Midterm II.

April 11, 2011

Name ____________________________ solutions

The five problems are worth 20 points each.

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1. Consider a two-dimensional (2D) film of atoms arranged in a regular simple cubic lattice. The lattice spacing is 2 Å. Let us assume that each atom contributes one "valence" electron that acts as a free electron in the 2D solid.

   a) What is the Fermi energy (in eV) of this 2D solid at T=0? Recall that

   \[ \frac{\hbar^2}{2m_e} = 3.845 \text{ eV} \cdot \text{Å}^2 \]

   \[ N = \int_0^{E_F} dE \, D(E) \quad \text{where} \]

   \[ D(E) = 2 \frac{dN}{dE} = 2 \frac{dN}{dk} \frac{dk}{dE}. \]

   In 2D, \[ N(k) = \frac{\pi k^2}{(2\pi L)^2} = \frac{L^2 k^2}{4\pi} \]

   \[ E = \frac{\hbar^2 k^2}{2m_e} \Rightarrow \frac{dE}{dk} = \frac{\hbar^2 k}{m_e}. \]

   So, \[ D(E) = 2 \frac{L^2 k}{2\pi} \frac{m_e}{\hbar^2 k} = \frac{L^2 m_e}{\pi \hbar^2} = \text{const}. \]

   Then \[ N = \frac{L^2 m_e}{\pi \hbar^2} E_F \Rightarrow E_F = \frac{N}{L^2} \frac{\pi \hbar^2}{m_e}. \]

   \[ n = \frac{1}{(2 \text{ Å})^2} = 0.25 \text{ Å}^{-2} \]

   \[ E_F = n \frac{\pi \hbar^2}{m_e} = 0.25 \text{ Å}^{-2} \times (2\pi) \times 3.845 \text{ eV} \cdot \text{Å}^2 \]

   \[ = 6.04 \text{ eV}. \]
b) Please calculate the average energy per electron in the 2D film, at T=0.

\[ \langle E \rangle = \int_0^{E_F} dE E D(E) = \frac{E_F^2}{2} \frac{L^2 m}{\hbar^2 \pi} \frac{1}{N/E_F} = \frac{E_F}{2} n \]

\( \frac{E_F}{n} \) is simply \( \langle E \rangle \), as expected since \( D(E) = \text{const.} \).

c) At room temperature (T=300K, \( k_B T=0.025 \) eV), what is the probability that a state 0.05 eV above the Fermi level is occupied by an electron?

This probab. is given by F-D distribution:

\[ f(E) = \frac{1}{e^{(E-E_F)/k_B T} + 1} \]

In this case,

\[ f(E) = \frac{1}{e^{0.05 \text{eV}/0.025 \text{eV}} + 1} = \frac{1}{e^2 + 1} \approx 0.12. \]
2. The diagram below shows the electronic band structure of some hypothetical one-dimensional (1D) solid. Will this solid be a metal or an insulator at T=0 if it has:

a) 1 electron/primitive unit cell?

b) 2 electrons/primitive unit cell?

c) 3 electrons/primitive unit cell?

d) 4 electrons/primitive unit cell?

Please justify your answers!

\[
\begin{align*}
1 \bar{E} / \text{cell} &\Rightarrow N \bar{E}'s \Rightarrow 1\text{st band } \frac{1}{2} \text{ full} \\
3 \bar{E} / \text{cell} &\Rightarrow 3N \bar{E}'s \Rightarrow 2\text{nd band } \frac{1}{2} \text{ full, 1\text{st band full}} \\
2 \bar{E} / \text{cell} &\Rightarrow 2N \bar{E}'s \Rightarrow 1\text{st band full} \\
4 \bar{E} / \text{cell} &\Rightarrow 4N \bar{E}'s \Rightarrow 1\text{st & 2\text{nd bands full}} \text{ insulator}
\end{align*}
\]
Key Points:

a) Each band accommodates $2N \tilde{e}$'s

b) $x \tilde{e}$'s/unit cell $\RightarrowNx$ total $\tilde{e}$'s

Full bands cannot carry electric current. To be a metal, some bands need to be partially occupied.
3. Please describe recent developments in the field of nanoelectronics. Please include some current challenges and future goals in your description, and use a minimum of 4 sentences in your response.

Recent developments include creation of nanometer-scale electronic devices such as transistors & diodes from organic molecules, carbon nanotubes and semiconductor nanowires. The current challenge is to wire some of these components together to create a functional device. Unlike current microelectronics produced in a top-down manufacturing process, nanoelectronics devices will be made in a bottom-up approach. Researchers will make building blocks first which will then either self-assemble or be assembled into larger structures.
4. a) Empirically speaking, what is the difference between a metal and an insulator?

Application of electric field to solid: current in metals, no current in insulators.

b) What is the criterion, based on the energy band theory, for distinguishing a metal from an insulator?

A solid behaves as a metal if some of its bands are partially occupied. In insulators, all bands are either full or empty. It takes \( 2N \) \( \tilde{e} \)'s to fill a band \( \rightarrow \) insulators must have an even \( \# \tilde{e} \)'s per unit cell.

c) From the point of view of band structure, why are some divalent elements such as Be or Mg metals rather than insulators?

In divalent metals some bands overlap, resulting in \( \tilde{e} \) transfer from one band \( \rightarrow \) band \( \tilde{e} \) filled, thus creating partially filled bands.
5. a) What is a semiconductor and how is it distinctive from a metal and from an insulator?

A semiconductor has a gap $\Delta E \leq 2 \text{ eV}$, so that $\tilde{E}$'s are thermally excited into the conduction band at high $T$. Therefore, unlike insulators, semiconductors are conducting at $T \geq 350 \text{ K}$ or so; however, the conductivity is substantially lower than with metals due to low carrier concentration.

b) Please sketch $n(T)$ vs. $T$ plot (temperature dependence of the carrier concentration) for an $n$-type semiconductor. Indicate and explain the three main temperature regimes.

\[ n \]

\[ N_d \]

\[ T \]

\[ T_1 \text{ freeze-out extrinsic} \]

\[ T_2 \text{ intrinsic} \]

$T < T_1$  

Donor $\tilde{E}$'s "frozen" at $T_1 \approx 100 \text{ K}$ impurity sites

$T_1 < T < T_2$  

Extrinsic regime, $n \sim N_d$ all donors ionized, all $\tilde{E}$'s from impurities are in conduction band

$T > T_2$  

Thermal activation of $\tilde{E}$'s: $\text{VB} \rightarrow \text{CB}$ becomes dominant
c) Use the Maxwell-Boltzmann approximation to the Fermi-Dirac distribution to compute the electron concentration as a function of Fermi energy and gap energy in the intrinsic semiconductor regime. Use

\[ n(E) = \frac{1}{2 \pi^2} \left( \frac{2 m e}{\hbar^2} \right)^{3/2} (E - E_g)^{3/2} \]

for the density of states on the bottom of the conduction band. 

Recall that

\[ \int_0^\infty dx \ x^{1/2} e^{-x} = \frac{\sqrt{\pi}}{2} \]

Using

\[ f(E) = e^{E_F/k_b T} e^{-E/k_b T} \]

we obtain:

\[ n = \int_{E_g}^{E_{c2}} \text{d}E f(E) g_\varepsilon(E) = \]

For energy at top of VB extend upper limit to \( \infty \) kx integrand \( \approx 0 \) there

\[ = \frac{1}{2 \pi^2} \left( \frac{2 m e}{\hbar^2} \right)^{3/2} \int_{E_g}^{E_{c2}} \text{d}E e^{E_F/k_b T} e^{-E/k_b T} (E - E_g)^{3/2} \]

\[ = \frac{1}{2 \pi^2} \left( \frac{2 m e}{\hbar^2} \right)^{3/2} e^{E_F/k_b T} e^{-E_g/k_b T} \int_0^{\infty} dx \ x^{1/2} e^{-x} \]

\[ x = \frac{E - E_g}{k_b T} \]

\[ \Rightarrow \frac{1}{4} \left( \frac{2 m e}{\pi \hbar^2} \right)^{3/2} (k_b T)^{3/2} e^{E_F/k_b T} e^{-E_g/k_b T} = \]

\[ = 2 \left( \frac{m e k_b T}{2 \pi \hbar^2} \right)^{3/2} e^{E_F/k_b T} e^{-E_g/k_b T} \]