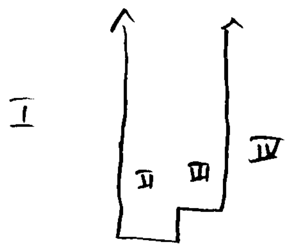
HW # 2

1) Find E_1, E_2, ψ_1, ψ_2

$$V(x) = \begin{cases} \infty & x < -d \\ 0 & -d < x < 0 \\ V_0 & 0 < x < d \\ \infty & x > d \end{cases}$$

Four regions:



In I, IV $\psi = 0$

In II, Schrodinger Eq is for free electron

$$\frac{\partial^2}{\partial x^2} \psi_{II} = \frac{-2m}{\hbar^2} E \psi_{II}$$

$$\boxed{\psi_{II} = A \sin Kx + B \cos Kx \qquad K = \sqrt{\frac{2mE}{\hbar^2}}}$$

In III, Schrodinger Eq is for free electron w/ lower energy $(E - V_0)$

$$\frac{\partial^2}{\partial x^2} \psi_{III} = \frac{-2m}{\hbar^2} \underbrace{(E - V_0)}_{\text{positive}} \psi_{III}$$

$$\boxed{\psi_{III} = C \sin \gamma x + D \cos \gamma x \qquad \gamma = \sqrt{\frac{2m(E-V_0)}{\hbar^2}}}$$

Boundary Conditions

① $\psi_{II}(-d) = 0 \qquad \psi_{III}(d) = 0$

② $\psi_{II}(0) = \psi_{III}(0)$

③ $\psi'_{II}(0) = \psi'_{III}(0)$

①

$$\psi_{II}(-d) = A \sin K(-d) + B \cos K(-d) = 0$$

$$\boxed{B \cos Kd = A \sin Kd}$$

$$\psi_{III}(d) = C \sin \gamma d + D \cos \gamma d$$

$$\boxed{D \cos \gamma d = -C \sin \gamma d}$$

②

$$\psi_{II}(0) = B \qquad \psi_{III}(0) = D$$

$$\boxed{B = D}$$

③

$$\psi'_{II}(0) = AK \cos K\cdot 0 - B\cancel{K} \sin K0 = AK$$

$$\psi'_{III}(0) = C\gamma \cos \gamma 0 - D\gamma \sin K 0 = C\gamma$$

$$\boxed{AK = C\gamma}$$

$$\tan Kd = \frac{B}{A} \qquad \tan \gamma d = \frac{-D}{C} \qquad B = D \qquad AK = C\gamma$$

$$\tan Kd = \frac{B}{A} \qquad \tan \gamma d = \frac{-B}{AK/\gamma} = \frac{-B\gamma}{AK}$$

$$\tan \gamma d = -\frac{\gamma}{K} \tan Kd$$

$$\tan\left[\sqrt{\frac{2m(E-V_0)}{\hbar^2}} \cdot d\right] = -\frac{\sqrt{\frac{\cancel{2m}(E-V_0)}{\cancel{\hbar^2}}}}{\sqrt{\frac{\cancel{2m}E}{\cancel{\hbar^2}}}} \tan \sqrt{\frac{2mE}{\hbar^2}}\, d$$

$$\tan\left(\sqrt{\frac{2m(E-V_0)}{\hbar^2}}\, d\right) = -\sqrt{1 - V_0/E}\ \tan\sqrt{\frac{2mE}{\hbar^2}}\, d$$

$$E = \varepsilon \cdot V_0$$

$$\tan \sqrt{\frac{2mV_0}{\hbar^2}(\varepsilon - 1)} \cdot d = -\sqrt{1 - \frac{V_0}{\varepsilon V_0}}\ \tan \sqrt{\frac{2m V_0 \varepsilon}{\hbar^2}}\, d$$

$$V = \sqrt{\frac{2mV_0 d^2}{\hbar^2}}$$

$$\tan(V\sqrt{\varepsilon - 1}) = -\sqrt{1 - 1/\varepsilon}\ \tan V\sqrt{\varepsilon}$$

$$V = \sqrt{\frac{2 \cdot 1\times10^{-31} \cdot (1\times10^{-9})^2}{(1.05\times10^{-34})^2}\, V_0}$$

$$V = 0.757$$

$$\tan(0.757\sqrt{\varepsilon - 1}) = -\sqrt{1 - 1/\varepsilon}\ \tan 0.757\sqrt{\varepsilon}$$

GRAPHICALLY: $\varepsilon_1 = 4.796$ $\varepsilon_2 = 17.6$

$E_1 = \varepsilon_1 V_0$ $E_2 = 17.6\, V_0$

$\boxed{E_1 = 0.96\,eV}$ $\boxed{E_2 = 3.52\,eV}$

$$\psi_1 = \begin{cases} A\sin kx + B\cos kx & k = \sqrt{\dfrac{2mE_1}{\hbar^2}} \quad -d < x < 0 \\ C\sin \gamma x + D\cos \gamma x & \gamma = \sqrt{\dfrac{2m(E_1 - V_0)}{\hbar^2}} \quad 0 < x < d \end{cases}$$

TO FIND A, B, C, D, USE

$B = D$ $Ak = C\gamma$,

AND

$|\psi_1|^2 = 1$ for $-d < x < d$

Follow same for ψ_2, but use E_2

(13) If $V_0 = 0$, THEN THIS IS SIMPLY AN INFINITE POTENTIAL WELL!

$$\psi_1 = \sqrt{\frac{2}{2d}} \cos Kx \qquad \psi_2 = \sqrt{\frac{2}{2d}} \sin Kx$$

$$K_1 d = \pi/2 \qquad K_2 d = \pi$$

$$\sqrt{\frac{2mE_1}{\hbar^2}} \cdot d = \frac{\pi}{2} \qquad \sqrt{\frac{2mE_2}{\hbar^2}} \cdot d = \pi$$

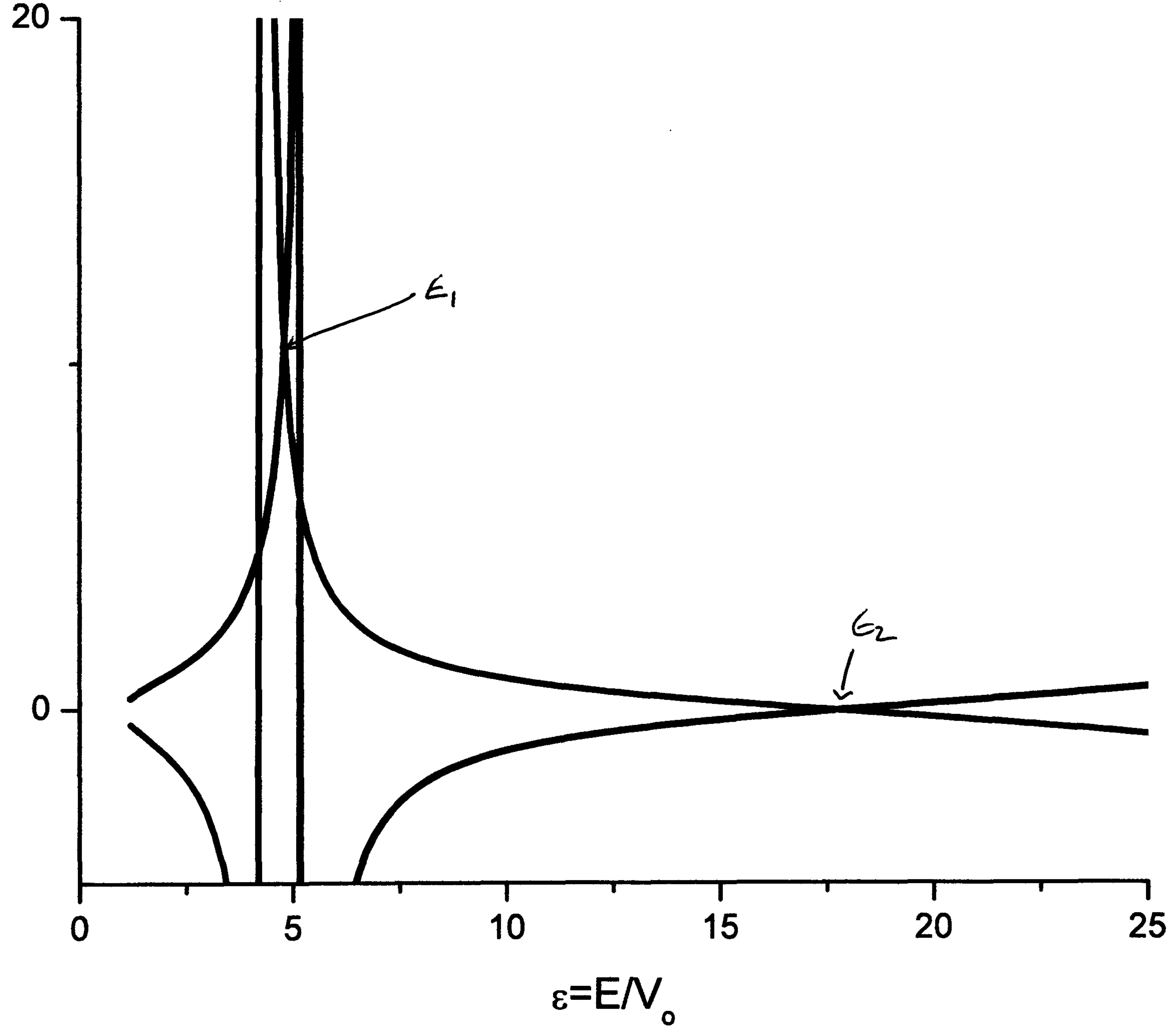
$$E_1 = \frac{\pi^2 \hbar^2}{4 \cdot 2md^2} \qquad E_2 = \frac{\pi^2 \hbar^2}{d^2 2m}$$

$$E_1 \quad \frac{\pi^2 \hbar^2}{8md^2} \qquad E_2 = 4E_1$$

$$\boxed{E_1 = 860\,meV} \qquad \boxed{E_2 = 3.44\,eV}$$

$$K_1 = 1.57 \times 10^9$$

$$\boxed{\psi_1 = 3.16 \times 10^{-5} \cos(1.57 \times 10^9 \cdot x)} \qquad \boxed{\psi_2 = 3.16 \times 10^{-5} \sin(3.14 \times 10^9 \cdot x)}$$



20
0
0
5
10
15
20
25
ε=E/V_o
ε1
ε2

2) QUANTUM BOX

$$\psi(x,y,z) = \psi_x(x)\,\psi_y(y)\,\psi_z(z)$$

$$\psi(x,y,z) = A \sin\frac{\pi n_x}{L_x}x \;\sin\frac{\pi n_y}{L_y}y\; \sin\frac{\pi n_z}{L_z}z$$

A found by normalization

$$\iiint_V \psi^*\psi = 1$$

$$\frac{L_x L_y L_z}{8}A^2 = 1$$

$$\boxed{A = \sqrt{\frac{8}{L_x L_y L_z}}}$$

B)

$$-\frac{\hbar^2}{2m}\cancel{\frac{\partial^2}{\partial}}\nabla^2\psi = E\psi$$

$$\nabla^2\psi = -\frac{\pi^2 n_x^2}{L_x^2} + -\frac{\pi^2 n_y^2}{L_y^2} + \frac{-\pi^2 n_z^2}{L_z^2}$$

$$E = +\frac{\hbar^2\pi^2}{2m}\left(\frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2} + \frac{n_z^2}{L_z^2}\right)$$

$L_x = 10nm \qquad L_y = 35nm \qquad L_z = 20nm$

$$\mathcal{E}_{n_x, n_y, n_z} = \frac{\hbar^2 \pi^2}{2m \cdot (10^{-9})^2} \left(\frac{n_x^2}{10^2} + \frac{n_y^2}{35^2} + \frac{n_z^2}{20^2} \right)$$

$\mathcal{E}_{111} \cong .0133$

$\mathcal{E}_{121} = .0157$

$\mathcal{E}_{131} = .0198$

$\mathcal{E}_{112} = .0208$

$\mathcal{E}_{122} = .023$

$\boxed{13}$ SEE CLASS NOTES