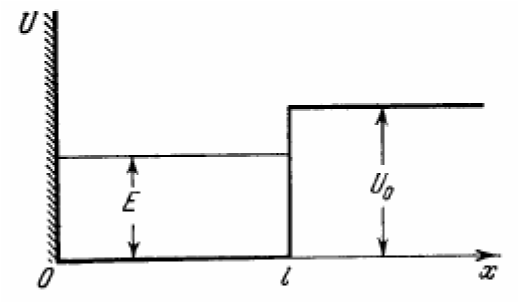


Fig. 6.2.

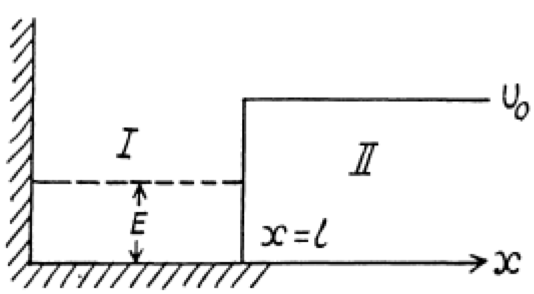
(a) the equation defining the possible values of energy of the particle in the region E < U_0; reduce that equation to the form

$\sin kl = \pm kl\sqrt{\hbar^2/2ml^2U_0},$

where $k = \sqrt{2mE}/\hbar$. **Solving this equation by graphical means, demonstrate that the possible values of energy of the particle form a discontinuous spectrum;**

(b) the minimum value of the quantity l^2U_0 at which the first energy level appears in the region E < U_0. At what minimum value of l^2U_0 does the nth level appear?

Ans.



(a) Starting from the Schrodinger equation in the regions l & II

$$\frac{d^2\psi}{dx^2} + \frac{2mE}{\hbar^2}\psi = 0 \quad x \text{ in } I \qquad (1)$$

$$\frac{d^2\psi}{dx^2} - \frac{2mE(U_0 - E)}{\hbar^2}\psi = 0 \quad x \text{ in } II \qquad (2)$$

where $U_0 > E > 0$, we easily derive the solutions in I & II

$$\Psi_I(x) = A\sin kx + B\cos kx \qquad (3)$$

$$\Psi_{II}(x) = Ce^{\alpha x} + De^{-\alpha x} \qquad (4)$$

where $k^2 = \frac{2mE}{\hbar^2},\ \alpha^2 = \frac{2m(U_0 - E)}{\hbar^2}.$

The boundary conditions are

$$\Psi(o) = 0 \qquad (5)$$

and $\Psi\ \&\ \left(\frac{d\psi}{dx}\right)$ are continuous at x = /, and ψ must vanish at x = + ∞ .

Then $\psi_I = A\sin kx$

and $\Psi_{II} = De^{-\alpha x}$

so $A\sin kl = De^{-\alpha l}$

$$kA\cos kl = -\alpha De^{-\alpha l}$$

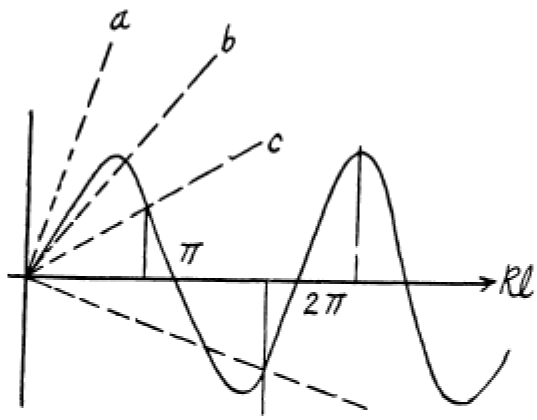
From this we get

$$\tan kl = -\frac{k}{\alpha}$$

or $\sin kl = \pm\, kl \Big/ \sqrt{k^2 l^2 + \alpha^2 l^2}$

$$= \pm\, kl \Big/ \sqrt{\frac{2mU_0 l^2}{\hbar^2}}$$

$$= \pm\, k\,l \sqrt{\hbar^2 / 2\,m\,U_0\,l^2} \quad (6)$$



Plotting the left and right sides of this equation we can find the points at which the straight lines cross the sine curve. The roots of the equation corresponding to the eigen values of energy E_i and found from the inter section points $(kl)_i$, for which tan $(kl)_i < 0$ (i.e. 2nd & 4th and other even quadrants). It ii seen that bound states do not always exist. For the first bound state to appear (refer to the line (b) above)

$$(k\,l)_{1,\,\min} = \frac{\pi}{2}$$

(b) Substituting, we get $(l^2 U_0)_{1,\min} = \dfrac{\pi^2 h^2}{8\,m}$

as the condition for the appearance of the first bound state. The second bound state will appear when Id is in the fourth quadrant The magnitude of the slope of the straight line must then be less than

$$\frac{1}{3\,\pi/2}$$

Corresponding to $(kl)_{2,\,\min} = \dfrac{3\,\pi}{2} = (3)\dfrac{\pi}{2} = (2 \times 2 - 1)\dfrac{\pi}{2}$

For n bound states, it is easy to convince one self that the slope of the appropriate

straight line (upper or lower) must be less than

$$(kl)_{n,\,\min} = (2n - 1)\frac{\pi}{2}$$

Then $(l^2U_0)_{n,\,\min} = \frac{(2n-1)^2\pi^2\hbar^2}{8m}$

Do not forget to note that for large n both + and - signs in the Eq. (6) contribute to solutions.

Q.86. Making use of the solution of the foregoing problem, determine the probability of the particle with energy E = U_0/2 to be located in the region $x > l,\ \text{if}\ l^2U_0 = \left(\frac{3}{4}\pi\right)^2\frac{\hbar^2}{m}.$

Ans.

$$U_0 l^2 = \left(\frac{3}{4}\pi\right)^2\frac{\hbar^2}{m}$$

and $$E\,l^2 = \left(\frac{3}{4}\pi\right)^2\frac{\hbar^2}{2m}$$

or $$k\,l = \frac{3}{4}\pi$$

It is easy to check that the condition of the boud state is satisfied. Also

$$\alpha\,l = \sqrt{\frac{2m}{\hbar^2}(U_0-E)\,l^2} = \sqrt{\frac{m\,U_0}{\hbar^2}l^2} = \frac{3}{4}\pi$$

Then from the previous problem

$$D = A\,e^{\alpha l}\sin k\,l = A\frac{e^{3\pi/4}}{\sqrt{2}}$$

By normalization

$$I = A^2\left[\int_0^l \sin^2 k\,x\,d\,x + \int_l^\infty \frac{e^{3\pi/2}}{2}\,e^{-(3\pi/2)x/l}\,d\,x\right]$$

$$= A^2\left[\frac{1}{2}\int_0^l (1-\cos 2kx)\,dx + l\int_0^\infty \frac{1}{2}e^{-\frac{3\pi}{2}y}\,dy\right]$$

$$= A^2\left[\frac{1}{2}\left[-\frac{\sin 2kl}{2k}\right] + \frac{1}{2}\cdot\frac{l}{\frac{3\pi}{2}}\right]$$

$$= A^2 l\left[\frac{1}{2}\left[1+\frac{1}{\frac{3\pi}{2}}\right] + \frac{1}{2}\,\frac{1}{\frac{3\pi}{2}}\right]$$

$$= A^2 l\left[\frac{1}{2}+\frac{2}{3\pi}\right] = A^2\frac{l}{2}\left(1+\frac{4}{3\pi}\right) \quad \text{or} \quad A = \sqrt{\frac{2}{l}}\left(1+\frac{4}{3\pi}\right)^{-1/2}$$

The probability of the particle to be located in the region x > l is

$$P = \int_l^\infty \psi^2\,dx = \frac{2}{l}\left(1+\frac{4}{3\pi}\right)^{-1}\int_l^\infty \frac{e^{3\pi/2}}{2}\,e^{-\frac{3\pi}{2}\frac{x}{l}}\,dx$$

$$= \left(1+\frac{4}{3\pi}\right)^{-1}\int_l^\infty e^{3\pi/2}\,e^{-(3\pi/2)y}$$

$$dy = \frac{2}{3\pi}\times\frac{3\pi}{3\pi+4} = 14{\cdot}9\,\%.$$

Q.87. Find the possible values of energy of a particle of mass m located in a spherically symmetrical potential well U (r) = 0 for r < r_o and U (r) = ∞ for r = r_0, in the case when the motion of the particle is described by a wave function ψ(r) depending only on r.
Instruction. When solving the Schrodinger equation, make the substitution ψ(r) = x (r)/r.

Ans. The Schrodinger equation is

$$\nabla^2\psi + \frac{2m}{\hbar^2}(E - U(r))\psi = 0$$

when ψ depends on r only, $\nabla^2 \psi = \frac{1}{r^2}\frac{d}{dr}\left(r^2 \frac{d\psi}{dr}\right)$

If we put $\psi = \frac{\chi(r)}{r},\ \frac{d\psi}{dr} = \frac{\chi'}{r} - \frac{\chi}{r^2}$

and $\nabla^2 \psi = \frac{\chi''}{r}$. Thus we get

$$\frac{d^2\chi}{dr^2} + \frac{2m}{\hbar^2}(E - U(r))\chi = 0$$

The solution is $\chi = A \sin kr,\ r < r_0$

$$k^2 = \frac{2mE}{\hbar^2}$$

and $\chi = 0 \quad r > r_0$

(For $r < r_0$ we have rejected a term 5 cos k r as it does not vanish at r = 0). Continuity of the wavefunction at $r = r_0$ requires

$$k r_0 = n\pi$$

Hence $E_n = \frac{n^2 \pi^2 \hbar^2}{2 m r_0^2}$.

Q.88. From the conditions of the foregoing problem find:
(a) normalized eigenfunctions of the particle in the states for which ψ(r) depends only on r;
(b) the most probable value r_{pr} for the ground state of the particle and the probability of the particle to be in the region $r < r_{pr}$.

Ans. (a) The nomalized wave functions are obtained from the normalization

$$1 = \int |\psi|^2 dV = \int |\psi|^2 4\pi r^2 dr$$

$$= \int_0^{r_0} A^2 4\pi \chi^2 dr = 4\pi A^2 \int_0^{r_0} \sin^2 \frac{n\pi r}{r_0} dr$$

$$= 4\pi A^2 \frac{r_0}{n\pi} \int_0^{n\pi} \sin^2 x \, dr = 4\pi A^2 \frac{r_0}{n\pi} \cdot \frac{n\pi}{2} = r_0 \cdot 2\pi A^2$$

Hence $A = \frac{1}{\sqrt{2\pi r_0}}$ and $\psi = \frac{1}{\sqrt{2\pi \cdot r_0}} \frac{\sin \frac{n\pi r}{r_0}}{r}$

(b) The radial probability distribution function is

$$P_n(r) = 4\pi r^2 (\psi)^2 = \frac{2}{r_0} \sin^2 \frac{n\pi r}{r_0}$$

For the ground state n = 1

so $P_1(r) = \frac{2}{r_0} \sin^2 \frac{\pi r}{r_0}$

By inspection this is maximum for $r = \frac{r_0}{2}$. Thus $r_{pr} = \frac{r_0}{2}$

The probability for the particle to be found in the region $r < r_{pr}$ is clearly 50 % as one can immediately see from a graph of $\sin^2 x$.

Q.89. A particle of mass m is located in a spherically symmetrical potential well U (r) = 0 for r < r_0 and U (r) = U_0 for r >

(a) By means of the substitution ψ(r) = x(r)/r find the equation defining the proper values of energy E of the particle for E < U_0, when its motion is described by a wave function ψ(r) depending only on r. Reduce that equation to the form

$$\sin kr_0 = \pm kr_0 \sqrt{\hbar^2/2mr_0^2 U_0}, \text{ where } k = \sqrt{2mE}/\hbar.$$

(b) Calculate the value of the quantity $r_0^2 U_0$ at which the first level appears.

Ans. If we put $\psi = \frac{\chi(r)}{r}$

the equation for X(r) has the from $\chi'' + \frac{2m}{\hbar^2}[E - U(r)]\chi(r) = 0$

which can be written as $\chi'' + k^2 \chi = 0, \; 0 \le r < r_0$

and $\chi'' - \alpha^2 \chi = 0 \quad r_0 < r < \infty$

where $k^2 = \frac{2mE}{\hbar^2}, \alpha^2 = \frac{2m(U_0 - E)}{\hbar^2}$.

The boundary condition is

$$\left.\begin{array}{c} \chi(0) = 0 \\ \text{and } \chi, \chi' \text{ are continuous at } r = r_0 \end{array}\right\}$$

These are exactly same as in the one dimensional problem in problem (6.85) Wc therefore omit further details

Q.90. The wave function of a particle of mass in in a unidimensional potential field U (x) = kx²/2 has in the ground state the form ψ(x) = Ae^{-αx²}, where A is a normalization factor and a is a positive constant. Making use of the Schrodinger equation, find the constant a and the energy E of the particle in this state.

Ans. The Schrodinger equation is $\frac{d^2\Psi}{dx^2} + \frac{2m}{\hbar^2}\left(E - \frac{1}{2}kx^2\right)\Psi = 0$

We are given $\Psi = A e^{-\alpha x^2/2}$

Then $\Psi' = -\alpha x A e^{-\alpha x^2/2}$

$$\Psi'' = -\alpha A e^{-\alpha x^2/2} + \alpha^2 x^2 A e^{-\alpha x^2/2}$$

Substituting we find that following equation must hold

$$\left[(\alpha^2 x^2 - \alpha) + \frac{2m}{\hbar^2}\left(E - \frac{1}{2}kx^2\right)\right]\Psi = 0$$

since $\Psi \neq 0$, the bracket must vanish identicall. This means that the coefficient of x^2 as well the term independent of x must vanish. We get

$$\alpha^2 = \frac{mk}{\hbar^2} \quad \text{and} \quad \alpha = \frac{2mE}{\hbar^2}$$

Putting k/m = ω^2, this leads to $\alpha = \frac{m\omega}{\hbar}$ and $E = \frac{\hbar\omega}{2}$

Q.91. Find the energy of an electron of a hydrogen atom in a stationary state for which the wave function takes the form $\psi(r) = A(1 + ar)e^{-\alpha r}$, where A, a, and α are constants.

Ans. The Schrodinger equation for the problem in Gaussian units

$$\nabla^2\psi + \frac{2m}{\hbar^2}\left[E + \frac{e^2}{r}\right]\psi = 0$$

In MKS units we should read $(e^2/4\pi\varepsilon_0)$ for e^2.

we put $\psi = \frac{\chi(r)}{r}$. Then $\chi'' + \frac{2m}{\hbar^2}\left[E + \frac{e^2}{r}\right]\chi = 0$ (1)

We are given that $\chi = r\psi = Ar(1 + ar)e^{-\alpha r}$

so $\chi' = A(1 + 2ar)\,e^{-\alpha r} - \alpha Ar(1 + ar)e^{-\alpha r}$

$$\chi'' = \alpha^2 Ar(1 + ar)e^{-\alpha r} - 2\alpha A(1 + 2ar)e^{-\alpha r} + 2aAe^{-\alpha r}$$

$$\alpha^2(r + ar^2) - 2\alpha(1 + 2ar) + 2a \quad + \frac{2m}{\hbar^2}(Er + e^2)\times(1 + ar) = 0$$

Equating the coefficients of r^2, r, and constant term to zero we get

$$2a - 2\alpha + \frac{2me^2}{\hbar^2} = 0 \quad (2)$$

$$a\alpha^2 + \frac{2m}{\hbar^2}Ea = 0 \quad (3)$$

$$\alpha^2 - 4a\alpha + \frac{2m}{\hbar^2}(E + e^2 a) = 0 \quad (4)$$

From (3) either a = 0, or $E = -\frac{\hbar^2\alpha^2}{2m}$

In the first case $\alpha = \frac{m e^2}{\hbar^2}, E = -\frac{\hbar^2}{2m}\alpha^2 = -\frac{m e^4}{2\hbar^2}$

This state is the ground state.

It n the second, case $a = \alpha - \frac{m e^2}{\hbar^2}, \ \alpha = \frac{1}{2}\frac{m e^2}{\hbar^2}$

$$E = -\frac{m e^4}{8\hbar^2} \quad \text{and} \quad a = -\frac{1}{2}\frac{m e^2}{\hbar^2}$$

This state is one with n = 2 (2s).

Q.92. The wave function of an electron of a hydrogen atom in the ground state takes the form $\psi(r) = Ae^{-r}/r_1$, where A is a certain constant, r_1 is the first Bohr radius. Find: (a) the most probable distance between the electron and the nucleus; (b) the mean value of modulus of the Coulomb force acting on the electron; (c) the mean value of the potential energy of the electron in the field of the nucleus.

Ans. We first find A by normalization

$$1 = \int_0^\infty 4\pi A^2 e^{-2r/r_1} r^2 dr = \frac{\pi A^2}{2} r_1^3 \int_0^\infty e^{-x} x^2 dx = \pi A^2 r_1^3$$

since the integral has the value 2.

Thus $A^2 = \frac{1}{\pi r_1^3}$ or $A = \frac{1}{\sqrt{r_1^3 \pi}}$.

(a) The most probable distance r_{pr} is that value of r for which

$$P(r) = 4\pi r^2 |\psi(r)|^2 = \frac{4}{r_1^3} r^2 e^{-2r/r_1}$$

is maximum. This requires

$$P'(r) = \frac{4}{r_1^3}\left[2r - \frac{2r^2}{r_1}\right] e^{-2r/r_1} = 0$$

or $r = r_1 = r_{pr}$.

(b) The coulomb force being given by $-e^2/r^2$, the mean value o f its modulus is

$$<F> = \int_0^\infty 4\pi r^2 \frac{1}{\pi r_1^3} e^{-2r/r_1} \frac{e^2}{r^2} dr$$

$$= \int_0^\infty \frac{4e^2}{r_1^3} e^{-2r/r_1} dr = \frac{2e^2}{r_1^2} \int_0^\infty e^{-x} dx = \frac{2e^2}{r_1^2}$$

In MKS units we should read $(e^2/4\pi\varepsilon_0)$ for e^2

(c) $$<U> = \int_0^\infty 4\pi r^2 \frac{1}{\pi r_1^3} e^{-2r/r_1} \frac{-e^2}{r} dr = -\frac{e^2}{r_1} \int_0^\infty x\, e^{-x}\, dx = -\frac{e^2}{r_1}$$

In MKS units we should read $(e^2/4\pi\varepsilon_0)$ for e^2.

Q.93. Find the mean electrostatic potential produced by an electron in the centre of a hydrogen atom if the electron is in the ground state for which the wave function is $\psi(r) = Ae^{-r}/r_1$, where A is a certain constant, r_1 is the first Bohr radius.

Ans. We find A by normalization as above. We get

$$A = \frac{1}{\sqrt{\pi r_1^3}}$$

Then the electronic charge density is

$$\rho = -e|\psi|^2 = -e\frac{e^{-2r/r_1}}{\pi r_1^3} = \rho(\vec{r})$$

The potential $\psi(\vec{r})$ due to this charge density is

$$\varphi(\vec{r}) = \frac{1}{4\pi\varepsilon_0} \int \frac{\rho(\vec{r}')}{|\vec{r} - \vec{r}'|} d^3 r'$$

so at the origin $\varphi(0) = \frac{1}{4\pi\varepsilon_0}\int_0^\infty \frac{\rho(r')}{r'} 4\pi r'^2 dr' = \frac{-e}{4\pi\varepsilon_0}\int_0^\infty \frac{4r'}{r_1^3} e^{-2r'/r_1} dr$

$$= -\frac{e}{4\pi\varepsilon_0 r_1}\int_0^\infty x e^{-x} dx = -\frac{e}{(4\pi\varepsilon_0) r_1}$$

Q.94. Particles of mass m and energy E move from the left to the potential barrier shown in Fig. 6.3. Find:
(a) the reflection coefficient R of the barrier for $E > U_0$;
(b) the effective penetration depth of the particles into the region $x > 0$ for $E < U_0$, i.e. the distance from the barrier boundary to the point at which the probability of finding a particle decreases e-fold.

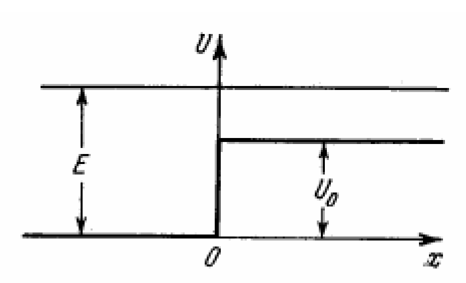


Fig. 6.3.

Ans. (a) We start from the Schrodinger equation $\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E - U(x))\psi = 0$

which we write as $\Psi_I'' + k^2\Psi_I = 0,\ x < 0$

$$k^2 = \frac{2mE}{\hbar^2}$$

and $\Psi_{II}'' + \alpha^2\Psi_{II} = 0 \quad x > 0$

$$\alpha^2 = \frac{2m}{\hbar^2}(E - U_0) > 0$$

It is convenient to look for solutions in the form

$$\psi_I = e^{ikx} + Re^{-ikx}\, x < 0$$

$$\Psi_{II} = A e^{i\alpha x} + B e^{-i\alpha x} \quad x > 0$$

In region I (x < 0), the amplitude of e^{ikx} is written as unity by convention. In II we expect only a transmitted wave to the right, B = 0 then. So

$$\Psi_{II} = A e^{ikx} \quad x > 0$$

The boundary conditions follow from the continuity of Ψ & $\frac{d\psi}{dx}$ at $x = 0$.

1 + R = A

$$iK(1 - R) = i\alpha A$$

Then $\frac{1-R}{1+R} = \frac{\alpha}{k}$ or $R = \frac{k-\alpha}{k+\alpha}$

The reflection coefficient is the absolute square of R:

$$r = |R|^2 = \left|\frac{k-\alpha}{k+\alpha}\right|^2$$

(b) In this case $E < U_0$, $\alpha^2 = -\beta^2 < 0$. Then Ψ_I is unchanged in form but

$$\Psi_{II} = A e^{-\beta x} + B e^{+\beta x}$$

we must have B = 0 since otherwise ψ(x) will become unbounded as $x \to \infty$ Finally

$$\Psi_{II} = A e^{-\beta x}$$

Inside the barrier, the particle then has a probability density equal to

$$|\psi_{II}|^2 = |A|^2 e^{-2\beta x}$$

This decreases to $\frac{1}{e}$ of its value in

$$x_{eff} = \frac{1}{2\beta} = \frac{\hbar}{2\sqrt{2m(U_0 - E)}}$$

Q.95. Employing Eq. (6.2e), find the probability D of an electron with energy E tunnelling through a potential barrier of width l and height U_0 provided the barrier is shaped as shown:
(a) in Fig. 6.4;
(b) in Fig. 6.5.

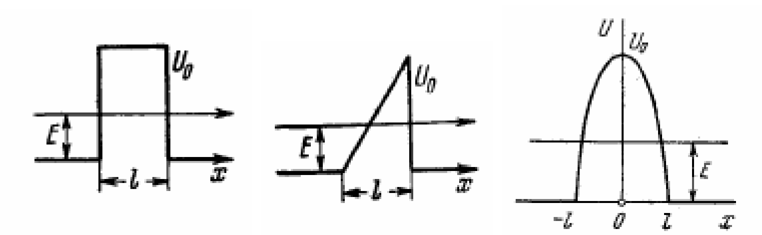


Fig. 6.4. Fig. 6.5. Fig. 6.6.

Ans. The formula is

$$D = \exp\left[-\frac{2}{\hbar}\int_{x_1}^{x_2} \sqrt{2m(V(x) - E)}\, dx\right]$$

Here $V(x_2) = V(x_1) = E$ and $V(x) > E$ in the region $x_2 > x > x_1$.

(a) For the problem, the integral is trivial

$$D = \exp\left[-\frac{2l}{\hbar} \sqrt{2m(U_0 - E)}\right]$$

(b) We can without loss of generality take x = 0 at the point the potential begins to climb. Then

$$U(x) = \begin{cases} 0 & x < 0 \\ U_0 \frac{x}{l} & 0 < x < l \\ 0 & x > l \end{cases}$$

Then $$D \approx \exp\left[-\frac{2}{\hbar}\int_{l\frac{E}{U_0}}^{l}\sqrt{2m\left(U_0\frac{x}{l}-E\right)}\,dx\right]$$

$$= \exp\left[-\frac{2}{\hbar}\sqrt{\frac{2mU_0}{l}}\int_{x_0}^{l}\sqrt{x-x_0}\,dx\right] x_0 = l\frac{E}{U_0}$$

$$= \exp\left[-\frac{2}{\hbar}\sqrt{\frac{2mU_0}{l}}\,\frac{2}{3}\,(x-x_0)^{3/2}\Big|_{x_0}^{l}\right]$$

$$= \exp\left[-\frac{4}{3\hbar}\sqrt{\frac{2mU_0}{l}}\left(l-l\frac{E}{U_0}\right)^{3/2}\right]$$

$$= \exp\left[-\frac{4l}{3\hbar U_0}(U_0-E)^{3/2}\sqrt{2m}\right]$$

Q.96. Using Eq. (6.2e), find the probability D of a particle of mass m and energy E tunnelling through the potential barrier shown in Fig. 6.6, where U(x) = U_0(1 — x^2/l^2).

Ans. The potential is $U(x) = U_0\left(1-\frac{x^2}{l^2}\right)$. The turning points are

$$\frac{E}{U_0} = 1-\frac{x^2}{l^2} \text{ or } x = \pm l\sqrt{1-\frac{E}{U_0}}.$$

Then $$D \approx \exp\left[-\frac{4}{\hbar}\int_0^{l\sqrt{1-(E/U_0)}}\sqrt{2m\left\{U_0\left(1-\frac{x^2}{l^2}\right)-E\right\}}\,dx\right]$$

$$= \exp\left[-\frac{4}{\hbar} \int_0^{l\sqrt{1-(E/U_0)}} \sqrt{2mU_0} \sqrt{1 - \frac{E}{U_0} - \frac{x^2}{l^2}}\, dx \right]$$

$$= \exp\left[-\frac{4l}{\hbar} \sqrt{2mV_0} \int_0^{x_0} \sqrt{x_0^2 - x^2}\, dx \right], \quad x_0 = \sqrt{1 - E/V_0}$$

The integral is

$$\int_0^{x_0} \sqrt{x_0^2 - x^2}\, dx = x_0^2 \int_0^{\pi/2} \cos^2\theta\, d\theta = \frac{\pi}{4} x_0^2$$

Thus

$$D = \exp\left[-\frac{\pi l}{\hbar} \sqrt{2mU_0} \left(1 - \frac{E}{U_0} \right) \right]$$

$$= \exp\left[-\frac{\pi l}{\hbar} \sqrt{\frac{2m}{U_0}} (U_0 - E) \right]$$