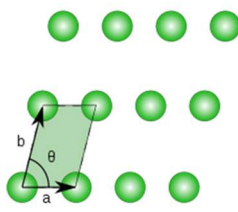
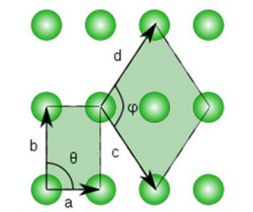
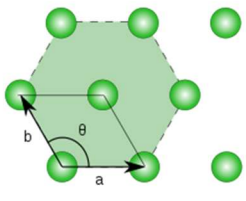
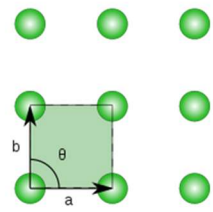


1. The following are the 5 Bravais lattices possible in two-dimensions (2D). Evaluate the highest packing fraction possible for a 2D Bravais lattice. (You may carefully eliminate options by qualitative arguments where possible, instead of calculating the packing fraction for each type.) [5]

 <p style="text-align: center;">Oblique</p>	 <p style="text-align: center;">Rectangular</p>	 <p style="text-align: center;">Hexagonal</p>	 <p style="text-align: center;">Square</p>
$ a \neq b , \theta \neq 90^\circ$ <p style="text-align: center;">m</p>	$ a \neq b , \theta = 90^\circ$ $ c = d , \phi \neq 90^\circ$ <p style="text-align: center;">o</p>	$ a = b , \theta = 120^\circ$ <p style="text-align: center;">h</p>	$ a = b , \theta = 90^\circ$ <p style="text-align: center;">t</p>

Packing fraction for lattice type:

- (i) Square: $(\pi a^2/4)/a^2 = \pi/4$ [1]
 (ii) Hexagonal: $(\pi a^2/4) / (\sqrt{3}a^2/2) = \pi / 2\sqrt{3}$ [1]
 (iii) Rhombic: Can be close packed only when $\phi = 60^\circ$, viz. the hexagonal case [1]

Similarly, rectangular and oblique can be close packed only in the cases where they reduce to the square or hexagonal case. [1+1]

Therefore, the maximal packing fraction is for the hexagonal.

2. Consider a particle of energy $E > 0$ impinging as a plane wave on a delta-function potential barrier $V = \alpha \cdot \delta(x)$, where $\alpha \in \mathbb{R}$ and $\alpha > 0$.
 (a) Derive the discontinuity in the first-derivative of the wavefunction at $x = 0$. [1]

The Schrödinger equation in this case is:

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

Let us integrate this in neighborhood of $x = 0$ from $x = -\varepsilon$ to $x = +\varepsilon$.

$$\int_{-\varepsilon}^{+\varepsilon} \frac{-\hbar^2}{2m} \frac{d^2\psi}{dx^2} dx + \int_{-\varepsilon}^{+\varepsilon} \alpha \delta(x) \psi dx = E \int_{-\varepsilon}^{+\varepsilon} \psi dx$$

[0.5]

Now as $\varepsilon \rightarrow 0$, we have:

$$\frac{-\hbar^2}{2m} \left[\Delta \left(\frac{d\psi}{dx} \right) \right]_{x=0} + \alpha \psi(0) = 0$$

$$\left[\Delta \left(\frac{d\psi}{dx} \right) \right]_{x=0} = \frac{2m\alpha}{\hbar^2} \psi(0)$$

[0.5]

(b) Derive the probabilities for transmission through, and reflection from, the barrier. [4]

The solutions to the Schrodinger Equation are plane- waves of the form $e^{\pm ikx}$, we assume a plane wave Ae^{ikx} incident from the left and no incident wave from the right. Let the reflected and transmitted wave be Be^{-ikx} and Fe^{ikx} respectively.

Now, continuity of the wave function at the origin implies:

$$A + B = F \quad [0.5]$$

The above calculated discontinuity in the derivative of the wavefunction implies:

$$ikF - ikA + ikB = (2m\alpha/\hbar^2)F \quad [0.5]$$

Putting these together and eliminating B :

$$F(1 - (m\alpha/ik\hbar^2)) = A \quad [1]$$

The transmission amplitude is:

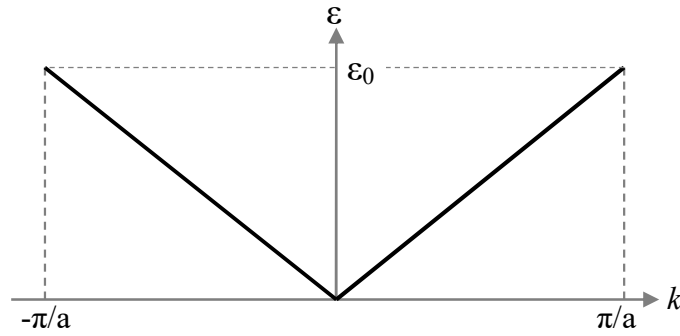
$$t = F/A = 1/(1 - (m\alpha/ik\hbar^2))$$

Therefore, the transmission and reflection probabilities are:

$$T = |t|^2 = 1/(1 + (m\alpha/k\hbar^2)^2) = 1/(1 + (m\alpha^2/2E\hbar^2)) \quad [1]$$

$$R = 1 - T = 1/(1 + (2E\hbar^2/m\alpha^2)) \quad [1]$$

3. Consider the linear dispersion relation for a one-dimensional crystalline solid shown below, shown in the reduced zone scheme. Symbols have their usual meaning. Ignore all other energy bands.



- (a) Write down the ε - k relation for all k . [1]

$$\varepsilon = \left(\frac{a\varepsilon_0}{\pi}\right) |k|, \text{ for } |k| \leq \frac{\pi}{a}$$

$$\varepsilon\left(k + \frac{2\pi}{a}\right) = \varepsilon(k) \quad [0.5+0.5]$$

- (b) Derive the expression for the group velocity of electrons in this band as a function of k . [2]

The following semiclassical equation relates the group velocity of the electron wave in the periodic crystal to the slope of the dispersion relation:

$$v = \frac{1}{\hbar} \frac{\partial \varepsilon}{\partial k}$$

$$v = \frac{1}{\hbar} \frac{\partial}{\partial k} \left(\frac{a\varepsilon_0}{\pi}\right) |k| = \left(\frac{a\varepsilon_0}{\pi\hbar}\right) \text{sgn}(k) \cong v_0 \text{sgn}(k), \text{ for } |k| \leq \frac{\pi}{a}$$

[1+1]

4. Consider the quantum well for electrons, with two bound states, formed in the heterostructure shown below. In the X-Y plane, electrons obey the dispersion relation:

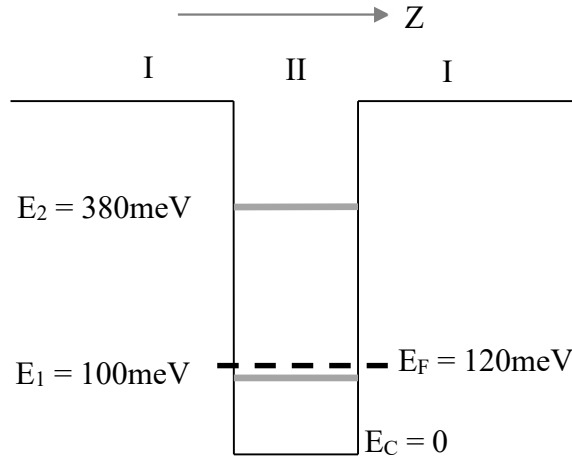
$$E = \frac{\hbar^2 k_x^2}{2m_1} + \frac{\hbar^2 k_y^2}{2m_2}$$

- (a) The ‘density of states (DOS) effective mass’ (viz. averaged effective mass to be used for a DOS calculation) is then given by $m_{dos}^* = \sqrt{m_1 m_2}$. Give a concise justification for this. [1]

If we consider the circle of equal area in k-space, we will have the same number of k-states therein, and therefore we will arrive at the same DOS. Thus, the DOS effective mass may be obtained from:

$$\begin{aligned}\pi k_{eff}^2 &= \pi k_1 k_2 \Rightarrow k_{eff}^2 = k_1 k_2 \\ \Rightarrow 2m_{eff}\varepsilon/\hbar^2 &= \sqrt{2m_1\varepsilon/\hbar^2} \cdot \sqrt{2m_2\varepsilon/\hbar^2} \quad [1] \\ \Rightarrow m_{eff} &= \sqrt{m_1 m_2}\end{aligned}$$

- (b) Suppose the 2D DOS $g \cong m_{dos}^*/\pi \hbar^2 = 10^{14} \text{cm}^{-2} \text{eV}^{-1}$. Calculate the 2D carrier density at 300K. Clearly justify any assumptions you make. [4]



The carrier density is given by:

$$n_{2D} \approx \int_{E_1}^{\infty} g_{2D}(E) f_{FD}(E) dE \quad [1]$$

$$n_{2D} \approx g \int_{E_1}^{\infty} f_{FD}(E) dE$$

Now,

$$\int_{E_1}^{\infty} f_{FD}(E) dE = \int_{E_1}^{\infty} \frac{1}{e^{(E-E_F)/kT} + 1} dE$$

It turns out the integral can be evaluated simply for this 2D case, using:

$$\int \frac{d\zeta}{e^{\zeta} + 1} = \zeta - \ln(1 + e^{\zeta}) + C \quad [1]$$

This yields:

$$\int_{E_1}^{\infty} f_{FD}(E) dE = \int_{E_1}^{\infty} \frac{1}{e^{(E-E_F)/kT} + 1} dE = kT [\ln(1 + e^{(E_1-E_F)/kT}) - (E_1 - E_F)/kT]$$

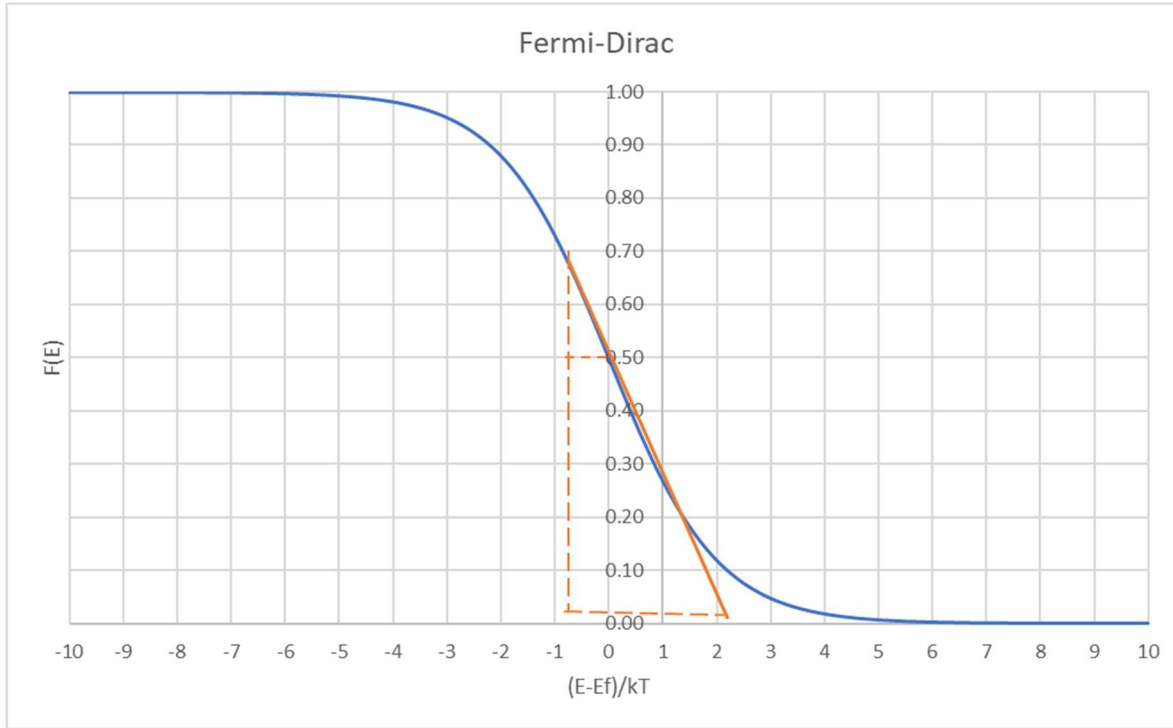
For the given values:

$$\int_{E_1}^{\infty} f_{FD}(E) dE = 1.15kT \quad [1]$$

$$n_{2D} \approx g \int_{E_1}^{\infty} f_{FD}(E) dE = 10^{14} \times 1.15 \times 0.026 \text{ cm}^{-2} = 3 \times 10^{12} \text{ cm}^{-2}$$

[1]

Alternatively, an approximate geometrical evaluation of the Fermi integral could also have been done as shown below, for full points. Extending the shown line to 2kT (or 3kT) on the X-axis introduces an underestimate of 14% (or, overestimate of 12%).



5. We have a thin sample of a semiconductor with bandgap 1eV, an intrinsic carrier concentration of 10^{10} cm^{-3} at room temperature, n-doping of 10^{15} cm^{-3} , and electron (hole) mobility of 1000 (500) $\text{cm}^2 \text{V}^{-1} \text{s}^{-1}$, and lifetime of 1ms. Suppose it is irradiated uniformly with light such that the steady-state electron-hole pair generation rate everywhere is $10^{20} \text{ s}^{-1} \text{ cm}^{-3}$.
- (a) Draw a quantitatively labeled band-diagram. Include the equilibrium Fermi level therein. [5]

First we need to calculate the excess carrier concentrations.

The low-level injection formula would yield a minority carrier concentration: $\delta n = \delta p = G\tau_p = 10^{17} \text{ cm}^{-3}$. This is clearly not a low-level injection scenario, but it would beget full points. [1]

It is possible to determine the minority carrier concentration for this high level injection case as follows.

$$R = \alpha(np - n_i^2)$$

$$\text{For low-level injection: } G = R_{low} = \alpha n_0 \delta p = \delta p / \tau$$

$$\text{Therefore, } \alpha = 1/(n_0 \tau) = 10^{-1} \text{ cm}^3 \text{ s}^{-1}$$

For high-level injection: $G = R_{high} = \alpha(\delta p)^2$

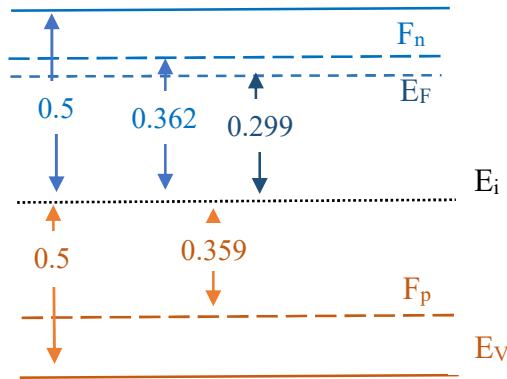
Therefore, $\delta n = \delta p = \sqrt{G/\alpha} = 10^{16} \text{ cm}^{-3}$

The semiconductor has a bandgap of 1eV.

Using the formulas:

$n_0 = n_i \exp((E_F - E_i)/kT)$ for the equilibrium electron concentration, and

$n = n_i \exp((F_n - E_i)/kT)$ and $p = n_i \exp((E_i - F_p)/kT)$ for the non-equilibrium distributions characterized by quasi-Fermi levels, the band diagram is as follows (with the high level injection formula; with the low-level injection formula, the energy difference between quasi-Fermi level and intrinsic Fermi level of 0.36eV would be about 0.42eV).



Marking: Ec, Ev, Ei placement [1]; Ef placement [1]; Fn placement [1]; Fp placement [1]

(b) What is the percentage change in the conductivity of the sample upon illumination? [2]

The fractional change in the conductivity is given by:

$$\frac{((n_0 + \delta n)q\mu_n + (p_0 + \delta p)q\mu_p) - (n_0q\mu_n + p_0q\mu_p)}{(n_0q\mu_n + p_0q\mu_p)}$$

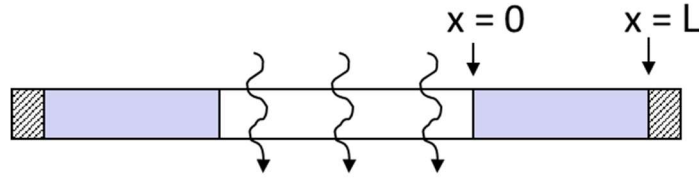
[1]

$$= \frac{(10^{16} \times 1100 + 10^{16} \times 500) - 10^{15} \times 1000}{10^{15} \times 1000} = 15$$

[1]

Therefore, the percentage change is 1400%. This is with the high-level injection formula. Going with the low-level injection formula, the fractional change would be 150, viz. 15000%.

6. Consider an n-doped semiconductor bar illuminated in the middle – as illustrated below. Assume steady-state conditions throughout this problem. Assume that the length of the unilluminated segment, L , is much less than the minority carrier diffusion length λ .



Suppose the generation rate everywhere in the illuminated segment is G , and the minority carrier lifetime everywhere is τ .

- (a) What is the excess minority carrier concentration at $x = 0$? [1]

The excess hole concentration at $x = 0$ is given by:

$$\delta p(0) = G \cdot \tau \dots (1) \quad [1]$$

- (b) The contact at $x = L$ has a hole surface recombination velocity S_p , defined below. Determine the excess minority carrier concentration profile for $x \in [0, L]$ in terms of the given parameters. [4]

$$S_p \cong \frac{\text{Hole current flowing into contact}}{\text{Excess hole charge at } x=L^-}$$

The steady-state hole continuity equation is:

$$-\frac{1}{q} \frac{\partial J_p}{\partial x} + G_p - R_p = 0 \dots (2)$$

$$\text{In the range } x \in [0, L], \text{ there is no G-R. Hence we have: } -\frac{1}{q} \frac{\partial J_p}{\partial x} = 0 \dots (3)$$

$$\text{The hole diffusion current is given by: } J_p = -qD_p \frac{\partial p}{\partial x} = -qD_p \frac{\partial (\delta p)}{\partial x} \dots (4)$$

$$\text{Substituting (4) in (3): } \frac{\partial^2 (\delta p)}{\partial x^2} = 0 \dots (5) \quad [1]$$

$$\text{Integrating twice, we get: } \delta p(x) = Ax + B \dots (6)$$

Using (1) for the boundary condition on the LHS, i.e. at $x = 0$, we get from (6):

$$B = G \cdot \tau \dots (7)$$

$$\text{Eq. (6) implies that the diffusion current is: } J_p = -qD_p \frac{\partial p}{\partial x} = -qD_p \cdot A \dots (8)$$

The boundary condition at $x = L$ is from the surface recombination velocity on the RHS contact:

$$S_p \cong \frac{\text{Hole current flowing into contact}}{\text{Excess hole charge at } x = L} = \frac{-qD_p A}{\delta p(L)} \quad [1]$$

$$\Rightarrow A = -\frac{S_p \delta p(L)}{qD_p} = \dots (9)$$

$$\text{Substituting (9) and (7) in (6) for } x = L: \delta p(L) = -\frac{S_p \delta p(L)}{qD_p} L + G\tau \dots (10) \quad [1]$$

$$\therefore \delta p(L) \left[1 + \frac{S_p L}{qD_p} \right] = G\tau \Rightarrow \delta p(L) = \frac{G\tau}{\left(1 + S_p L / qD_p \right)} \Rightarrow A = -\frac{G\tau \cdot S_p / qD_p}{\left(1 + S_p L / qD_p \right)} \dots (11)$$

$$\text{Finally: } \delta p(x) = G\tau \left[1 - \frac{S_p x / qD_p}{\left(1 + S_p L / qD_p \right)} \right] \quad [1]$$

{Note that for an ideal contact, $S_p \rightarrow \infty$, $\delta p(L) \rightarrow 0$ as expected. While for a contact which cannot source or sink any carriers, $S_p \rightarrow 0 \Rightarrow \delta p(x) = G\tau \forall x$ as expected.}