Assignment - 1

Shivam Kumar

2311166

(1.) (a.) For a spherically symmetric potential $V(r)$, the scattering amplitude in 1^{st} Born order app. is :

$$f(q) = \frac{-m}{2\pi\hbar^2} \int e^{iq\cdot r} V(r)\, d^3 r$$

$\because$ Here the potential depends only on r, we convert to spherical co-ordinates .

Now; since, $\int e^{iq\cdot r}\, d\Omega = 4\pi \frac{\sin(qr)}{qr}$

$\Downarrow$

$$\therefore f(q) = \frac{-m}{2\pi\hbar^2} \cdot 4\pi \int_0^\infty V(r) \frac{\sin(qr)}{qr} r^2 dr$$

$$f(q) = -\frac{2m}{\hbar^2} \frac{1}{q} \int_0^\infty r V(r) \sin(qr)\, dr$$

Now, we put $V(r) = V_0 \dfrac{e^{-r/R}}{r} \Rightarrow rV(r) = V_0 e^{-r/R}$

$$\therefore \; f(q) = -\frac{2mV_0}{\hbar^2} \frac{1}{q} \underbrace{\int_0^\infty e^{-r/R} \sin(qr)\,dr}_{\to \left(\frac{q}{q^2 + 1/R^2}\right) \text{ (given)}}$$

$$= -\frac{2mV_0}{\hbar^2} \cdot \frac{1}{q} \cdot \left(\frac{q}{q^2 + \frac{1}{R^2}}\right)$$

So ; Scattering amplitude $= f(q) = \dfrac{-2mV_0}{\hbar^2} \dfrac{1}{q^2 + \frac{1}{R^2}}$

For differential cross-section, we have :

$$\frac{d\sigma}{d\Omega} = |f(q)|^2$$

Thus ; $\boxed{\dfrac{d\sigma}{d\Omega} = \left(\dfrac{2mV_0}{\hbar^2}\right)^2 \dfrac{1}{\left(q^2 + \frac{1}{R^2}\right)^2}}$ where, $q = 2K\sin\frac{\theta}{2}$ & $K = \dfrac{\sqrt{2mE}}{\hbar}$

(b.) For total scattering cross-section

we have, $\sigma = \int \underbrace{\left(\frac{d\sigma}{d\Omega}\right)}_{\downarrow \text{ put}} d\Omega$

$$\sigma = \left(\frac{2mV_0}{\hbar^2}\right)^2 \int \frac{d\Omega}{\left(q^2 + \frac{1}{R^2}\right)^2}$$

$\because$ $\boxed{d\Omega = 2\pi \sin\theta \, d\theta}$ & $\boxed{q = 2k \sin\left(\frac{\theta}{2}\right)}$

& Also; $\boxed{\sin\theta \, d\theta = 2 \sin\frac{\theta}{2} \cos\theta/_2 \, d\theta}$

$\therefore$ Let $u = \sin\left(\frac{\theta}{2}\right) \Rightarrow du = \frac{1}{2}\cos\left(\frac{\theta}{2}\right) d\theta$

So:

$$\sigma = \left(\frac{2mV_0}{\hbar^2}\right)^2 2\pi \int_0^1 \frac{4u \, du}{\left(4k^2u^2 + \frac{1}{R^2}\right)^2}$$

Now, let $\frac{1}{R^2} = a$ & ~~t~~ $4k^2u^2 + a = t$

$$\therefore \int_0^1 \frac{u\,du}{(4k^2u^2+a)^2} =$$

$$\Rightarrow dt = 8k^2 u\,du \Rightarrow \boxed{u\,du = \frac{dt}{8k^2}}$$

~~so~~ &

$$u = 0 \Rightarrow t = a$$

$$u = 1 \Rightarrow t = 4k^2 + a$$

So;

$$\int_a^{4k^2+a} \frac{(t)^{-2}\,dt}{8k^2} = \frac{1}{8k^2}\left[\frac{t^{-1}}{-1}\right]_a^{4k^2+a}$$

$$= \frac{-1}{8k^2}\left[\frac{1}{4k^2+a} - \frac{1}{a}\right]$$

$$= \frac{-1}{8k^2}\left[\frac{\cancel{a} - 4k^2 - \cancel{a}}{(4k^2+a)(a)}\right] = \frac{\cancel{4k^2}}{\underset{2}{\cancel{8k^2}}(4k^2+a)(a)}$$

$$= \frac{1}{2a(4k^2+a)}$$

So,

$$\sigma = \left(\frac{2mV_0}{\hbar^2}\right)^2 \cancel{2}\pi \times 4 \times \frac{R^2}{\cancel{2}\left(4K^2 + \frac{1}{R^2}\right)}$$

$$\boxed{\sigma_{total} = \frac{16\pi m^2 V_0^2 R^4}{\hbar^4 \left(4K^2R^2 + 1\right)}}$$

↳ Total cross-section

(2.) We have;

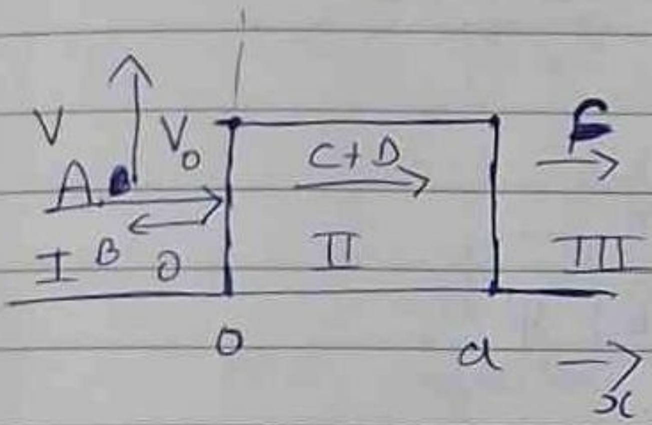
$$V(x) = \begin{cases} V_0 , & 0 \leq x \leq a \\ 0 , & \text{otherwise} \end{cases}$$

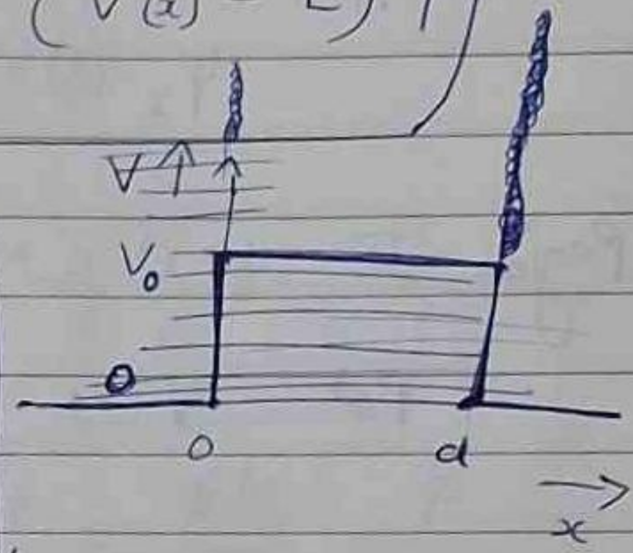
Here, we take $E < V_0$

We have; 1D time independent Schrodinger Eq^n; as

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

$$\Rightarrow \quad \boxed{\frac{\partial^2 \psi}{\partial x^2} = \frac{2m}{\hbar^2}\left(V(x) - E\right)\psi}$$





Now; we'll solve this eq^n in all different regions :

$\underline{R-1}$: $\boxed{x < 0}$

$V(x) = 0$

$$\Rightarrow \quad \frac{\partial^2 \psi}{\partial x^2} + \frac{2mE}{\hbar^2}\psi = 0$$

& Let $\quad K = \frac{\sqrt{2mE}}{\hbar}$

$\therefore \quad \frac{d^2\psi}{dx^2} + K^2\psi = 0 \Rightarrow$ Characteristic eq^n:

$$r^2 + K^2 = 0$$

$$\boxed{r = \pm iK}$$

Important Notes:

Hence, general solution is ;

$$\psi_I(x) = Ae^{ikx} + Be^{-ikx}$$

Region - II : $0 \leq x \leq a$

Pot: $V(x) = V_0$

& $\frac{\partial^2 \psi}{\partial x^2} = \frac{2m(V_0 - E)}{\hbar^2}\psi$

$\because E < V_0$, we let, $\beta = \frac{\sqrt{2m(V_0 - E)}}{\hbar}$

$\therefore \frac{\partial^2 \psi}{\partial x^2} - \beta^2 \psi = 0$

↳ Characteristic eqn: $r^2 - \beta^2 = 0$

$\boxed{r = \pm \beta}$

$\therefore$ general soln

$$\psi_{II} = Ce^{\beta x} + De^{-\beta x}$$

Region : III : $x > a$

Pot. $\Rightarrow V(x) = 0$

$$\Rightarrow \frac{\partial^2 \psi}{\partial x^2} + k^2 \psi = 0$$

$$\therefore \boxed{\psi_{III}(x) = F e^{ikx}}$$

No, reflected term because there is no source of particles to the right of the barrier, therefore no wave will travel to the left in this region.

Now;

Boundary conditions :

$\because$ Potential is finite every where, the boundary conditions are :

1. ψ is continuous
2. $\frac{d\psi}{dx}$ is continuous

Important Notes:

M / T / W / T / F / S / S

So, at $x=0$ continuity of ψ:

$$\psi_{I}(0) = \psi_{II}(0)$$

$$\boxed{A+B = C+D}$$

& for $\frac{d\psi}{dx}$: $\psi_{I}'(0) = \psi_{II}'(0)$

$$\Rightarrow \boxed{ik(A-B) = \beta(C-D)}$$

& at $\boxed{x=a}$ $\Rightarrow$ Continuity of ψ:

$$\psi_{II}(a) = \psi_{III}(a)$$

$$\Rightarrow \boxed{Ce^{\beta a} + De^{-\beta a} = Fe^{ika}}$$

& continuity of derivative:

$$\psi_{II}'(a) = \psi_{III}'(a)$$

$$\Rightarrow \beta\left(Ce^{\beta a} - De^{-\beta a}\right) = ikFe^{ika}$$

(b) <u>Probability current density :</u>

$$j = \frac{i\hbar}{2m}\left(\psi \frac{\partial \psi^*}{\partial x} - \psi^* \frac{\partial \psi}{\partial x}\right) \rightarrow \text{(i)}$$

$\Rightarrow$ <u>Current for a right-moving plane wave :</u>

Let we have a plane wave ; $\psi(x) = Ae^{iKx}$

$$\Rightarrow \frac{d\psi(x)}{dx} = iKAe^{iKx} \quad , \quad \frac{d\psi^*(x)}{dx} = -iKAe^{-iKx}$$

<u>Putting in (i) :</u>

$$j = \frac{i\hbar}{2m}\left(-iKA^2 - iKA^2\right)$$

$$\boxed{j = \frac{\hbar K}{m}|A|^2}$$

Date ________ M/T/W/T/F/S/S

Now, incident & transmitted currents :

Region 1 (Incident wave) :

$$\psi_{in} = A e^{ikx} \Rightarrow j_{in} = \frac{\hbar k}{m} |A|^2$$

Region 3 (Transmitted wave) :

$$\psi_t = F e^{ikx} \Rightarrow j_t = \frac{\hbar k}{m} |F|^2$$

$$T = \text{Transmission coff.} = \frac{j_t}{j_{in}} = \frac{|F|^2}{|A|^2}$$

Boundary conditions

we use $A + B = C + D$

$$\& \quad ik(A-B) = \beta(C-D)$$

$$\Downarrow$$

$$C = \frac{1}{2}\left[(A+B) + \frac{ik}{\beta}(A-B)\right]$$

$$D = \frac{1}{2}\left[(A+B) - \frac{ik}{\beta}(A-B)\right]$$

Important Notes:

Date

Putting the value of C & D in :

$$C e^{\beta a} + D e^{-\beta a} = F e^{ika}$$

$$\beta \left(C e^{\beta a} - D e^{-\beta a} \right) = ik F e^{ika}$$

After simplifying we get :

$$\boxed{\begin{aligned} e^{\beta a} + e^{-\beta a} &= 2\cosh(\beta a) \\ e^{\beta a} - e^{-\beta a} &= 2\sinh(\beta a) \end{aligned}}$$

$$\frac{F}{A} = \frac{4ik\beta e^{-ika}}{(k+i\beta)^2 e^{\beta a} - (k-i\beta)^2 e^{-\beta a}}$$

Now,

$$\left| \frac{F}{A} \right|^2 = \frac{4 k^2 \beta^2}{(k^2+\beta^2)^2 \sinh^2(\beta a) + 4k^2\beta^2}$$

$$\Rightarrow \boxed{T = \frac{1}{1 + \frac{(k^2+\beta^2)^2 \sinh^2(\beta a)}{4k^2\beta^2}}} \rightarrow (ii)$$

Now : $\because k^2 = \frac{2mE}{\hbar^2}$, $\beta^2 = \frac{2m(V_0 - E)}{\hbar^2}$

$$\Rightarrow \boxed{k^2 + \beta^2 = \frac{2mV_0}{\hbar^2}}$$

Important Notes:

Date

M/T/W/T/F/S/S

Putting in eq^n (ii)

$$\boxed{T = \left[1 + \frac{V_0^2}{4E(V_0 - E)} \sinh^2(\beta a)\right]^{-1}}$$

Transmission coefficient

2. (b.) ⇒ Comment on Transmission probability:

⇒ We see that even for $E < V_0$, the transmission probability is non-zero, which different of classical prediction i.e $T = 0$ for $E < V_0$.

⇒ It also decreases exponentially with barrier width a:

$$T \sim e^{-2\beta a}$$

⇒ Increasing V_0, increases β, which in turn reduces transmission probability.

(3.) $$H = \frac{1}{2}\left(p_x^2 + p_y^2\right) + \frac{1}{2}\left(x^2+y^2\right)$$

(a) $$= \frac{1}{2}\left(p_x^2 + x^2\right) + \frac{1}{2}\left(p_y^2+y^2\right)$$

$$\boxed{H_{(x,y)} = H_x + H_y}$$

So, since Hamiltonian separates:

$$\psi(x,y) = \psi_{n_x}(x) \cdot \psi_{n_y}(y)$$

The energy is: $$E_{n_x,n_y} = E_{n_x} + E_{n_y}$$

As; the normalized 1D harmonic oscillator wavefunctions are:

$$\boxed{\psi_n(x) = \frac{1}{\sqrt{2^n n! \sqrt{\pi}}} H_n(x) e^{-x^2/2}}, \quad H_n(x) = \text{Hermite polynomials}$$

& $\boxed{E_{n(x)} = \left(n + \frac{1}{2}\right)}$, $n = 0, 1, 2, \ldots$

$$H_0(x) = 1, \quad H_1(x) = 2x, \quad H_2(x) = 4x^2 - 2,$$

So, for ground state $(n_x, n_y) = (0,0)$

Energy: $\cancel{E_{00} =}$ $$E_{n_x,n_y} = \left(n_x + \frac{1}{2}\right) + \left(n_y + \frac{1}{2}\right)$$

$$= \left(n_x + n_y + 1\right)$$

$$\Rightarrow E_{0,0} = 0 + 0 + 1 = 1$$

& wavefunc^n $$\psi_{0,0}(x,y) = \psi_0(x) \; \psi_0(y)$$

$$\psi_{0,0}(x,y) = \frac{1}{\sqrt{\pi}} e^{-(x^2+y^2)/2}$$

(*) 1^{st} excited level $(n_x + n_y = 1)$ $\xrightarrow{\text{which is}}$ degenerate.

Energy $\Rightarrow$ $E_{10} = E_{01} = 2$

& State $\Rightarrow$ $(n_x, n_y) = (1,0) \Rightarrow \psi_{10}(x,y) = \psi_1(x)\ \psi_0(y)$

$$= \sqrt{\frac{2}{\pi}}\, x\, e^{-(x^2+y^2)/2}$$

& for $(0,1) \Rightarrow \psi_{10}(x,y) = \psi_0(x)\ \psi_1(y)$

$$= \sqrt{\frac{2}{\pi}}\, y\, e^{-(x^2+y^2)/2}$$

(*) 2nd excited state:

$(n_x + n_y = 2) \rightarrow$ 3 fold degenerate $\Rightarrow$ $\boxed{E_{20} = E_{11} = E_{02} = 3}$

(i) state $\Rightarrow$ $(2,0)$ $\Rightarrow$ $\psi_{20}(x,y) = \psi_2(x)\ \psi_0(y)$

$$\psi_{20}(x,y) = \frac{1}{\sqrt{2\pi}}(2x^2-1)\, e^{-(x^2+y^2)/2}$$

(ii) state $\Rightarrow$ $(1,1) \Rightarrow$ $\psi_{11}(x,y) = \psi_1(x)\ \psi_1(y)$

$$\psi_{11}(x,y) = \frac{2}{\sqrt{\pi}}\, xy\, e^{-(x^2+y^2/2)}$$

(iii) state $(0,2) \Rightarrow$ $\psi_{02}(x,y) = \psi_0(x)\ \psi_2(y)$

$$\psi_{02}(x,y) = \frac{1}{\sqrt{2\pi}}(2y^2-1)\, e^{-(x^2+y^2)/2}$$

(b.) For Variational calculation of ground-state energy:

Trial func^n $\Rightarrow$ $\psi(x,y) = A\, e^{-b(x^2+y^2)}$

Normalisation :
$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} |\psi|^2\, dx\, dy = 1$$

$$A^2 \int e^{-2b(x^2+y^2)}\, dx\, dy = 1$$

Now in polar co-ordinates:

$$x^2+y^2 = r^2 , \quad dx\,dy = r\,dr\,d\theta$$

$$A^2 \int_0^{2\pi} d\theta \int_0^{\infty} e^{-2br^2} r\,dr = 1$$

$$\Rightarrow \int_0^{\infty} r e^{-2br^2} dr = \frac{1}{4b}$$

$$\Rightarrow \text{so,} \quad A^2 (2\pi) \frac{1}{4b} = 1 \Rightarrow A = \sqrt{\frac{2b}{\pi}}$$

Now; Expectation value of energy $\Rightarrow E(b) = \langle \psi | H | \psi \rangle = \langle T \rangle + \langle V$

for K.E $\Rightarrow T = -\frac{1}{2}\left(\partial_x^2 + \partial_y^2\right)$

$$\Rightarrow \partial_x \psi = -2bx\psi \quad \& \quad \partial_x^2 \psi = \left(4b^2x^2 - 2b\right)\psi$$

Similarly for y:

$$\Rightarrow \left(\partial_x^2 + \partial_y^2\right)\psi = \left(4b^2\left(x^2+y^2\right) - 4b\right)\psi$$

So:

$$\langle T \rangle = \int \psi^* \left[-\frac{1}{2}\left(4b^2 r^2 - 4b\right)\right] \psi\, dx\,dy$$

$$\Rightarrow \langle T \rangle = 2b - 2b^2 \langle r^2 \rangle$$

& for Potential Energy:

$$V = \frac{1}{2}\left(x^2+y^2\right) = \frac{1}{2} r^2$$

$$\langle V \rangle = \frac{1}{2}\langle r^2 \rangle$$

thus, $\langle r^2 \rangle = \int r^2 |\psi|^2 dx\,dy = A^2 \int_0^{2\pi} d\theta \int_0^{\infty} r^3 e^{-2br^2} dr$

On solving, we get;

$$\int_0^{\infty} r^3 e^{-2br^2} dr = \frac{1}{8b^2}$$

So; $$\langle r^2 \rangle = \cancel{2\pi} \times \frac{1}{8b^{\cancel{2}}} \times \left(\frac{2\cancel{b}}{\cancel{\pi}}\right)$$

$$= \frac{1}{2b}$$

Thus; Total kinetic energy $\Rightarrow \langle T \rangle = 2b - \cancel{2}b^{\cancel{2}} \cdot \left(\frac{1}{\cancel{2b}}\right)$

$$= b$$

$$\& \langle V \rangle = \frac{1}{4b}$$

$$\therefore \boxed{E(b) = b + \frac{1}{4b}}$$

Now, we'll minimize energy;

$$\frac{\partial E}{\partial b} = 1 - \frac{1}{4b^2} = 0$$

$$\Rightarrow \boxed{b = +\frac{1}{2}} \quad (\because E(b) \text{ can't be } -ve)$$

So: $E_0^{\text{Variational}} = \frac{1}{2} + \frac{1}{4 \times \left(\frac{1}{2}\right)} = 1$

(c) For Perturbation:

$$V_1 = \frac{1}{2} \epsilon xy (x^2 + y^2), \text{ where } \epsilon \ll 1$$

First-order Correction:

$$E^{(1)} = \langle \psi_0 | V_1 | \psi_0 \rangle = \frac{\epsilon}{2} \int xy (x^2 + y^2) |\psi_0|^2 dx dy$$

ψ_0 = unperturbed Ground state wavefuncn

$\because \quad \psi_0(x,y) = \frac{1}{\sqrt{\pi}} e^{-(x^2+y^2)/2}$

So:
$$E^{(1)} = \frac{\varepsilon}{2\pi} \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} xy\,(x^2+y^2)\, e^{-(x^2+y^2)}\, dx\, dy$$

$$= \frac{\varepsilon}{2\pi}\left[\int x^3 y\, e^{-(x^2+y^2)}\, dx\,dy + \int xy^3\, e^{-(x^2+y^2)}\, dx\,dy\right]$$

So;
$$\int x^3 y\, e^{-x^2} e^{-y^2}\, dx\,dy = \left(\int x^3 e^{-x^2} dx\right)\left(\int y\, e^{-y^2} dy\right)$$

&
$$\int xy^3\, e^{-x^2} e^{-y^2}\, dx\,dy = \left(\int x\, e^{-x^2} dx\right)\left(\int y^3 e^{-y^2} dy\right)$$

$\left(\because \int_{-\infty}^{\infty} x\, e^{-x^2} dx = 0 \text{ (odd func}^n) \quad \& \int_{-\infty}^{\infty} x^3 e^{-x^2} dx = 0 \text{ (odd ,,)} \right)$

$\therefore \boxed{E^{(1)} = 0}$

Also, by Variational principle;

$$\psi_{trial}(x,y) = A\, e^{-b(x^2+y^2)}, \quad A = \sqrt{\frac{2b}{\pi}}$$

$$E^{(1)}_{varia} = \frac{\varepsilon}{2}\int xy\,(x^2+y^2)\, |\psi_{trial}|^2\, dx\,dy$$

$$= \frac{\varepsilon}{2}\left(\frac{2b}{\pi}\right)\int xy\,(x^2+y^2)\, e^{-b(x^2+y^2)}\, dx\,dy$$

Again on expanding; each term factorizes into odd integrals, as before:

$\therefore \boxed{E^{(1)}_{vari} = 0}$

So; from ~~the~~ exact perturbation theory:

~~$\psi_{0,0}$ is even func~~

$$\langle \psi_{00} | V_1 | \psi_{00} \rangle = 0$$

So, the 1^{st}- order correct is zero, which is in aggrement with the Variational result.