Solution of Problem Set 2

Problem 1) (20 marks)

Consider a one-dimensional step potential that is depicted in Fig P-1 .

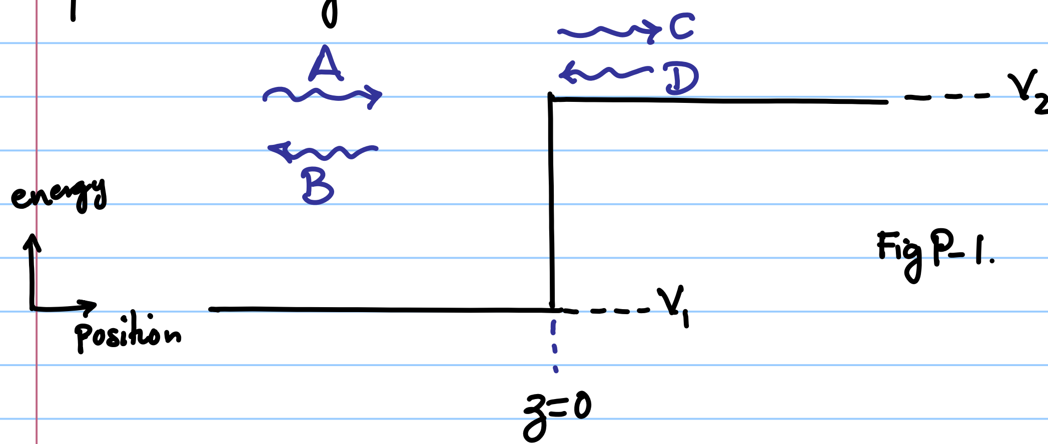


Fig P-1.

If we consider that the energy of the object $E > V_2$ then :

$$\psi_1 = \frac{1}{\sqrt{k_1}} \left(A e^{ik_1 z} + B e^{-ik_1 z} \right) \qquad k_1 = \frac{\sqrt{2m(E-V_1)}}{\hbar}$$

$$\psi_2 = \frac{1}{\sqrt{k_2}} \left(C e^{ik_2 z} + D e^{-ik_2 z} \right) \qquad k_2 = \frac{\sqrt{2m(E-V_2)}}{\hbar}$$

Note that factor $\frac{1}{\sqrt{k}}$ is necessary to have the conservation of current probability since :

$$J_1 = \frac{e\hbar}{m} \left(|A|^2 - |B|^2 \right) \quad \& \quad J_2 = \frac{e\hbar}{m} \left(|C|^2 - |D|^2 \right)$$

forcing the unimodularity of transfer matrix as $|M| = 1$.

If k is imaginary then $|M| = \pm i$.

Applying the boundary condition $\psi_1 = \psi_2$ & $m_1 \frac{d\psi_1}{dt} = m_2 \frac{d\psi_2}{dt}$ at $z=0$, we yield:

$$\frac{A}{\sqrt{k_1}} + \frac{B}{\sqrt{k_1}} = \frac{C}{\sqrt{k_2}} + \frac{D}{\sqrt{k_2}}$$

$$\Rightarrow$$

$$\frac{A}{\sqrt{k_1}} - \frac{B}{\sqrt{k_1}} = \frac{k_2}{k_1}\frac{C}{\sqrt{k_2}} - \frac{k_2}{k_1}\frac{D}{\sqrt{k_2}}$$

$$\begin{pmatrix} A \\ B \end{pmatrix} = \frac{1}{2\sqrt{k_1 k_2}} \begin{pmatrix} k_1+k_2 & k_1-k_2 \\ k_1-k_2 & k_1+k_2 \end{pmatrix} \begin{pmatrix} C \\ D \end{pmatrix}$$

$$M_{step} = \frac{1}{2\sqrt{k_1 k_2}} \begin{pmatrix} k_1+k_2 & k_1-k_2 \\ k_1-k_2 & k_1+k_2 \end{pmatrix}$$

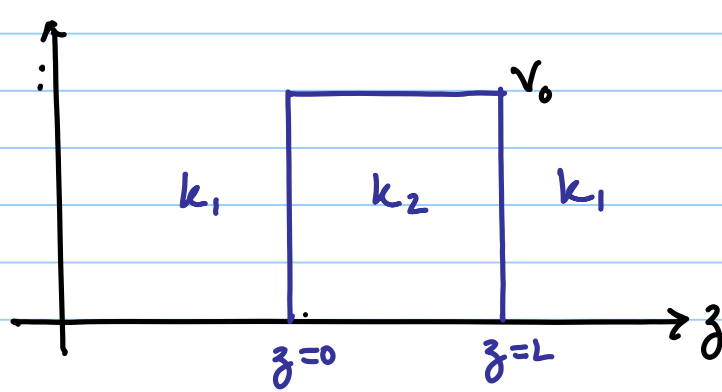
For free propagation to the right for distance $\underline{z}$, we have

$$M_{free} = \begin{pmatrix} e^{-ikz} & 0 \\ 0 & e^{-ikz} \end{pmatrix}$$

a)

Now a potential barrier can be considered as shown in Fig

$$k_1^2 = k_2^2 + \frac{2mV_0}{\hbar^2}$$



$$M_{barrier} = M_{step(1\to2)} \; M_{free} \; M_{step(2\to1)}$$

$$= \frac{1}{2\sqrt{k_1k_2}} \begin{pmatrix} k_1+k_2 & k_1-k_2 \\ k_1-k_2 & k_1+k_2 \end{pmatrix} \begin{pmatrix} e^{-ik_2L} & 0 \\ 0 & e^{-ik_2L} \end{pmatrix}$$

$$\times \frac{1}{2\sqrt{k_1k_2}} \begin{pmatrix} k_2+k_1 & k_2-k_1 \\ k_2-k_1 & k_2+k_1 \end{pmatrix} = \begin{pmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{pmatrix}$$

$$m_{11} = m_{22}^* = \cos(k_2L) - i\,\frac{k_1^2+k_2^2}{2k_1k_2}\sin(k_2L)$$

$$m_{12} = m_{21}^* = -i\,\frac{k_2^2-k_1^2}{2k_1k_2}\sin(k_2L)$$

if $E < V_0 \longrightarrow k_2 \to ik_2$

b)

The delta function limit can be reached where $V_0 \to \infty$ & $L \to 0$, also $k_2 \to ik_2$ $\therefore$

$$m_{11} = 1 + i\,\frac{k_0}{k_1} \qquad k_0 \triangleq \frac{mV_0L}{\hbar^2} \qquad (V_0L = cte)$$

$$m_{12} = \frac{ik_0}{k_1}$$

$$\rightarrow M_\delta = \begin{pmatrix} 1+i\frac{k_0}{k_1} & \frac{ik_0}{k_1} \\ -\frac{ik_0}{k_1} & 1-i\frac{k_0}{k_1} \end{pmatrix}$$

Problem 2) (20 marks)

First, we cast the potential energy barriers in the proper coordinate system, as shown in Fig 2-1.

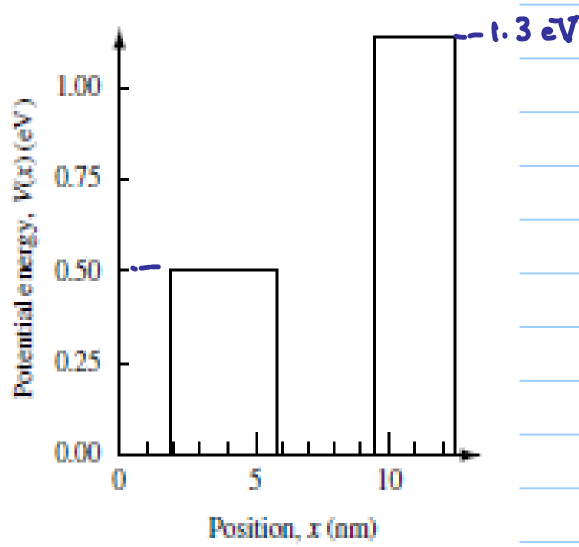


Fig 2-1) Potential Barrier

a)

We apply the transmission matrix method and then find the following energy vs. transmission in linear plot. shown in Fig 2-2.

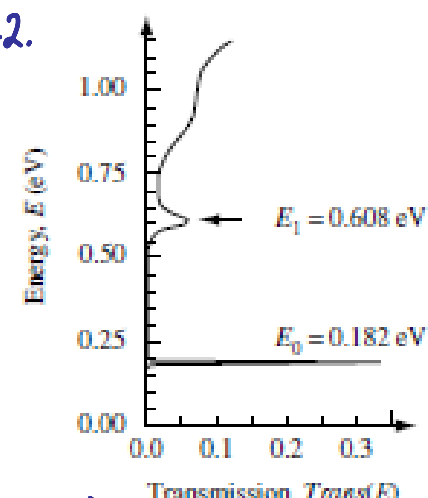


Fig 2-2)

The resolution for getting Fig 2-2) is about 6 meV.

To better observe the two resonant peaks, we plot E vs. $-\ln[\text{Transmission}]$, in Fig 2-3.

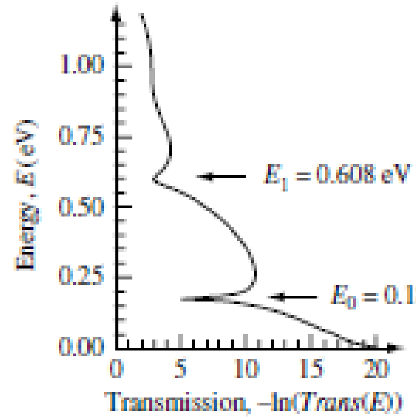


Fig 2-3)

b) Resonances occur at $\boxed{E_0 = 0.182 \text{ eV}}$ & $\boxed{E_1 = 0.608 \text{ eV}}$

c) To get the lifetime at both resonances, we get a better look at resonances like the following fig. 2-4 for $E_0 = 0.182$ eV.

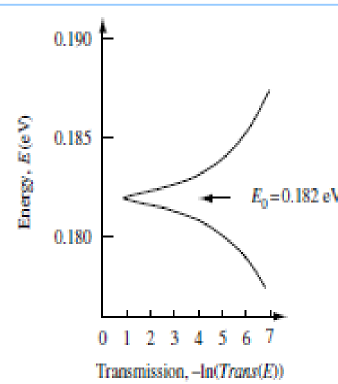


Fig 2-4)

The width of the peak, FWHM $\simeq$ 0.5 meV $\Rightarrow$

$$\tau \simeq \frac{\hbar}{FWHM} \simeq 1.3 \text{ psec.}$$

For $E_1 = 0.608$ eV, the life time is ill-defined as this resonance happens at energy greater than the lowest potential barrier, so it is not well-localized. Therefore energy band is broad and the resonance life time is much shorter than E_0.

Problem 3)

(20 marks)

Fig P2, shows the band gaps E_{g1} & E_{g2} along with pass bands E_{b1}, E_{b2} & E_{b3} up to energy 15 eV.

The velocity of the electron is expected to be slower near pass band edges since one can not expect a sudden discontinuity in the velocity, since the electron velocity is zero in the band gaps. Electron velocity should be greatest for energies near the middle of the pass bands.

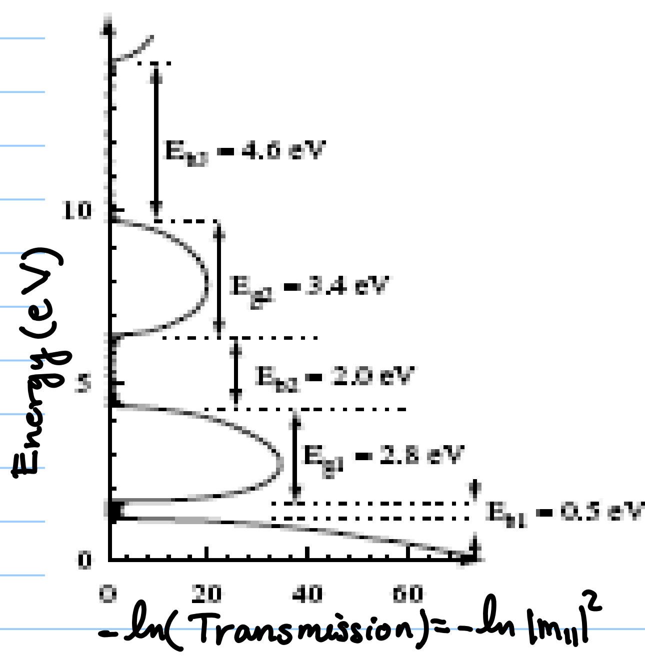


Fig P2

Problem 4) (20 marks)

$\psi_n(z) = A \sin(k_n z)$ where $A = \sqrt{\frac{2}{L}}$ & $k_n = \frac{n\pi}{L}$

After imparting momentum p_0, the new wavefunction will be $\psi_{p_0}(z) = e^{-i\frac{p_0}{\hbar}z}\, \psi_n(z)$.

$$\psi_{p_0}(z) = \sum_n c_n \psi_n(z) = \exp\left(-\frac{i}{\hbar}p_0 z\right) \psi_n(z) \implies$$

$$c_n = |A|^2 \int_{-L/2}^{L/2} \exp\left(-\frac{i}{\hbar}p_0 z\right) \sin^2 k_n z \, dz$$

$$\boxed{C_n = |A|^2 \int_{-L/2}^{L/2} \cos\left(\frac{p_0}{\hbar}z\right) \sin^2 k_n z \, dz}$$

$$\int_{-L/2}^{L/2} \cos\left(\frac{p_0}{\hbar}z\right) \sin^2 k_n z \, dz = \int_{-L/2}^{L/2} \cos\left(\frac{p_0}{\hbar}z\right)\left[\frac{1}{2} - \frac{1}{2}\cos 2k_n z\right] dz$$

$$= \frac{\hbar}{p_0} \sin \frac{p_0 L}{2\hbar} - \int_0^{L/2} \cos\left(\frac{p_0}{\hbar}z\right) \cos 2k_n z \, dz$$

$$= \frac{\hbar}{p_0} \sin \frac{p_0 L}{2\hbar} - I$$

If $2k_n = \pm \frac{p_0}{\hbar} \implies I_1 = \frac{1}{2}\left\{\frac{L}{2} + \frac{\hbar}{2p_0} \sin \frac{p_0 L}{\hbar}\right\}$

If $2k_n \neq \frac{p_0}{\hbar} \implies I_1 = \frac{1}{2}\left\{\frac{1}{p_0/\hbar - 2k_n} \sin\left(\frac{p_0}{\hbar} - 2k_n\right) L/2 + \frac{1}{p_0/\hbar + 2k_n} \sin\left(\frac{p_0}{\hbar} + 2k_n\right) L/2\right\}$

There fore

If $\frac{P_0}{\hbar} = \pm \frac{2n\pi}{L} \Rightarrow$ $\boxed{|C_n|^2 = \left[\frac{\sin P_0 L/2\hbar}{P_0 L/2\hbar} - \frac{\sin (P_0 L/\hbar)}{2 P_0 L/\hbar} - \frac{1}{2} \right]^2}$

If $\frac{P_0}{\hbar} \neq \pm \frac{2\pi n}{L} \Rightarrow$

$$|C_n|^2 = \left[\frac{\sin (P_0 L/2\hbar)}{P_0 L/2\hbar} - \frac{1}{\left(\frac{P_0}{\hbar} - \frac{2n\pi}{L}\right) L} \sin\left(\frac{P_0}{\hbar} - \frac{2n\pi}{L}\right) L/2 - \frac{1}{\left(\frac{P_0}{\hbar} + \frac{2n\pi}{L}\right) L} \sin\left(\frac{P_0}{\hbar} + \frac{2n\pi}{L}\right) L/2 \right]^2$$

$|C_n|^2$ is the probability of having the same energy after imparting momentum P_0.

As sanity check if $\hbar \to 0$ then $C_n \to 0$ which is correct for both cases.

Problem 5)

$$\Psi(x, t=0) = A\sum_{n=0}^{N} c^n \psi_n(x) \qquad , \quad |c| < 1$$

a) $\displaystyle\int_{-\infty}^{+\infty} \Psi^*(x, t=0)\, \Psi(x, t=0)\, dx = 1 \Rightarrow$

$$A^{-2} = \int_{-\infty}^{+\infty} \sum_{n=0}^{N} |c|^{2n} \psi_n^*(x)\, \psi_n(x)\, dx$$

$$A^{-2} = \sum_{n=0}^{N} |c|^{2n} \underbrace{\int_{-\infty}^{+\infty} \psi_n^*(x)\, \psi_n(x)\, dx}_{1}$$

$$\sum_{n=0}^{N} |c|^{2n} = \frac{1-|c|^{2N}}{1-|c|^2} = A^{-2} \Rightarrow$$

$$A = \sqrt{\frac{1-|c|^2}{1-|c|^{2(N+1)}}}$$

b)

The time-evolved wave function is

$$\Psi(x,t) = A e^{-\frac{i\omega t}{2}} \sum_{n=0}^{N} c^n e^{-in\omega t} \psi_n(x)$$

since $E_n = (n+\frac{1}{2})\hbar\omega$

c)

The probability amplitude to find the system at later time in $\Psi(x,0)$ is

$$\langle \Psi(t=0) | \Psi(t) \rangle^2 = P(t)$$

Thus $P(t) = |A|^4 \left| \sum_{n=0}^{N} |c|^{2n} e^{-in\omega t} \right|^2$

$$\boxed{P(t) = \left(\frac{1-|c|^2}{1-|c|^{2(N+1)}}\right)^2 \left|\frac{1-|c|^{2N+2} e^{-i(N+1)\omega t}}{1-|c|^2 e^{-i\omega t}}\right|^2}$$

d)

$$\langle H \rangle = |A|^2 \sum_{n=0}^{N} E_n |c|^{2n} = |A|^2 \sum_{n=0}^{N} (n+\tfrac{1}{2})\hbar\omega \, |c|^{2n}$$

$$= \frac{\hbar\omega}{2}\left[1 + \frac{1-|c|^2}{1-|c|^{2N+2}} \sum_{n=0}^{N} 2n|c|^{2n}\right]$$

$$= \frac{\hbar\omega}{2}\left[1 + |c| \frac{1-|c|^2}{1-|c|^{2N+2}} \frac{\partial}{\partial |c|} \sum_{n=0}^{N} |c|^{2n}\right]$$

$$\boxed{\langle H \rangle = \frac{\hbar\omega}{2}\left[1 + \frac{2|c|^2(1-|c|^{2N+2}) - 2(N+1)|c|^{2N+2}(1-|c|^2)}{1-|c|^2}\right]}$$