

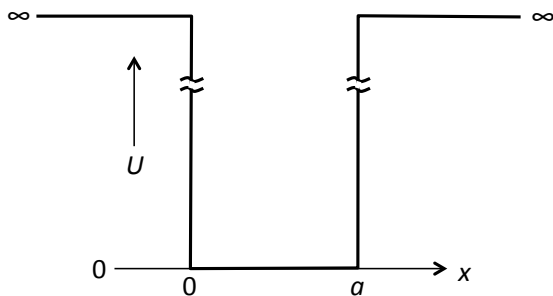
Homework #2

Solutions

Quantum (Energy Band) Theory of Solids – **100 points****DUE @ Beginning of Class: Thursday, September 14**

1) To help you establish some background of basic quantum mechanics and the wave-like nature of electrons, consider the familiar “particle-in-a-box” shown below. The particle has a mass m and is confined in the box between 0 and a in 1-dimension. The potential energy (U) is infinite outside of the box and 0 within the box. Beginning with the time-independent Schrödinger equation shown below, complete the following parts: **(14 points)**

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}[E - U(x)]\psi = 0$$



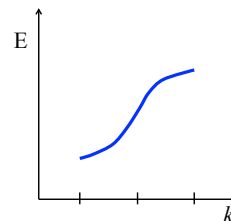
- Define the wavenumber, k , and substitute it into the Schrödinger equation.
- Using the boundary conditions of the box, determine the allowed values for k . Hint: There should be an integer multiple.
- What is the expression for the wavefunction ψ corresponding to a certain k for this particle?
- What is the expression for the quantized energy levels E_n (n being some integer multiple) for the particle?
- Sketch the first four energy levels within the box and the corresponding wavefunctions at each level.

2) In lecture, the 3D DOS (density of states) function was derived for a parabolic dispersion relation. Now consider a 2D material that also has a parabolic dispersion relation (E - k): **(18 points)**

- Derive the DOS for this 2D material (HINT: assume the size of the crystal to be length L in x and y).
- Plot this 2D DOS on a plot and the 3D DOS on another plot (use software such as MATLAB). Use $m^* = 0.5m_0$ for the effective mass. Include a printout of your plot with labels for the axes. Final units for the DOS should be $\text{cm}^{-3}\text{eV}^{-1}$ or $\text{cm}^{-2}\text{eV}^{-1}$. Use energy axis range of 0 to 5 eV.
- What is unique about the 2D DOS expression's dependence on energy compared to 3D? Why would this matter?

3) Given the approximate E - k plot to the right: **(10 points)**

- Sketch approximate plots of dE/dk and d^2E/dk^2 .
- What is the significance of each of these plots?



4) E-Book, problem 3.13 **(6 points)**

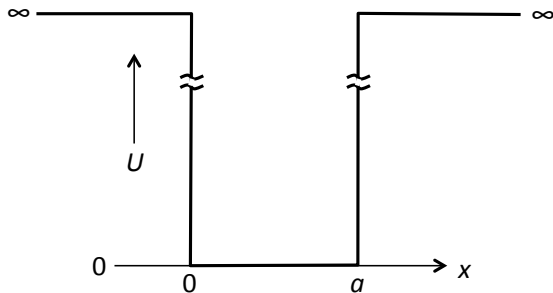
**CONTINUED**

- 5) E-Book, problem 3.15 (12 points)
- 6) E-Book, problem 3.18 (8 points)
- 7) E-Book, problem 3.26 (12 points)
- 8) E-Book, problem 3.32 (6 points)
- 9) E-Book, problem 3.45 (14 points)

(each problem is provided on an individual page below; feel free to use if you'd like)

1) To help you establish some background of basic quantum mechanics and the wave-like nature of electrons, consider the familiar "particle-in-a-box" shown below. The particle has a mass m and is confined in the box between 0 and a in 1-dimension. The potential energy (U) is infinite outside of the box and 0 within the box. Beginning with the time-independent Schrödinger equation shown below, complete the following parts: (14 points)

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}[E - U(x)]\psi = 0$$



- Define the wavenumber, k , and substitute it into the Schrödinger equation.
- Using the boundary conditions of the box, determine the allowed values for k . Hint: There should be an integer multiple.
- What is the expression for the wavefunction ψ corresponding to a certain k for this particle?
- What is the expression for the quantized energy levels E_n (n being some integer multiple) for the particle?
- Sketch the first four energy levels within the box and the corresponding wavefunctions at each level.

a) For everywhere inside the potential well, the potential energy (U) of the particle is: $U(x) = 0$ [$0 \leq x \leq a$]

giving: $\frac{\partial^2 \psi}{\partial x^2} + \frac{2mE}{\hbar^2} \psi = 0$

Define wavenumber:

$$k = \sqrt{\frac{2mE}{\hbar^2}}$$

2

$$\frac{\partial^2 \psi}{\partial x^2} + k^2 \psi = 0$$

2

b) Boundary conditions: $\psi(0) = 0$ and $\psi(a) = 0$ [the particle is contained in the "box"]

$$\psi(x) = A \sin kx + B \cos kx$$

← general solution for this differential equation

Apply the B.C.s: $\psi(0) = B = 0$, $\psi(a) = A \sin ka = 0$

to satisfy this condition, ka must be a multiple of π

∴ allowed values of k :

$$k = \frac{n\pi}{a}, n = \pm 1, \pm 2, \pm 3, \dots$$

4

c) corresponding wave function since $B=0$ and $k = \frac{n\pi}{a}$:

$$\psi_n(x) = A_n \sin \frac{n\pi x}{a}$$

2

d) Quantized energy levels:

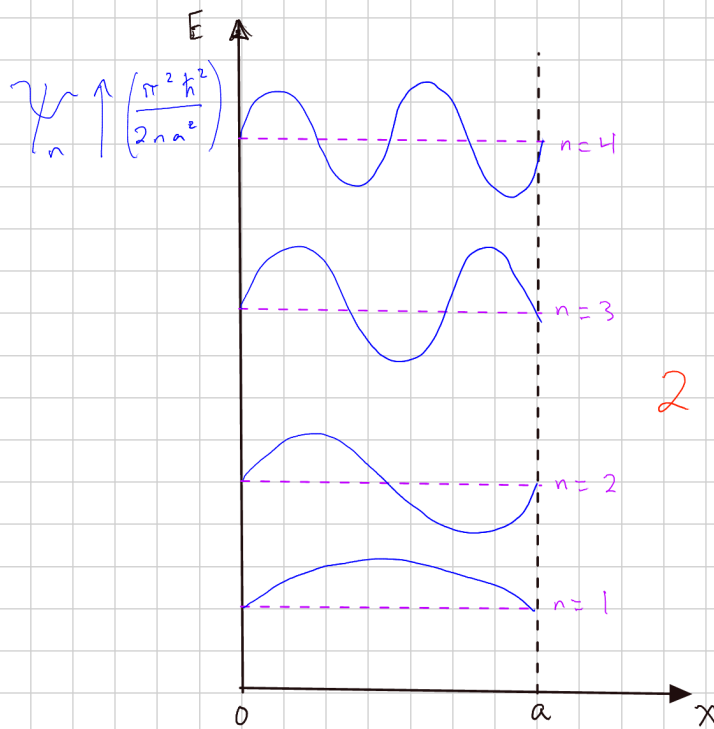
Since: $k = \sqrt{\frac{2mE}{\hbar^2}}$, then: $E = \frac{\hbar^2 k^2}{2m}$

Apply restricted values for k giving:

$$E_n = \frac{n^2 \pi^2 \hbar^2}{2ma^2}$$

2

e) First four E-levels in box with wavefunctions:



Notice how the wave functions must be able to "fit" within the box — this is why they are quantized.

2) In lecture, the 3D DOS (density of states) function was derived for a parabolic dispersion relation. Now consider a 2D material that also has a parabolic dispersion relation (E-k): (18 points)

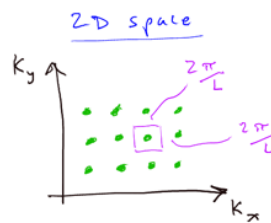
- Derive the DOS for this 2D material (HINT: assume the size of the crystal to be length L in x and y).
- Plot this 2D DOS on a plot and the 3D DOS on another plot (use software such as MATLAB). Use $m^* = 0.5m_0$ for the effective mass. Include a printout of your plot with labels for the axes. Final units for the DOS should be $\text{cm}^{-3}\text{eV}^{-1}$ or $\text{cm}^{-2}\text{eV}^{-1}$. Use energy axis range of 0 to 5 eV.
- What is unique about the 2D DOS expression's dependence on energy compared to 3D? Why would this matter?

a) 1. Determine # states per unit volume k-space

Based on the periodicity of the wave numbers: $k = \frac{2\pi}{L}n$

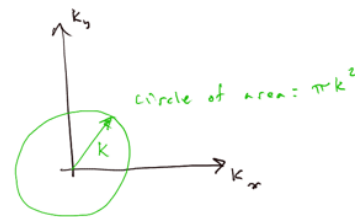
$$\Rightarrow \frac{1 \text{ state}}{\left(\frac{2\pi}{L}\right)^2} = \frac{1}{\frac{4\pi^2}{A}} = \frac{A}{4\pi^2} \times 2 = \frac{A}{2\pi^2} \quad 2$$

area of 2D crystal, $A = L^2$



2. Find total # states up to a value k

$$N(k) = \left(\frac{A}{2\pi^2}\right)(\pi k^2) = \frac{A k^2}{2\pi} \quad 2$$



3. Convert to total # states up to energy E

used the parabolic E-k: $k = \sqrt{\frac{2mE}{\hbar^2}}$

$$N(E) = \frac{A}{2\pi} \left(\sqrt{\frac{2mE}{\hbar^2}}\right)^2 = \frac{A}{2\pi} \left(\frac{2mE}{\hbar^2}\right) = \frac{A m E}{\pi \hbar^2} \quad 2$$

4. Differentiate and divide by area for DOS per unit area:

$$g(E) = \frac{1}{A} \frac{d}{dE} N(E) = \frac{1}{A} \left(\frac{A m}{\pi \hbar^2}\right) = \frac{m}{\pi \hbar^2} \quad 4$$

Notes: other forms of this could also work depending on unit conversions to J or Joules

b) 3D: $g_{3D}(E) = \frac{m \sqrt{2mE}}{\pi^2 \hbar^3} = \frac{[0.5(9.11 \times 10^{-31} \text{ kg})]^{3/2} \sqrt{2}}{\pi^2 (6.63 \times 10^{-34} \text{ J}\cdot\text{s})^3} \sqrt{E} \left(\frac{1 \text{ J}}{6.24 \times 10^{18} \text{ eV}}\right) \left(\frac{1 \text{ m}^3}{10^6 \text{ cm}^3}\right) = (2.42 \times 10^{28}) \sqrt{E} \frac{\text{states}}{\text{cm}^3 \text{ eV}}$

This is actually 'h' instead of 'h-bar' so slightly different.

units: $\frac{\text{kg}^{3/2}}{\text{J}^3 \cdot \text{s}^3} = \frac{\text{kg}^{3/2} \cdot \text{s}^6}{\text{kg}^3 \cdot \text{m}^4 \cdot \text{s}^3} = \frac{\text{s}^3}{\text{kg}^{3/2} \cdot \text{m}^4} \cdot \frac{\text{kg}^{1/2} \cdot \text{m}}{\text{s}} = \frac{\text{s}^2}{\text{kg} \cdot \text{m}^3} = \frac{\text{states}}{\text{m}^3 \cdot \text{J}} \cdot \frac{\text{J}}{\text{eV}} \cdot \frac{\text{m}^3}{\text{cm}^3} = \frac{\text{states}}{\text{cm}^3 \cdot \text{eV}}$

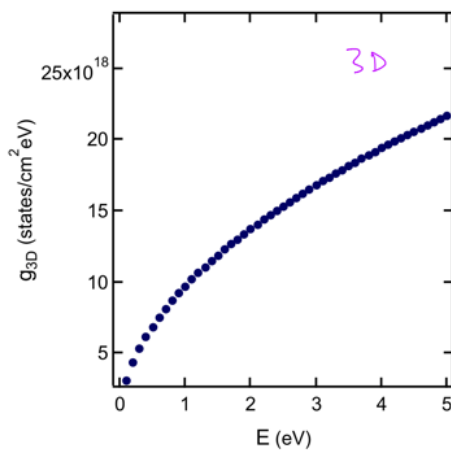
$\text{J} = \frac{\text{kg} \cdot \text{m}^2}{\text{s}^2}$

2D: $g_{2D}(E) = \frac{m}{\pi \hbar^2} = \frac{0.5(9.11 \times 10^{-31} \text{ kg})}{\pi (6.63 \times 10^{-34} \text{ J}\cdot\text{s})^2} \left(\frac{1 \text{ J}}{6.24 \times 10^{18} \text{ eV}}\right) \left(\frac{1 \text{ m}^2}{10^4 \text{ cm}^2}\right) = 2.11 \times 10^{14} \frac{\text{states}}{\text{cm}^2 \text{ eV}}$

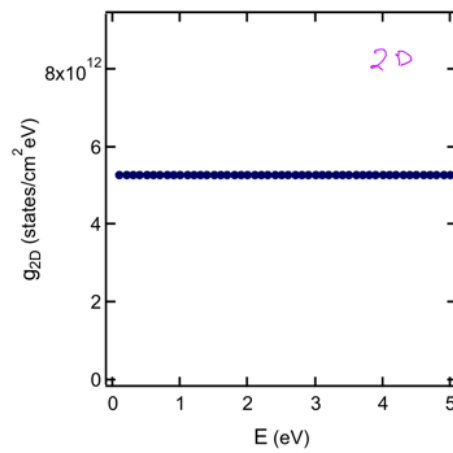
(see next page for plots)

2) (continued)

b) (continued)



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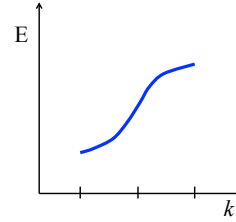


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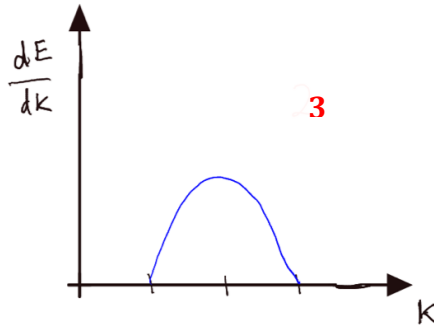
Note: the value
you should be:
 2.11×10^{14} rather
than what is shown
in this plot

- c) What is unique about the 2D DOS is that it is independent of energy! |
Compared to the 3D case where there is a dependence on \sqrt{E} . So, in 2D,
no matter where you are in energy space, the density of states is
constant for a parabolic dispersion relation.

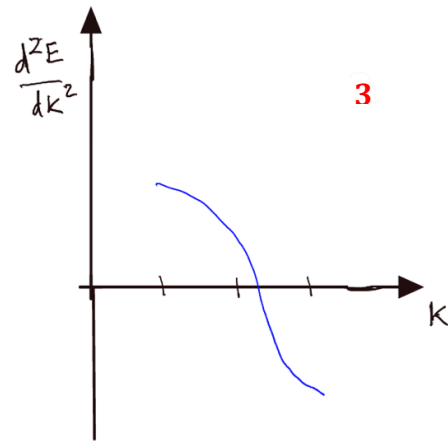
- 3) Given the approximate E-k plot to the right: (10 points)
a) Sketch approximate plots of dE/dk and d^2E/dk^2 .
b) What is the significance of each of these plots?



a)



3



3

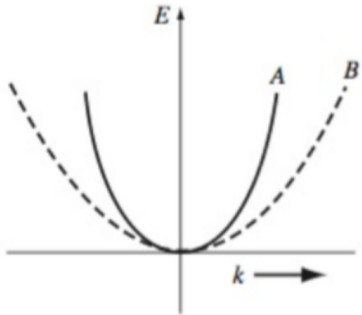
- b) Significance is that:

Velocity: $v = \frac{1}{\hbar} \frac{dE}{dk}$ 2

Ans
effective mass: $m^* = \hbar^2 \left(\frac{d^2E}{dk^2} \right)^{-1}$ 2

4) E-Book, problem 3.13 (6 points)

3.13 Two possible conduction bands are shown in the E versus k diagram given in Figure P3.13. State which band will result in the heavier electron effective mass; state why.



$$m^* = \hbar^2 \left(\frac{d^2 E}{dk^2} \right)^{-1} \quad 2$$

Since the curvature A > curvature B

$$\left(\frac{d^2 E}{dk^2} \right)_A > \left(\frac{d^2 E}{dk^2} \right)_B$$

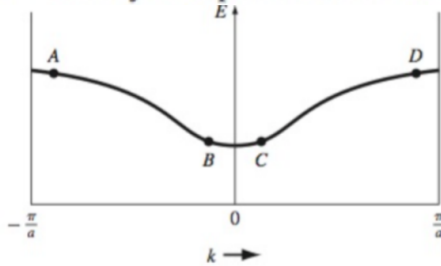
$$\therefore m_A^* < m_B^* \quad 2$$

Why?

Because of m^* dependence on the inverse curvature of the $E-k$ relation. 2

5) E-Book, problem 3.15 (12 points)

3.15 The E versus k diagram for a particular allowed energy band is shown in Figure P3.15. Determine (a) the sign of the effective mass and (b) the direction of velocity for a particle at each of the four positions shown.



$$m^* = \hbar^2 \left(\frac{d^2 E}{dk^2} \right)^{-1}$$

$$v = \frac{1}{\hbar} \frac{dE}{dk}$$

a) sign of the m^* ?		b) velocity direction?	
Point A	$\left. \frac{d^2 E}{dk^2} \right _A < 0 \Rightarrow -m^* \quad 1.5$	$\left. \frac{dE}{dk} \right _A < 0 \Rightarrow -x \text{ direction} \quad 1.5$	
B	$\left. \frac{d^2 E}{dk^2} \right _B > 0 \Rightarrow +m^* \quad 1.5$	$\left. \frac{dE}{dk} \right _B < 0 \Rightarrow -x \text{ direction} \quad 1.5$	
C	$\left. \frac{d^2 E}{dk^2} \right _C > 0 \Rightarrow +m^* \quad 1.5$	$\left. \frac{dE}{dk} \right _C > 0 \Rightarrow +x \text{ direction} \quad 1.5$	
D	$\left. \frac{d^2 E}{dk^2} \right _D < 0 \Rightarrow -m^* \quad 1.5$	$\left. \frac{dE}{dk} \right _D > 0 \Rightarrow +x \text{ direction} \quad 1.5$	

6) E-Book, problem 3.18 (8 points)

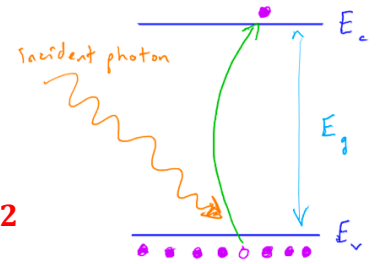
- 3.18** (a) The forbidden bandgap energy in GaAs is 1.42 eV. (i) Determine the minimum frequency of an incident photon that can interact with a valence electron and elevate the electron to the conduction band. (ii) What is the corresponding wavelength?
(b) Repeat part (a) for silicon with a bandgap energy of 1.12 eV.

a) $E_g = 1.42 \text{ eV}$ for GaAs

i. Energy of a photon: $E = h\nu$

Photon must give sufficient energy for e^- to cross E_g :

$$\nu = \frac{E_g}{h} = \frac{1.42 \text{ eV}}{4.14 \times 10^{-15} \text{ eV}\cdot\text{s}} = 3.43 \times 10^{14} \text{ Hz} \quad 2$$



$$\text{ii. } \lambda = \frac{hc}{E} = \frac{c}{\nu} = \frac{3 \times 10^{10} \text{ cm/s}}{3.43 \times 10^{14} \text{ s}^{-1}} = 8.75 \times 10^{-5} \text{ cm} = 875 \text{ nm} \quad 2$$

b) $E_g = 1.12 \text{ eV}$ for Si

$$\text{i. } \nu = \frac{E_g}{h} = \frac{1.12 \text{ eV}}{4.14 \times 10^{-15} \text{ eV}\cdot\text{s}} = 2.71 \times 10^{14} \text{ Hz} \quad 2$$

$$\text{ii. } \lambda = \frac{c}{\nu} = \frac{3 \times 10^{10} \text{ cm/s}}{2.71 \times 10^{14} \text{ s}^{-1}} = 1.11 \times 10^{-4} \text{ cm} = 1109 \text{ nm} \quad 2$$

7) E-Book, problem 3.26 (12 points)

3.26 (a) Determine the total number (#/cm³) of energy states in silicon between E_c and $E_c + 2kT$ at (i) $T = 300$ K and (ii) $T = 400$ K. (b) Repeat part (a) for GaAs.

a) Si: effective mass for e^- near E_c : $m_n^* = 1.08 m_0$

i. $T = 300$ K

$g_c(E) = \frac{4\pi(2m_n^*)^{3/2}}{h^3} \sqrt{E - E_c}$ — density of states in conduction band

total # of states: $N(E) = \int_{E_c}^{E_c + 2kT} \frac{4\pi(2m_n^*)^{3/2}}{h^3} \sqrt{E - E_c} dE$

Units: $\left(\frac{\text{kg}^{3/2}}{\text{s}^3 \cdot \text{s}^3} \right) = \frac{\text{kg}^{3/2} \cdot \text{s}^6}{\text{kg}^3 \cdot \text{m}^6 \cdot \text{s}^3} = \frac{\text{s}^3}{\text{kg}^{3/2} \cdot \text{m}^6}$

$A = \frac{4\pi [2(1.08)(9.11 \times 10^{-31})]^{3/2}}{(6.625 \times 10^{-34})^3} = 1.19 \times 10^{56}$

$N(E) = (1.19 \times 10^{56}) \int_{E_c}^{E_c + 2kT} \sqrt{E - E_c} dE = (1.19 \times 10^{56}) \left[\frac{2}{3} (E - E_c)^{3/2} \right]_{E_c}^{E_c + 2kT}$

$= (1.19 \times 10^{56}) \frac{2}{3} (2kT)^{3/2}$

Units: $\frac{\text{s}^3}{\text{kg}^{3/2} \cdot \text{m}^6} \cdot \text{s}^{3/2} = \frac{\text{s}^3}{\text{kg}^{3/2} \cdot \text{m}^6} \cdot \frac{\text{kg}^{3/2} \cdot \text{m}^6}{\text{s}^3} = \text{m}^{-3}$

$= (7.93 \times 10^{55}) [2(1.38 \times 10^{-23} \text{ J/K})(300 \text{ K})]^{3/2}$

$= 5.97 \times 10^{25} \text{ m}^{-3} = 6.0 \times 10^{19} \text{ states/cm}^3$ **4**

ii. $T = 400$ K

$N(E) = (7.93 \times 10^{55}) [2(1.38 \times 10^{-23})(400 \text{ K})]^{3/2} = 9.2 \times 10^{19} \text{ states/cm}^3$ **2**

b) Repeat for GaAs, $m_n^* = 0.067 m_0$

i. $T = 300$ K $N(E) = 9.27 \times 10^{17} \text{ states/cm}^3$ **1**

ii. $T = 400$ K $N(E) = 1.43 \times 10^{18} \text{ states/cm}^3$ **1**

8) E-Book, problem 3.32 (6 points)

3.32 Determine the probability that an energy level is occupied by an electron if the state is above the Fermi level by (a) kT , (b) $5kT$, and (c) $10kT$.

a) kT above E_F

$$f(E) = \frac{1}{1 + \exp\left(\frac{E - E_F}{kT}\right)} \rightarrow E - E_F = kT$$

$$= \frac{1}{1 + \exp\left(\frac{kT}{kT}\right)} = \frac{1}{1 + e^1} = 0.269 = \boxed{26.9\%} \quad 2$$

b) $5kT$ above E_F

$$E - E_F = 5kT$$

$$\Rightarrow f(E) = \frac{1}{1 + \exp\left(\frac{5kT}{kT}\right)} = \frac{1}{1 + e^5} = 6.69 \times 10^{-3} = \boxed{0.67\%} \quad 2$$

c) $10kT$ above E_F

$$E - E_F = 10kT$$

$$\Rightarrow f(E) = \frac{1}{1 + e^{10}} = 4.54 \times 10^{-5} = \boxed{4.54 \times 10^{-3}\%} \quad 2$$

9) E-Book, problem 3.45 (14 points)

3.45 Assume that the Fermi energy level is exactly in the center of the bandgap energy of a semiconductor at $T = 300$ K. (a) Calculate the probability that an energy state in the bottom of the conduction band is occupied by an electron for Si, Ge, and GaAs. (b) Calculate the probability that an energy state in the top of the valence band is empty for Si, Ge, and GaAs.

a) Since E_F at mid gap, $E - E_F = E_g/2$ for $E = E_c$ and:

$$f(E_c) = \frac{1}{1 + \exp\left(\frac{E_g/2}{kT}\right)}, \quad \text{also, } kT @ 300K = (8.617 \times 10^{-5} \text{ eV/K})(300K) = 0.026 \text{ eV}$$

for Si: $E_g = 1.12 \text{ eV}$

$$f(E_c) = \frac{1}{1 + \exp\left(\frac{1.12 \text{ eV}/2}{0.026 \text{ eV}}\right)} = 4.07 \times 10^{-10} \quad 4$$

Ge: $E_g = 0.66 \text{ eV}$

$$f(E_c) = \frac{1}{1 + \exp\left(\frac{0.66 \text{ eV}/2}{0.026 \text{ eV}}\right)} = 2.93 \times 10^{-6} \quad 3$$

GaAs: $E_g = 1.42 \text{ eV}$

$$f(E_c) = \frac{1}{1 + \exp\left(\frac{1.42 \text{ eV}/2}{0.026 \text{ eV}}\right)} = 1.24 \times 10^{-12} \quad 3$$

b) * Will be same for E_v as for E_c since E_F is at mid gap and $f(E)$ is symmetrical about E_F . 4