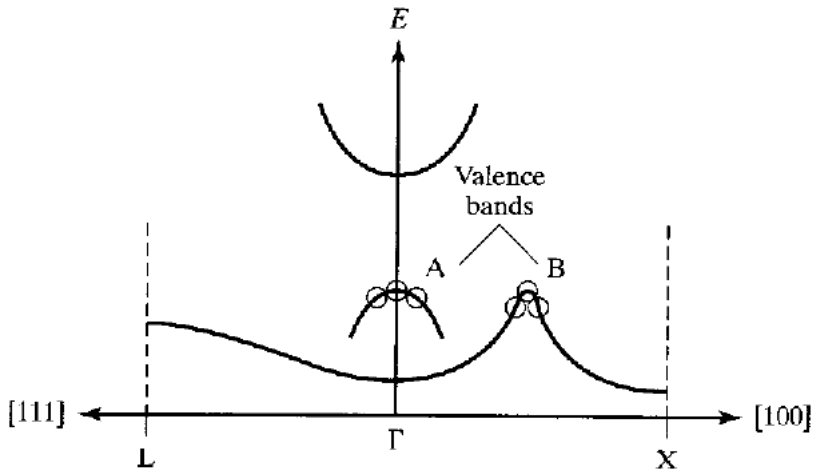
Assignment 2 (Maximum Marks: 50)

General Instructions:

1) The submission deadline is 27th August 2018 (Monday), 11:59pm.
2) Please state clearly the assumptions and the values of the constants used while solving the problems.
3) Please submit Matlab codes along with the solutions in PDF format.

Q. 1) The E-k plot of a material is as shown in the figure below:



Which set of holes, band A or band B will exhibit greater [100] direction effective mass? **(2 marks)**

Sol) Holes in band A will exhibit greater [100] direction effective mass because

$$m^* = \frac{\hbar^2}{\left(\partial^2 E / \partial k^2\right)}$$

Q. 2) The E-k band diagram of 1D periodic lattice can be defined as $E_k = E_o - 2E_1\cos(ka)$, where $E_o = 2E_1$. An electric field of magnitude $-\xi_o$ is applied across the solid. Derive and plot the expressions for the group velocity and the trajectory of the electron movement in the solid under the effect of electric field. Comment on the movement of electrons. **(3+2 = 5 marks)**

Sol)

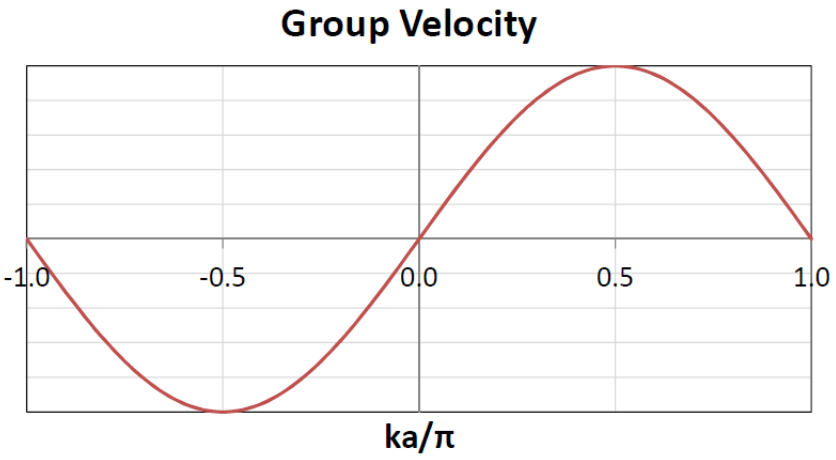
$$\hbar\frac{dk}{dt} = -eE = eE_0$$

$$\Rightarrow k = k(0) + \left(\frac{eE_0}{\hbar}\right)\cdot t = \frac{eE_0 t}{\hbar}$$

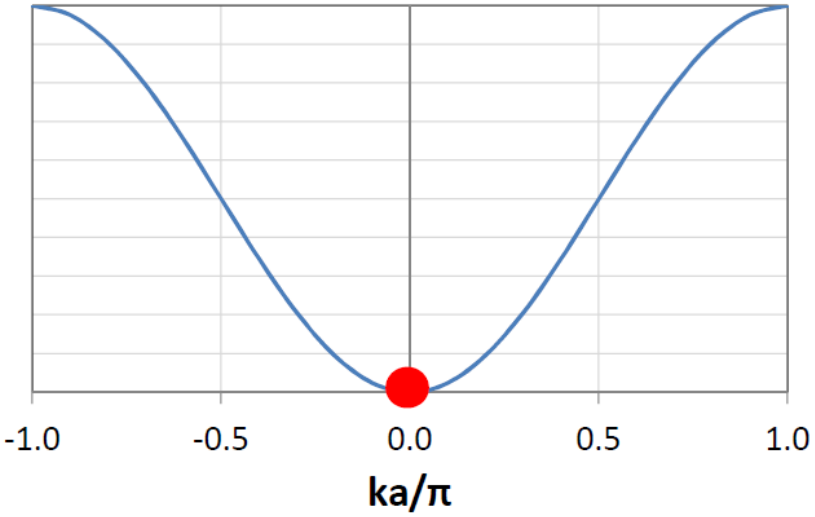
$$v = \frac{1}{\hbar}\frac{\partial \varepsilon_k}{\partial k} = \frac{2\varepsilon_1 a}{\hbar}\sin\left(\frac{eE_0 a}{\hbar}\cdot t\right) = v_0 \sin\omega t$$

$$v = \frac{\mathrm{dr}}{dt} \Rightarrow r = \frac{v_0}{\omega}(1-\cos\omega t)$$

$$r = \frac{v_0}{\omega}(1-\cos\omega t) \qquad v = \frac{2\varepsilon_1 a}{\hbar}\sin\left(\frac{eE_0 a}{\hbar}\cdot t\right) = v_0 \sin\omega t$$



$$r = \frac{v_0}{\omega}(1-\cos\omega t) \qquad v = \frac{2\varepsilon_1 a}{\hbar}\sin\left(\frac{eE_0 a}{\hbar}\cdot t\right) = v_0 \sin\omega t$$



Q. 3) The E-k relationship characterizing an electron confined to a two-dimensional surface layer is of the form $E - E_C = \frac{\hbar^2 k_x^2}{2m_x} + \frac{\hbar^2 k_y^2}{2m_y}$.

a) If DOS of the material is $\frac{m^*}{\pi\hbar^2}$, then find the value of m^*.

b) An electric field is applied in x-y plane at a 45° angle to x-axis. Assuming electron to be at rest initially, find the acceleration of the electron along with its direction. **(2+3 = 5 marks)**

Sol) a)

Consider electrons in a 2D material satisfying the dispersion relation: $E = E_C + \frac{\hbar^2 k_x^2}{2m_1} + \frac{\hbar^2 k_y^2}{2m_2}$

Equal energy surface is given by:

$$\frac{k_x^2}{2m_1(E-E_C)/\hbar^2} + \frac{k_y^2}{2m_2(E-E_C)/\hbar^2} = 1$$

We want to transform this ellipse into a circle:

$$\frac{k_x^2}{2m^*(E-E_C)/\hbar^2} + \frac{k_y^2}{2m^*(E-E_C)/\hbar^2} = 1$$

To keep the area constant: $\pi ab = \pi r^2 \Rightarrow (m^*)^2 = m_1 m_2$

b)

$$\hbar\dot{\vec{k}} = \vec{F}_{ext} = \mathbf{M}\cdot\vec{a}$$

$$\vec{F}_{ext} = -qE_0\begin{bmatrix}\cos 45^0\\ \sin 45^0\end{bmatrix} = \frac{-qE_0}{\sqrt{2}}\begin{bmatrix}1\\1\end{bmatrix}$$

$$\vec{a} = \mathbf{M}^{-1}\cdot\vec{F}_{ext} = \frac{-qE_0}{\sqrt{2}}\begin{bmatrix}m_1^{-1} & 0\\ 0 & m_2^{-1}\end{bmatrix}\begin{bmatrix}1\\1\end{bmatrix}$$

$$\vec{a} = -\frac{eE_0}{\sqrt{2}m_1}\hat{x} - \frac{eE_0}{\sqrt{2}m_2}\hat{y}$$

Q. 4) Find the density of states for 0D and 1D materials and plot DOS vs E for each case. Give some examples for these systems. **(3+3+1+1 = 8 marks)**

Sol)

- **1D DOS:**
  Consider a 1D element at k and thickness dk in k-space.
  The total number of states in k to k+dk is:

  $$dN = spin\ degeneracy * \frac{length\ of\ the\ structure\ with\ thickness\ dk}{area\ of\ each\ k-state},$$

  $$dN = 2 * \frac{2dk}{\frac{2\pi}{L_x}}.$$

  Using dispersion relation

  $$E = \frac{\hbar^2(k_x^2+k_y^2+k_z^2)}{2m} = \frac{\hbar^2k^2}{2m} + \frac{\hbar^2\left[\left(\frac{n_y\pi}{L_y}\right)^2+\left(\frac{n_z\pi}{L_z}\right)^2\right]}{2m},$$

  where n_y, n_z are quantum numbers for states in quantized axis (here y- and z-axis).
  we can write, 1D DOS as following.

  $$g_{1D} = \frac{dn}{dE} = \frac{dN}{(L_xL_y)dE} = \frac{1}{\pi\hbar}\sqrt{\frac{2m}{E-\frac{\hbar^2\left[\left(\frac{n\pi}{L_y}\right)^2+\left(\frac{n\pi}{L_z}\right)^2\right]}{2m}}}.$$

Examples are: CNTs, nanowires, nanofibers.

- **0D DOS:**
  Available states exist only at discrete energies due to the fact that no free motion of electron is possible in a 0D structure. There is no k-space to be filled and hence,
  $g_{0D} = 2\delta(E - E_n)$.

Examples are: C_{60}, quantum dots, metal nanoparticles.

Q. 5) The dispersion relation of electrons in a 2D material is given as $E = \hbar v_F|k|$. Find the expression for density of states for the material. **(4 marks)**

Sol)

Number of states in a given k-space volume : $\Delta N = \frac{\Delta k}{\delta k} \times 2 = \left(\frac{L}{2\pi}\right)^2 \Delta k \times 2$

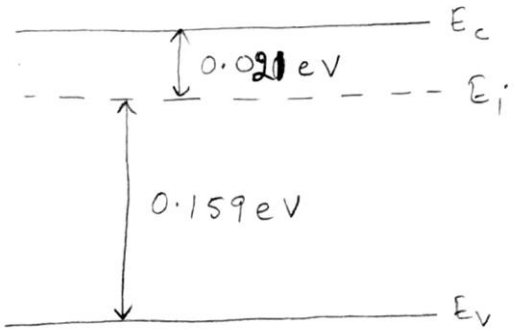
$$dN = \frac{L^2}{4\pi^2} 2 \cdot 2\pi k dk \xrightarrow{\text{per unit real-space volume}} dn = \frac{1}{\pi} k dk$$

$$g = \frac{dn}{d\varepsilon} = \frac{dn}{dk}\frac{dk}{d\varepsilon} \xrightarrow{\varepsilon = \frac{\hbar^2 k^2}{2m^*}} g = \frac{k}{\pi}\frac{m^*}{\hbar^2 k} = \frac{m^*}{\pi\hbar^2}$$

$$g = \frac{dn}{d\varepsilon} = \frac{dn}{dk}\frac{dk}{d\varepsilon} \xrightarrow{\varepsilon = \hbar v_F|\vec{k}|} g = \frac{k}{\pi}\frac{1}{\pm\hbar v_F} = \frac{\varepsilon}{\pi\hbar^2 v_F^2}$$

Q. 6) In InSb at 300 K, E_g = 0.18 eV (smallest band gap of all the semiconductor compounds), $m_n^* = 0.0116m_o$, $m_p^* = 0.4m_o$ and $n_i = 1.6 \times 10^{16}$ /cm^3. Find the position of intrinsic Fermi level (E_i) and comment on its position. Draw the energy band diagram indicating the position of E_i. **(4 marks)**

Sol)



$$E_i = \frac{E_g}{2} + \frac{k_B T}{2} \ln\left(\frac{N_v}{N_c}\right)$$

$$= 0.09 + \frac{0.026}{2} \cdot \frac{3}{2} \ln\left(\frac{m_p^*}{m_n^*}\right)$$

$$\Rightarrow E_i = 0.09 + 0.0195 \ln\left(\frac{0.4}{0.0116}\right)$$

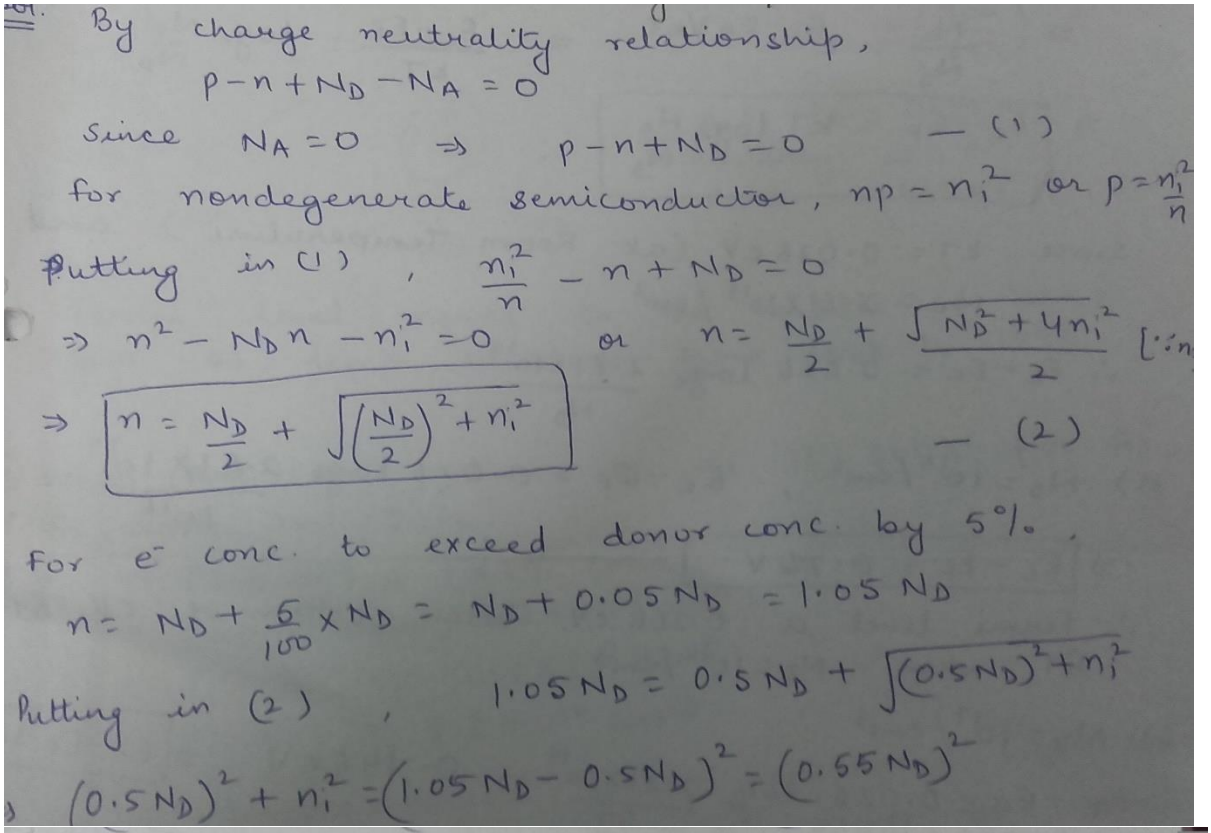
$$= (0.09 + 0.069)\,eV$$

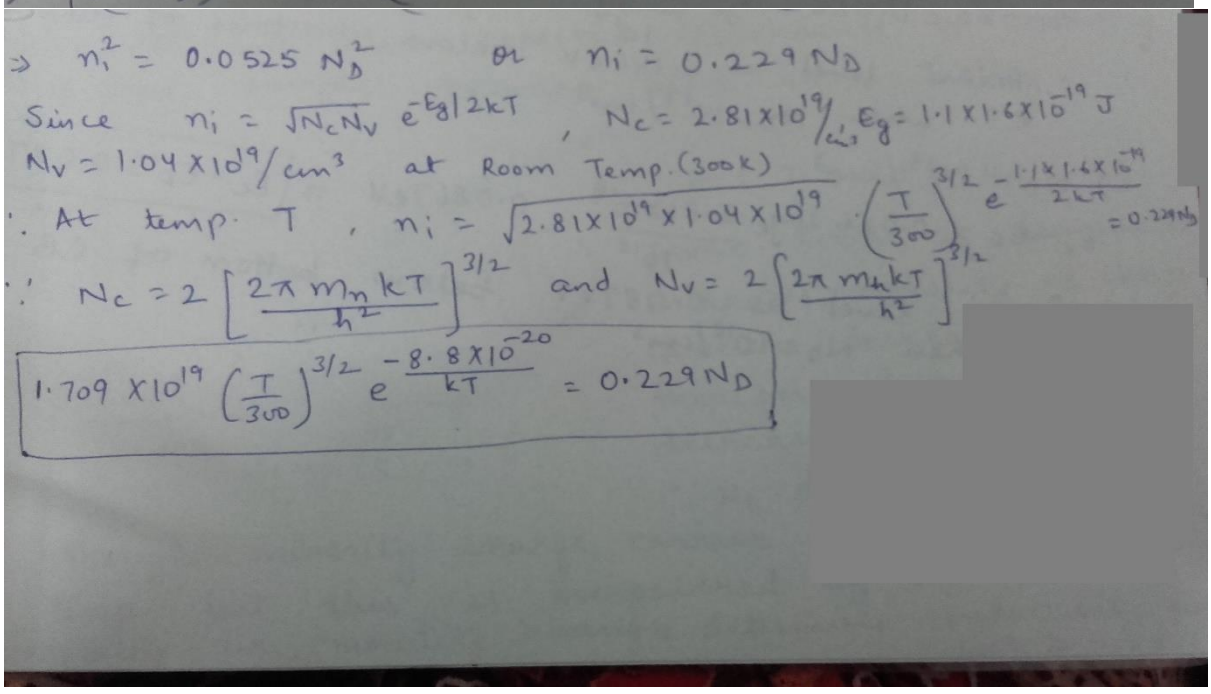
$$= 0.159\,eV$$

The intrinsic Fermi level is near the conduction band of InSb.

Q. 7) Calculate a general expression for electron concentration for a silicon sample doped with a shallow donor dopant density N_d/cm^3. At what temperature, the electron concentration will exceed the donor concentration by 5%? (Note: You may want to use a software to solve the final equation. Please explain the method used.) **(4 marks)**

Sol)





Putting value of $N_D = 10^{16}$ cm^{-3}, we get

$$1.709 \times 10^{19} \left(\frac{T}{300}\right)^{\frac{3}{2}} e^{-\frac{8.8 \times 10^{-20}}{1.38 \times 10^{-23} T}} = 2.29 \times 10^{15}$$

$$\Rightarrow 1.709 \times 10^{19} \left(\frac{T}{300}\right)^{\frac{3}{2}} e^{-\frac{6376.8}{T}} = 2.29 \times 10^{15}$$

Solving using Matlab, we get T = 635 K.

Q. 8) Silicon is used as dopant to GaAs by adding a concentration of 10^{10} cm^{-3}. Find the number of electrons and holes in the material assuming that silicon acts as fully ionized dopants with 20% replacing Ga, and 80% replacing As atoms. Use $n_{i,GaAs} = 2.5 \times 10^6$ cm^{-3}. **(4 marks)**

Sol)

$$n - p + N_A^- - N_D^+ = 0$$

$$Q \cong N_A^- - N_D^+$$

$$n - p + Q = 0$$

$$\left(n_i^2/p\right) - p + Q = 0 \;\|\; n - \left(n_i^2/n\right) + Q = 0$$

$$p^2 - Qp - n_i^2 = 0 \;\|\; n^2 + Qn - n_i^2 = 0$$

$$p = \frac{Q}{2} + \sqrt{\left(\frac{Q}{2}\right)^2 + n_i^2} \qquad \| \; n = \sqrt{\left(\frac{Q}{2}\right)^2 + n_i^2} - \frac{Q}{2}$$

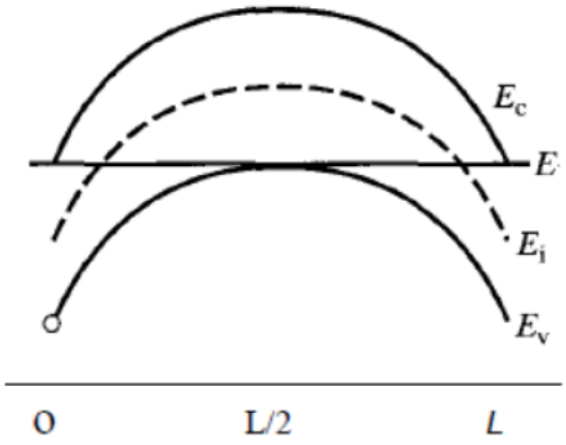
Q= $0.8 \times 2.5 \times 10^6 - 0.2 \times 2.5 \times 10^6 = 0.6 \times 2.5 \times 10^6 = 1.5 \times 10^6$ cm^{-3}

After solving,

Number of electrons, n = 1.86×10^6 cm^{-3}

Number of holes, p = 3.36×10^6 cm^{-3}

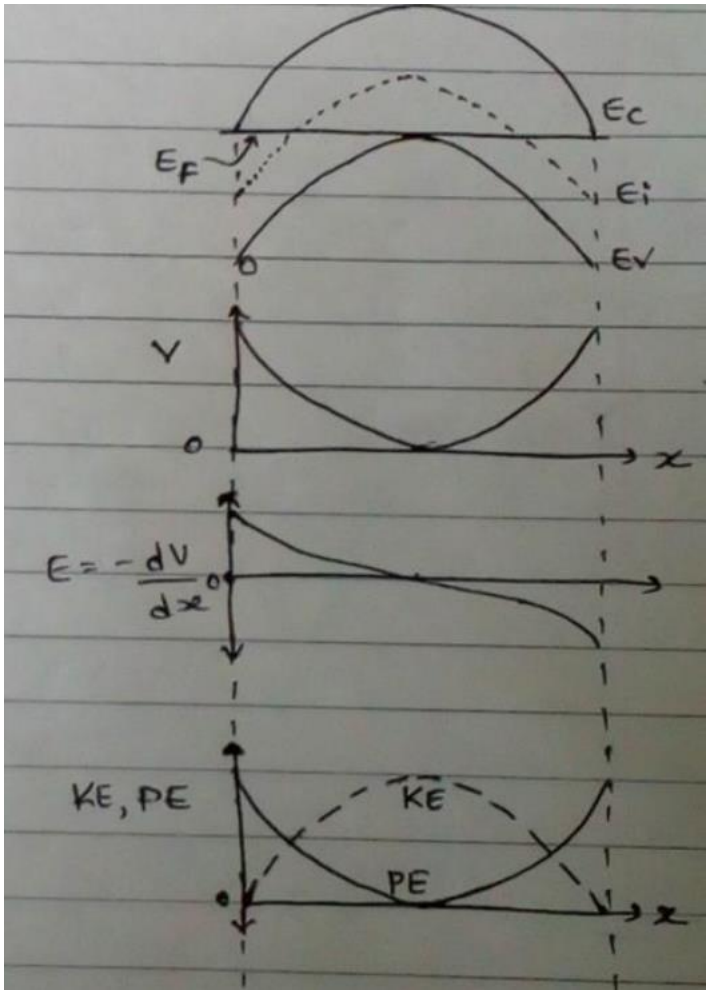
Q. 9) For the band diagram given below, answer the following questions:



a) Is the semiconductor in equilibrium? Justify.
b) Sketch the electrostatic potential, electric field, potential and kinetic energies as a function of x inside the semiconductor.

Assume E_F as the reference level and particle shown in hollow circle moves back and forth between x = 0 and x = L without changing the total energy. **(2+6 = 8 marks)**

Sol) a) Yes, semiconductor is in equilibrium



Please note that here minimum voltage is taken as zero. The offset can be taken as any value without affecting the shape and relative change in potential. E_F is taken as reference energy for calculating kinetic energy (KE) and potential energy (PE).

Q. 10) Write a Matlab code to compare and plot the difference in the charge carrier statistics (f(E)) vs E calculated using Fermi-Dirac and Maxwell-Boltzmann equations with variation in

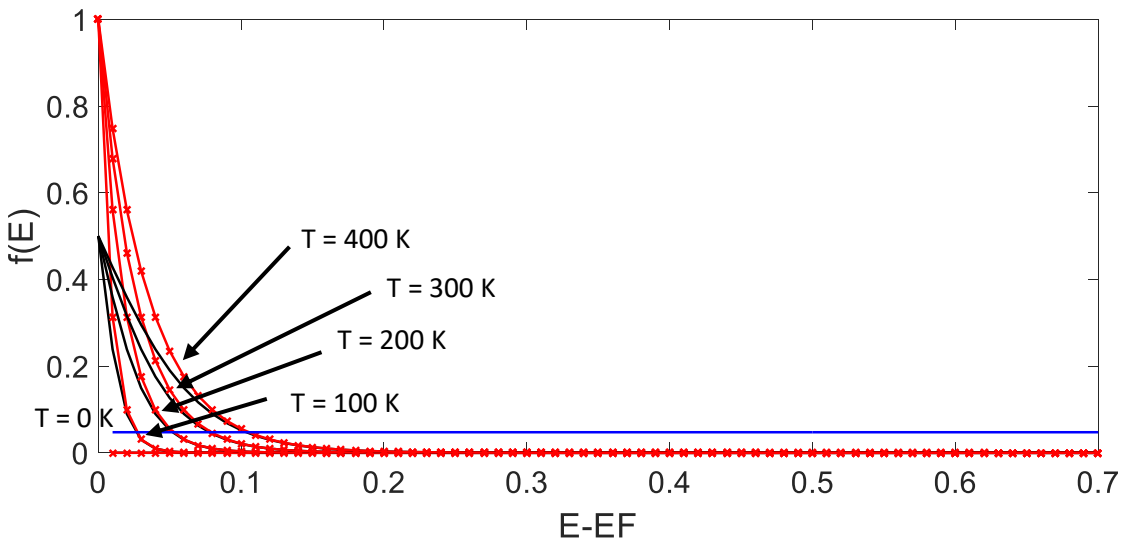
1) temperature ranging from 0 K to 400 K.

2) ($E-E_F$) varying from 0 eV to 0.7 eV

Calculate the range of temperature and ($E-E_{F)}$ where the error in the Maxwell-Boltzmann distribution w.r.t. to Fermi-Dirac distribution is less than 5%. **(3+3 = 6 marks)**

Sol) The Matlab code is:

```
clc;
clf;
clear all;
k=8.625e-5;
for T=0:100:400
    x=0:0.01:0.7; % x= E-E_F
        f1=1./(1+exp(x./(k*T)));
        f2=exp(-(x./(k*T)));
    plot(x,f1,'k','LineWidth',2);
    hold on;
    plot(x,f2,'xr',x,f2,'r','LineWidth',2);
    hold on;
    xlabel('E-EF');
    ylabel('f(E)');
end
T=0:5.714:400; %to maintain matrix size consistent with E-E_F matrix
y=3*k*T;
f3=1./(1+exp(y./(k*T)));      %5 percent error
plot(x,f3,'b','LineWidth',2);
hold on;
```



The black lines show the Fermi-Dirac distribution and red line (with cross) show Maxwell Boltzmann distribution.

As depicted in the graph, with increasing temperature, the difference $E-E_F$ required for close match between two distributions increases. The blue coloured line shows the 5% mismatch in the two distributions. Below the blue coloured line, the difference between the two distributions is less than 5%.

For 400 K, the $E-E_F$ value of 0.1 eV is required for both the distributions to yield same results. On the other hand, for 100 K, the value required for Maxwell-Boltzmann

approximation to hold is 0.026 eV. This justifies that the above ($E-E_F$) = $3k_BT$, both the distributions give almost equivalent results with 5% error bar

Similarly, at a constant value of $E-E_F$, the difference in the value of both the distributions increases with temperature. For instance, at $E-E_F$ value of 0.03 eV, temperature less than 100 K satisfies less than 5% error. For higher temperatures, deviations in the Maxwell Boltzmann distribution with respect to Fermi Dirac distributions is larger.