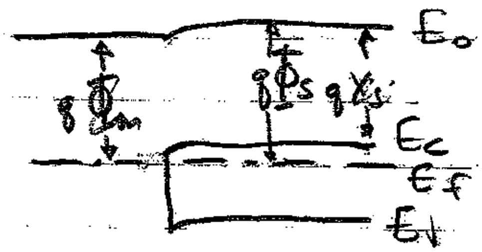
Homework #2 Solutions

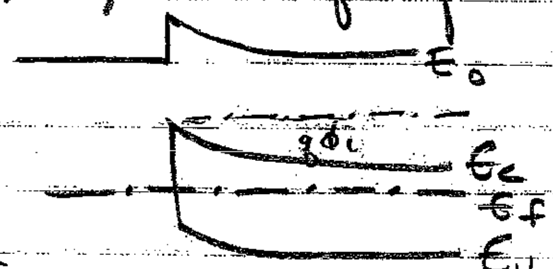
2. $\Phi_s = \chi_s + \frac{kT}{q}\ln\left(\frac{N_c}{N_d}\right) = 4.14V$

(a) $\Phi_{ms} = 4.1 - 4.14 = -0.04V = \phi_i$ $\Rightarrow$ no barrier (accumulation)



$\Phi_b = \Phi_M - \chi_s = 0.05 V$

(b) Very large density of surface states $\Rightarrow$ E_f pinned at neutrality level



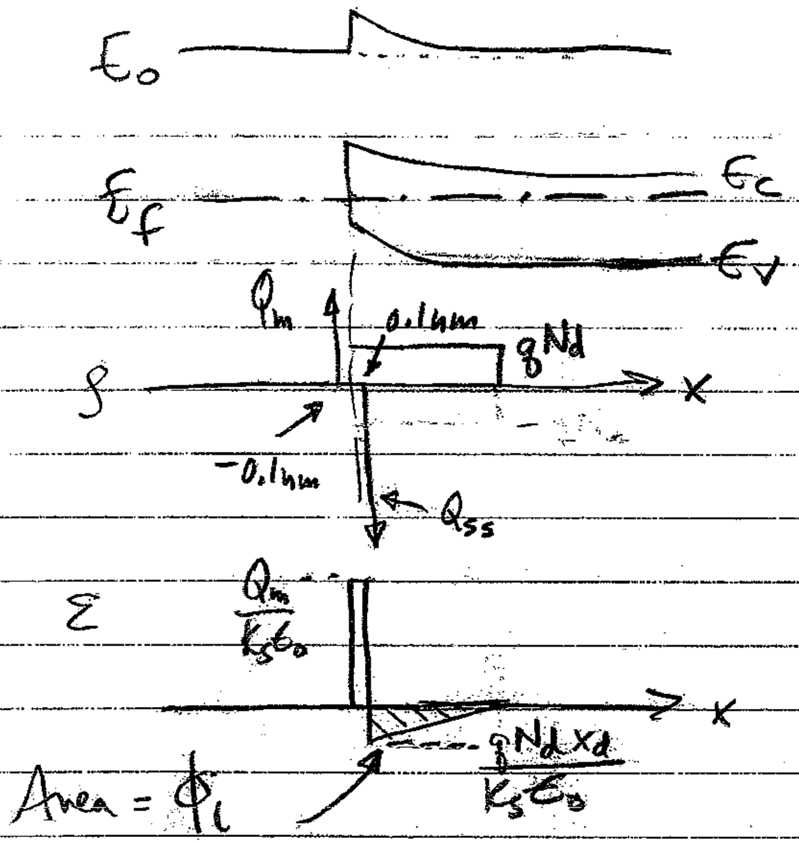
$$\phi_i = \frac{1}{q}\left[(E_c - E_f)_{surface} - (E_c - E_f)_{bulk}\right]$$

$$= \frac{1}{q}\left[(1.12eV - 0.5eV) - 0.09eV\right] = 0.53V$$

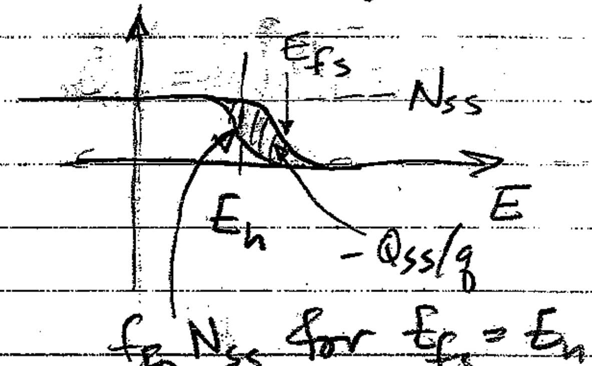
(c) Finite density of surface states

Expect $-0.04 < \phi_i < 0.53$

Assume $\phi_i > 0$, substrate depleted



$$Q_m = -Q_{ss} - qN_d x_d$$



$$\phi_i = \frac{qN_d x_d^2}{2K_s\epsilon_0}$$

$$Q_{ss}' = -q\int\left[f_{FD}(E, E_{fs}) - f_{FD}(E, E_{fs} = E_n)\right]N_{ss}(E)\,dE$$

$$\approx -q\,(E_{fs} - E_n)\,N_{ss}(E) = -q\left[(1.03\text{eV} - 0.5\text{eV} - q\phi_i)\,7\times10^{14}\,\text{cm}^{-2}\text{eV}^{-1}\right]$$

$$\left.\begin{aligned} E_{fs} - E_v &= (E_f - E_v)_{bulk} - q\phi_i \\ &= (1.12 - 0.09)\text{eV} - q\phi_i \end{aligned}\right\}$$

$$Q_{ss}' = -1.1\times10^{-4}(0.53\text{eV} - q\phi_i)\frac{C}{\text{cm}^2\text{eV}}$$

$$Q_m = 1.1\times10^{-4}(0.53\text{eV} - q\phi_i) - qN_d\sqrt{\frac{2K_s\epsilon_0}{qN_d}}\;\phi_i^{1/2}$$

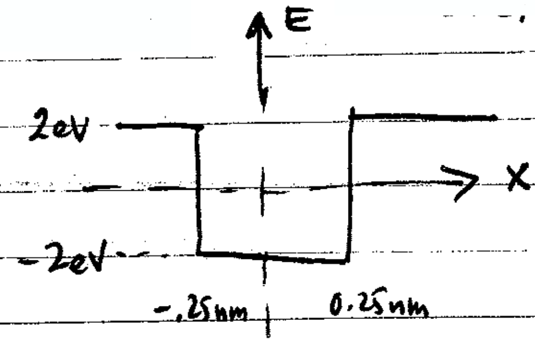
$$= 1.1\times10^{-4}(0.53\text{V} - \phi_i)\frac{C}{\text{cm}^2\text{V}} - \underbrace{5.8\times10^{-7}\frac{C}{\text{cm}^2\text{V}^{1/2}}\;\phi_i^{1/2}}_{\text{assume negligible}}$$

$$\phi_{ms} = -0.04\text{V} = V_{dipole} + \phi_i = -\frac{Q_m(0.2\times10^{-7}\text{cm})}{K_s\epsilon_0} + \phi_i$$

$$-0.04\text{V} = -2.1(0.53\text{V} - \phi_i) + \phi_i \Rightarrow \underline{\underline{\phi_i = 0.35\text{V}}}$$

3. in 1D:

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



$$\frac{d^2\psi}{dx^2} + \frac{2m_0}{\hbar^2}\left(E - V(x)\right)\psi = 0$$

$-a$ $\quad +a$

$a \equiv 0.25\ \text{nm}$

For bound states: $-2\text{eV} < E < 2\text{eV}$

Inside $(|x| < 0.25\text{nm})$ $\quad E > V_i = -2\text{eV}$

$$\frac{d^2\psi_i}{dx^2} + k^2\psi_i = 0$$

$$k^2 = \frac{2m_0}{\hbar^2}(E + 2\text{eV})$$

$$\frac{2m}{\hbar^2} = \frac{2(9.11\times10^{-31}\text{kg})(2\pi)^2}{(6.63\times10^{-34}\text{ J}\cdot\text{s})^2}$$

$$\psi_i = A\sin kx + B\cos kx$$

$$1\text{ J} = 1\ \frac{\text{kg m}^2}{\text{s}^2} = \frac{1}{1.6\times10^{-19}}\text{eV}$$

Outside $(|x| > 0.25\text{nm})$ $\quad E < V_0 = 2\text{eV}$

$$\frac{2m_0}{\hbar^2} = 2.62\times10^{19}\ \text{m}^{-2}\text{eV}^{-1}$$
$$= 26.2\ \text{nm}^{-2}\text{eV}^{-1}$$

$$\frac{\partial^2\psi_0}{\partial x^2} - \alpha^2\psi_0 = 0$$

$$\alpha^2 = \frac{2m_0}{\hbar^2}(2\text{eV} - E)$$

$$\psi_0 = Ce^{-\alpha x} + \underbrace{\cancel{De^{\alpha x}}}_{\to 0\ (x\to\infty)} = Ce^{-\alpha x} = C'e^{-\alpha(x-a)} \quad (x>a)$$

$$= \underbrace{\cancel{Ee^{-\alpha x}}}_{\to 0\ (x\to-\infty)} + Fe^{\alpha x} = Fe^{\alpha x} = F'e^{\alpha(x+a)} \quad (x<a)$$

BCs: $\psi_i(\pm 0.25\text{nm}) = \psi_0(\pm 0.25\text{ nm})$

$$\frac{\partial\psi_i}{\partial x}(\pm 0.25\text{nm}) = \frac{\partial\psi_0}{\partial x}(\pm 0.25)$$

$\underline{\psi_i = \psi_o}$

[1] @ $x=a$ $\quad A\sin ka + B\cos ka = C'$

[2] @ $x=-a$ $\quad A\sin(-ka) + B\cos(-ka) = F' = -A\sin ka + B\cos ka$

$\underline{\partial\psi_i/\partial x = \partial\psi_o/\partial x}$

[3] @ $x=a$ $\quad kA\cos ka - kB\sin ka = -\alpha C'$

[4] @ $x=-a$ $\quad kA\cos(-ka) - kB\sin(-ka) = \alpha F' = kA\cos(ka) + kB\sin ka$

[1] → [3] $\quad kA\cos ka - kB\sin ka = -\alpha\left(A\sin ka + B\cos ka\right)$

$$A(k\cos ka + \alpha\sin ka) = B[k\sin ka - \alpha\cos ka] \quad [5]$$

[2] → [4] $\quad kA\cos ka + kB\sin ka = \alpha(-A\sin ka + B\cos ka)$

$$A(k\cos ka + \alpha\sin ka) = B(\alpha\cos ka - k\sin ka) \quad [6]$$

[5] + [6] $\quad 2A(k\cos ka + \alpha\sin ka) = 0 \Rightarrow A = 0$ or

$0 = (k\cos ka + \alpha\sin ka$

If $A=0$, then $k\sin ka - \alpha\cos ka = 0$ since both A & B can't $= 0$

Thus, $\tan(ka) = -\frac{k}{\alpha}$ or $\frac{\alpha}{k}$

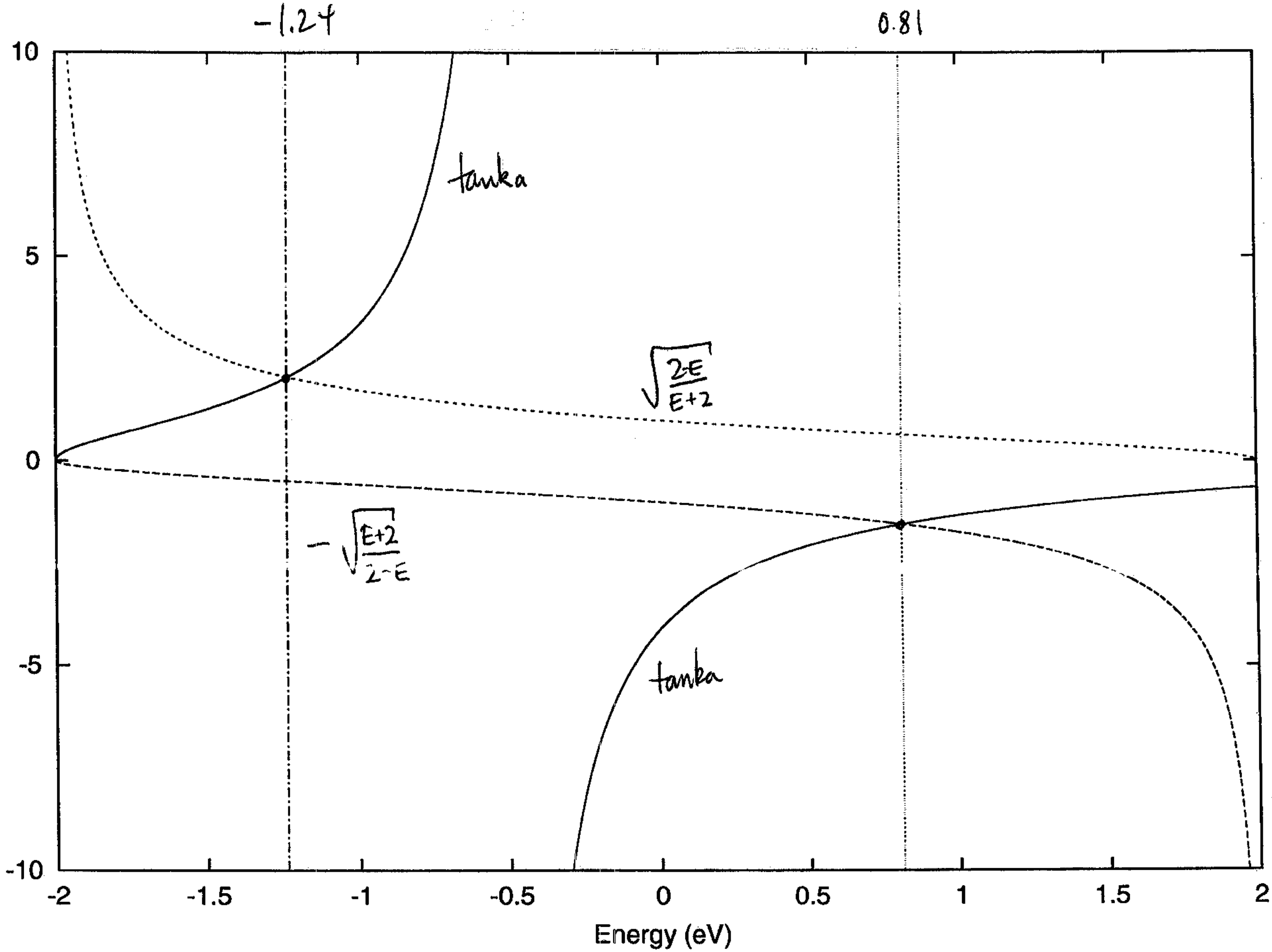
In terms of energy,

$$\tan\left(\sqrt{26.2}\,(0.25)\sqrt{E+2}\right) = -\sqrt{\frac{E+2}{2-E}} \text{ or } \sqrt{\frac{2-E}{E+2}} \quad (E \text{ in eV})$$

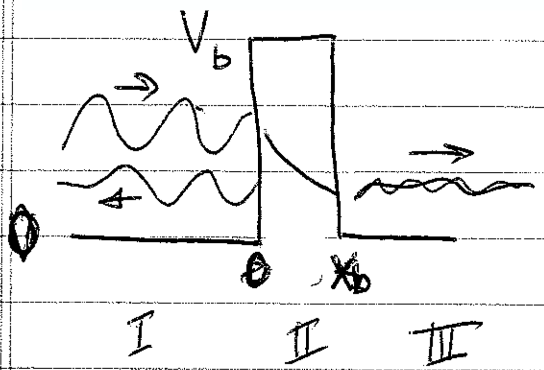
From graph:

$E = -1.24\text{eV}$ or

0.81eV


-1.24
0.81
10
5
0
-5
-10
-2
-1.5
-1
-0.5
0
0.5
1
1.5
2
Energy (eV)
tanka
tanka
$\sqrt{\frac{2-E}{E+2}}$
$-\sqrt{\frac{E+2}{2-E}}$

4.



In regions I & III

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} E \psi = 0$$

$$\psi_I = Ae^{ik_1x} + Be^{-ik_1x}$$

where $k_1 = \sqrt{\frac{2mE}{\hbar^2}}$

$$\psi_{III} = Ce^{ik_1x} + De^{-ik_1x}$$

In region II, $\frac{d^2\psi}{dx^2} - \frac{2m}{\hbar^2}(V_b - E)\psi = 0$

$$\psi_{II} = Ee^{k_2x} + Fe^{-k_2x}, \text{ where } k_2 = \sqrt{\frac{2m}{\hbar^2}(V_b - E)}$$

If we have incident wave from left, then there is only positive-going wave in region III, as there is no reflection from right (no change in potential), so $D = 0$

Also since we are looking at ratios to get transmission or reflection coefficients, the magnitude on incoming wave is irrelevant and we can take $A = 1$ to simplify

Match BC (continuity of ψ & ψ') at $x=0$ & $x=x_b$ to get 4 equations and 4 unknowns (B, C, E, F).

At $x=0$: $1+B = E+F \Rightarrow B = E+F-1$ [1]

$ik_1(1-B) = k_2(E-F)$ [2]

$ik_1(2-E-F) = k_2(E-F)$ [1] in [2]

$(k_2 - ik_1)F + 2ik_1 = (k_2+ik_1)E$

At $x=x_b$: $Ee^{k_2x_b} + Fe^{-k_2x_b} = Ce^{ik_1x_b} = C'$ [3]

$k_2[Ee^{k_2x_b} - Fe^{-k_2x_b}] = ik_1C'$ [4]

$2k_2Ee^{k_2x_b} = (k_2+ik_1)C'$ k_2[3]+[4]

$2k_2Fe^{-k_2x_b} = (k_2-ik_1)C'$ k_2[3]−[4]

$$(k_2-ik_1)\frac{(k_2-ik_1)C'}{2k_2e^{-k_2x_b}} + 2ik_1 = (k_2+ik_1)\frac{(k_2+ik_1)C'}{2k_2e^{k_2x_b}}$$

$$C' = \frac{(2ik_1)(2k_2)}{(k_2+ik_1)^2e^{-k_2x_b} - (k_2-ik_1)^2e^{k_2x_b}}$$

$$= \frac{4ik_1k_2}{(k_2^2+2ik_1k_2-k_1^2)e^{-k_2x_b} - (k_2^2+2ik_1k_2-k_1^2)e^{k_2x_b}}$$

$$= \frac{2\cancel{4}ik_1k_2}{2\cancel{4}ik_1k_2\cosh(k_2x_b) - \cancel{2}(k_2^2-k_1^2)\sinh(k_2x_b)}$$

Since $A=1$, $$T = |C'|^2 = \frac{4k_1^2k_2^2}{4k_1^2k_2^2\cosh^2(k_2x_b) + (k_2^2-k_1^2)^2\sinh^2(k_2x_b)}$$

For $x_b \gg \frac{1}{k_2}$, $\cosh(k_2x_b) \cong \sinh(k_2x_b) \cong \frac{1}{2}e^{k_2x_b}$

so $$T \cong \frac{16k_1^2k_2^2}{(k_1^2+k_2^2)^2}e^{-2k_2x_b} = \frac{16(E)(E-V_b)}{V_b^2}e^{-2k_2x_b}$$