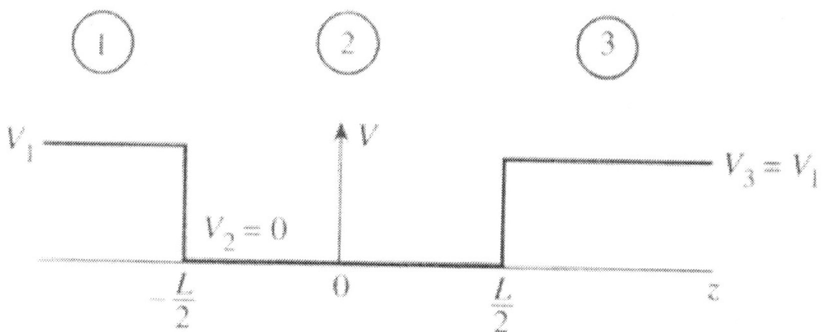
ECE 3080 Homework 2 Solutions

1.) An electron is contained in a FINITE potential well as shown below. As discussed in class, the finite potential barriers result in the electron wave function penetrating in to the barriers a small distance. Use the Schrödinger equation to solve for the allowable energy values inside the well for a.) Electron wave function solution for electron energy, $E>V_1$ and b.) Use a well width, L=5 angstroms and potential, V1=1.6e-18 Joules, to find the Electron energy, $E<V_1$.

Hints for part a: Very similar to what was done in class. There is no need to find all the coefficients.

Hints for part b: Assume a symmetric solution in region 2 of the General form: Ψ=Acos(kz) (actually there are also asymmetric solutions of the form, Ψ=Asin(kz), but we will ignore those in this homework). Use the normalization condition to show that the wave function must be finite at +/- infinity, thus eliminating two coefficients from the total number of general solution coefficients. Then use the continuity of the wave function and continuity of it's derivative as it passes through a boundary to solve for the remaining coefficients. Your final answer will be a transcendental equation in energy (what you are asked to find) and may be solved numerically or graphically for a series of allowable energy values.



2.) Describe the effect of band curvature on the effective mass.
3.) Describe the effect of band slope on the particle velocity.
4.) What is the effect of confining a particle in a localized region as opposed to allowing it to travel throughout free space? Explain by drawing an E-k relationship for both cases.
5.) How is a direct bandgap material different from an indirect bandgap material.
6.) If a state is above the fermi energy, is it likely to be empty or filled?
7.) Briefly describe the various ways a quantum particle can be reflected or transmitted at a potential barrier.

1.d) For $E > V_1$ any allowed Energy is possible

Region 1 = Region 3:

$$\psi_1(z) = \psi_3(z) = Ae^{+ik_1 z} + Be^{-ik_1 z}$$

where $k_1 = \frac{2\pi}{\lambda_1} = \sqrt{\frac{2m(E-V_1)}{\hbar^2}}$

Region 2:

$$\psi_2(z) = Ce^{+ik_2 z} + De^{-ik_2 z}$$

where $k_2 = \frac{2\pi}{\lambda_2} = \sqrt{\frac{2m}{\hbar^2} E}$

Note: I did not ask you to solve for the coefficients $A \to D$.

1.b) See next page

You may show your work here

1. b) Region 1: $\psi_1(z) = Ce^{-k_1 z} + De^{+k_1 z}$

Region 3: $\psi_3(z) = Ee^{-k_1 z} + Fe^{+k_1 z}$

where $k_1 = \sqrt{\frac{2m}{\hbar^2}(V_1 - E)}$

Region 2: $\psi_2(z) = A\cos k_2 z$

where $k_2 = \sqrt{\frac{2m}{\hbar^2}E}$

- Since $\int_{-\infty}^{\infty} \psi^*(z)\psi(z)dz = 1$, $\psi(z)$ can not "blow up" @ $z = \infty$ or $z = -\infty$. Thus, $C = F = 0$ otherwise $\psi(z \to \pm\infty) \to \infty$

- Since Cosine is an even function, at the boundaries $\pm\frac{L}{2}$ $\psi_1(-\frac{L}{2}) = \psi_3(\frac{L}{2})$ since $\underbrace{\psi_2(-\frac{L}{2}) = \psi_2(\frac{L}{2})}_{\text{cosine is even}}$ and $\underbrace{\psi_1(-\frac{L}{2}) = \psi_2(-\frac{L}{2}) \text{ and } \psi_3(\frac{L}{2}) = \psi_2(\frac{L}{2})}_{\text{Boundry continuity}}$

$\Longrightarrow$ $\underline{D = E}$ and $\psi_1(z) = \psi_2(-z)$

Now we can apply boundary continuity:

$\psi_2(\frac{L}{2}) = \psi_3(\frac{L}{2}) \Rightarrow A\cos(k_2\frac{L}{2}) = Ee^{-(k_1\frac{L}{2})}$

From the continuity of the derivative,

$\left.\frac{d\psi_2}{dz}\right|_{z=\frac{L}{2}} = \left.\frac{d\psi_3}{dz}\right|_{z=\frac{L}{2}} \Rightarrow Ak_2\sin(k_2\frac{L}{2}) = -Ek_1e^{-k_1 z}$

1.b cont'd)

You may show your work here

Thus, $A\cos\left(k_2 \frac{L}{2}\right) - E e^{-\left(k_1 \frac{L}{2}\right)} = 0$

$A\, k_2 \sin\left(k_2 \frac{L}{2}\right) + E\, k_1 e^{-\left(k_1 \frac{L}{2}\right)} = 0$

To solve, take the determinant $= 0$

$$\begin{vmatrix} \cos\left(k_2 \frac{L}{2}\right) & -e^{-\left(k_1 \frac{L}{2}\right)} \\ k_2 \sin\left(k_2 \frac{L}{2}\right) & +k_1 e^{-\left(k_1 \frac{L}{2}\right)} \end{vmatrix} = 0$$

$$k_1 \cos\left(k_2 \frac{L}{2}\right) e^{-\left(k_1 \frac{L}{2}\right)} + k_2 \sin\left(k_2 \frac{L}{2}\right) e^{-\left(k_1 \frac{L}{2}\right)} = 0$$

Divide by $\cos\left(k_2 \frac{L}{2}\right) e^{-\left(k_1 \frac{L}{2}\right)}$

$$-k_1 = k_2 \tan\left(k_2 \frac{L}{2}\right)$$

Substituting for k_1 and k_2,

$$-\cancel{\sqrt{\frac{2m}{\hbar^2}}}\sqrt{(V_1 - E)} = \cancel{\sqrt{\frac{2m}{\hbar^2}}}\sqrt{E}\ \tan\left(\sqrt{\left(\frac{2m}{\hbar^2}\right) E}\left(\frac{L}{2}\right)\right)$$

For values given:

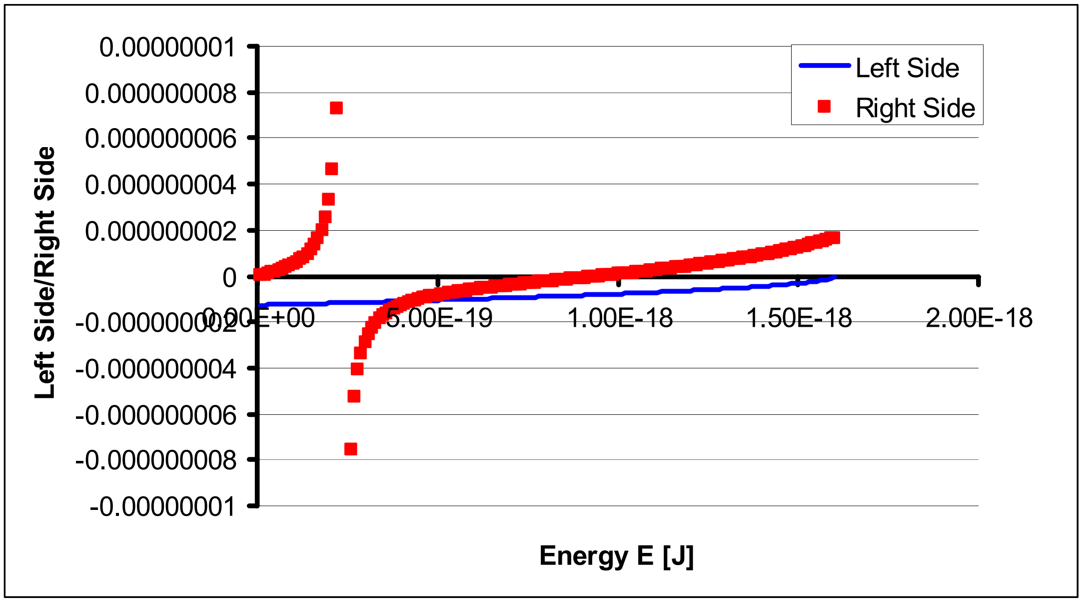
$m = 9.1 \times 10^{-31}$ kg $\quad \hbar = 1.05 \times 10^{-34}$ Js

$\frac{L}{2} = 5 \times 10^{-10}$ m $\quad , V_1 = 1.6 \times 10^{-18}$ J

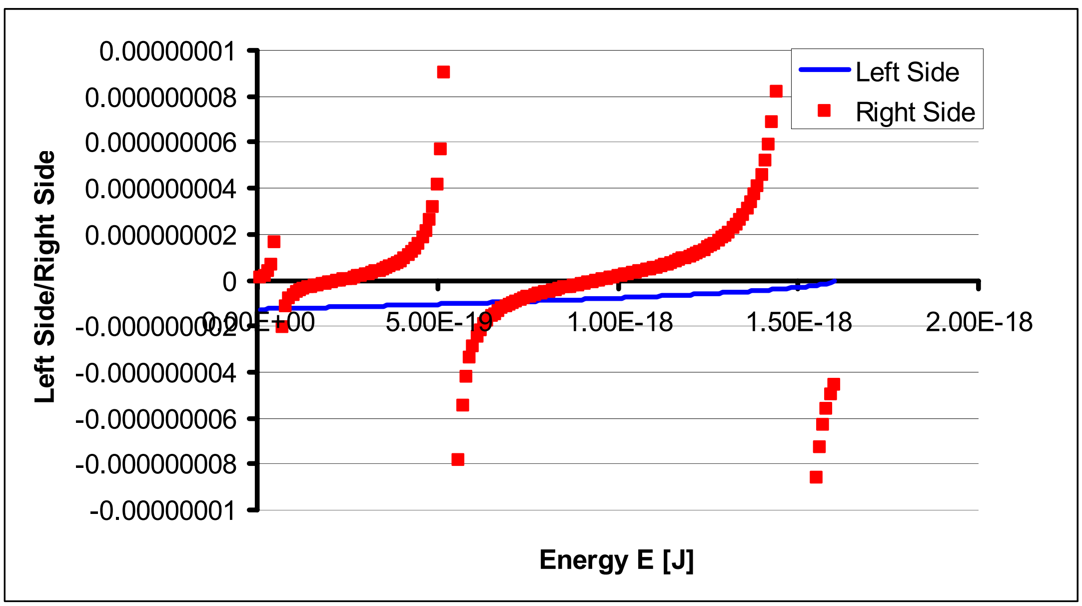
$$-\sqrt{1.6 \times 10^{-18} - E} = \sqrt{E}\ \tan\left(\left(2.5 \times 10^{-10}\right)\sqrt{1.65 \times 10^{38}}\sqrt{E}\right)$$

$$\boxed{E \approx (4.3 - 4.4\text{e-}19 \text{ J}}$$

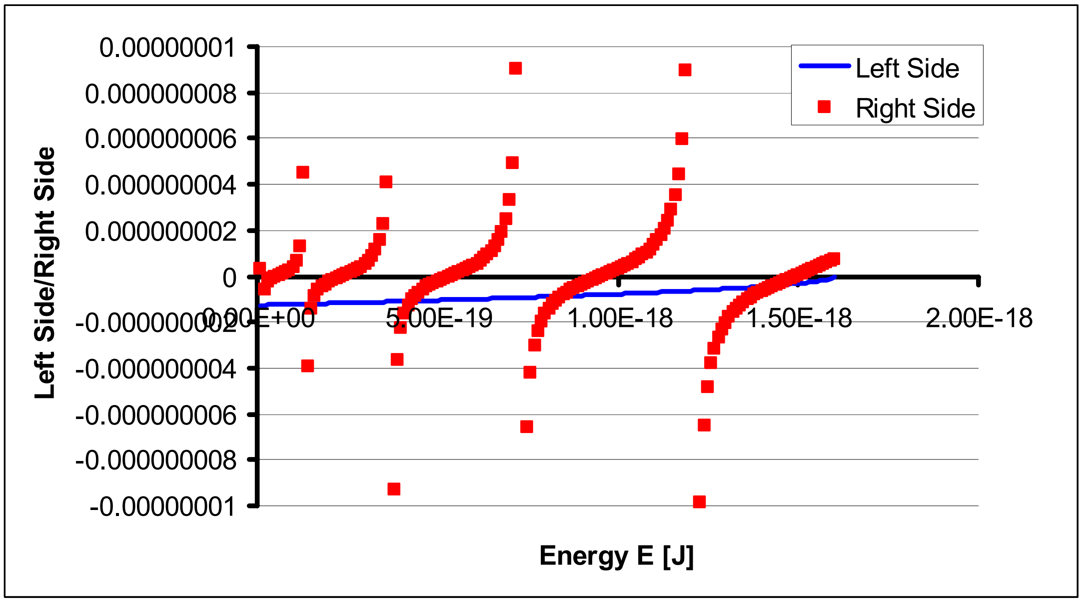
The plot of the left side verses right side is shown below. Note that there is only one intersection of the blue/red curve so we have only one solution for E~(4.3-4.5)x10^{-19} J.



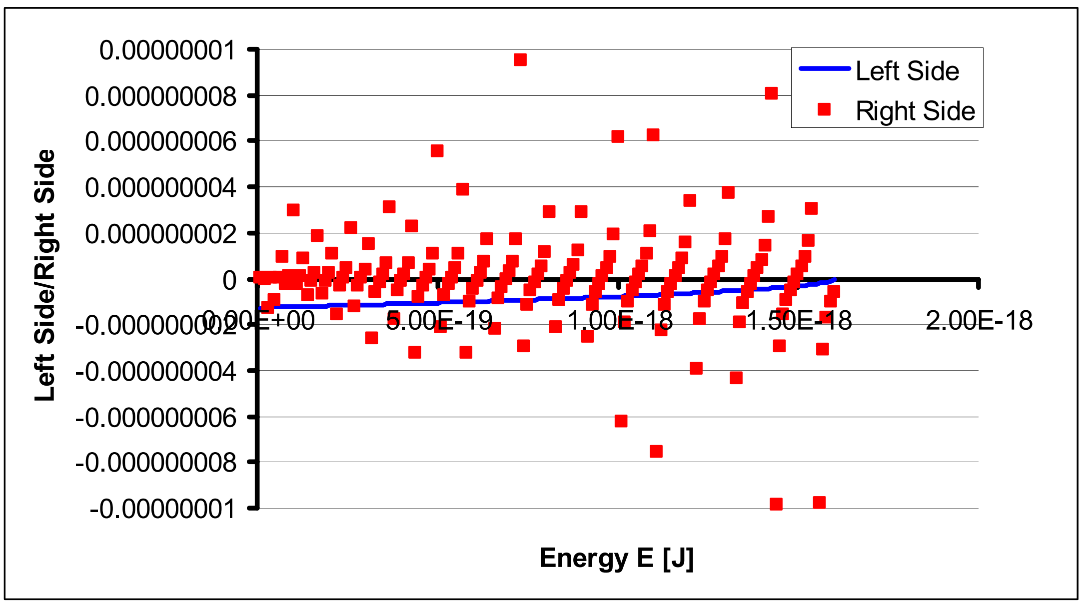
The following three plots are for L=10e-10 m, 20e-10 m and 100e-10 m. Note how more allowed energy values result as the particle is less constrained in space (i.e. exists in a bigger well width).



...L=10e-10 m results in 2 solutions...



...L=20e-10 m results in 4 solutions...



...L=100e-10 m results in >20 solutions...

Thus, as we move toward larger sizes for a confined particle, we loose quantization and start to result in very closely spaced energies that approximate a continuum. This occurs at fairly small distances on the order of ~100 angstroms (~100e-10 m).

2.) Higher curvature results in smaller effective mass since

$$m^* = \frac{\hbar^2}{\underbrace{\left(\frac{d^2E}{dk^2}\right)}_{=\text{ curvature}}}$$

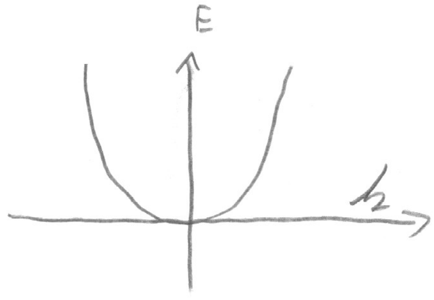
3.) Higher slope results in a higher group velocity since

$$v_g = \frac{1}{\hbar}\underbrace{\frac{dE}{dk}}_{\Downarrow \text{ slope}}$$

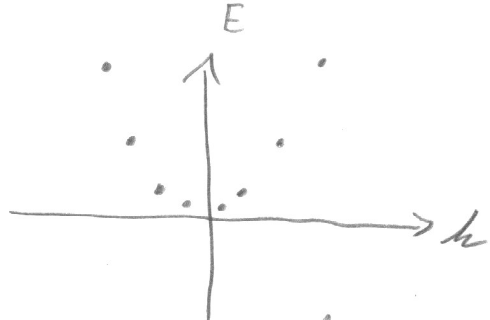
4.) When the particle is confined in a small space the allowed energies and momentum values are "quantized" (i.e. can only take on certain values).

In free space any energy/momentum value is allowed as long as it satisfies

$$E = \frac{\hbar^2 k^2}{2m} = \frac{\langle p \rangle^2}{2m}$$

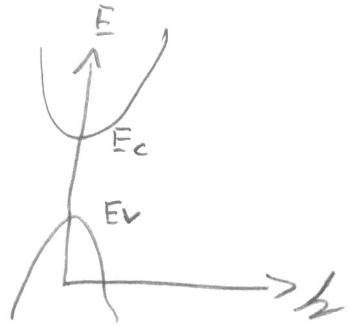


Free space

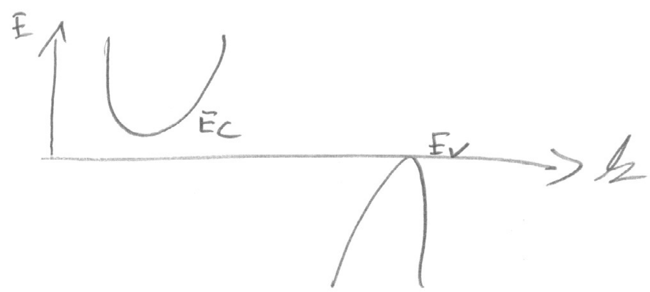


Confined particle

5.) A direct bandgap material has the momentum of electrons in the conduction band valley equal to the momentum of holes at the peak of the valence band such as,

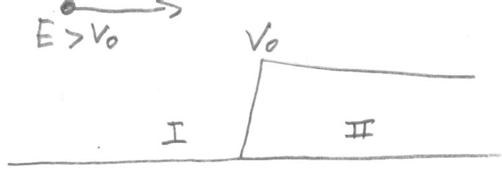


An indirect bandgap material has the momentum of electrons in the conduction band valley differing from the momentum of holes at the peak of the valence band.



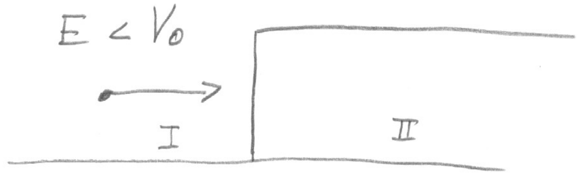
6.) A state above the fermi energy is most likely empty.

7.)



case 1) For $E > V_0$, the particle can be reflected or transmitted. If it is transmitted only it's wavelength changes.

Case 2)



For $E < V_0$, the particle can still penitrate into a shallow region of the barrier but it's wavefunction dies off exponentially with distance. The electron can also be reflected.

The probability of reflection in either case is:

$$R^*R \quad \text{where } R = \frac{k_I - k_{II}}{k_I + k_{II}}$$

The probability of transmission in either case is:

$$T^*T \quad \text{where } T = \frac{2k_I}{k_I + k_{II}}$$

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

$$k_2 = \sqrt{\frac{2m}{\hbar^2}(E-V)} = \frac{2\pi}{\lambda_{II}}$$