Physics 406, Spring 2013

Midterm II

April 11, 2013

Name solutions

The five problems are worth 20 points each.

Problem	Score
1	20
2	20
3	20
4	20
5	20
Total	100

1. Consider a three-dimensional (3D) crystal with atoms arranged in a bcc lattice. The lattice spacing is 4 Å. Let us assume that each atom contributes one valence electron that becomes a free electron in the 3D solid.

a) What is the Fermi energy (in eV) of this 3D solid at T=0?

Recall that

$$E_F = \frac{\hbar^2}{2m_e}\left(3\pi^2 n\right)^{2/3}, \quad \text{where}$$

n is $\bar{e}$ density & m_e is $\bar{e}$ mass.

In a bcc lattice, there are 2 $\bar{e}$'s per unit cell: $n = \frac{2}{a^3}$, where $a = 4\,\text{Å}$.

Plugging in the #'s, we obtain:

$$E_F = \frac{(1.054 \times 10^{-34}\ \text{J}\cdot\text{s})^2}{2 \times 9.11 \times 10^{-31}\ \text{kg}}\left(3\pi^2 \times 3.125 \times 10^{28}\ \text{m}^{-3}\right)^{2/3}$$ ⑪

↗

$$n = 3.125 \times 10^{28}\ \text{m}^{-3}$$

$$\textcircled{=}\ 5.79 \times 10^{-19}\ \text{J} = \underline{\underline{3.61\,\text{eV}}}.$$

b) Please calculate the average energy per electron (in eV) in this solid, at T=0.

Recall that $\mathcal{E}_k = \dfrac{\hbar^2 k^2}{2m_e}$

$$\langle \mathcal{E} \rangle = \frac{\hbar^2}{2m_e} \frac{\int_0^{k_F} dk\, k^4}{\int_0^{k_F} dk\, k^2} =$$

$$= \frac{\hbar^2}{2m} \frac{3}{5} k_F^2 = \underline{\underline{\frac{3}{5} E_F}}.$$

Here, $\langle \mathcal{E} \rangle = 2.17\ eV.$

c) At room temperature (T=300K, k_BT=0.025 eV), what is the probability that a state 0.1 eV above the Fermi level is occupied by an electron? What about a state 1.0 eV above the Fermi level?

Recall that $f(E) = \dfrac{1}{e^{(E-E_F)/k_BT} + 1}.$

Then

$$f(\underbrace{E_F + 0.1\,eV}_{E}) = \frac{1}{e^{0.1/0.025} + 1} \simeq 1.8 \times 10^{-2},$$

$$f(E_F + 1.0\,eV) = \frac{1}{e^{1.0/0.025} + 1} \simeq 4.2 \times 10^{-18}.$$

2. 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.

Some of the recent developments are:

(1) Single-ē transistors composed of metallic carbon nanotubes

(2) Self-assembly of nanowires and nanoarrays into functional components

(3) Molecular electronics

The challenges are to downsize electronics and improve performance using devices & approaches listed above. There are many technical difficulties such as robust self-assemly.

3. a) What are the empirical definitions of a metal, an insulator, and a semiconductor?

There is no current in an insulator when electric field is applied. In metals, current will flow. Semiconductors are insulators with smaller gaps (typically < 2 eV) between conductance and valence bands. As a result, $\bar{e}$'s are thermally excited across the gap at room T's.

b) What is the criterion, based on the energy band theory, for distinguishing a metal, an insulator, and a semiconductor? From the point of view of band structure, how can some divalent elements such as Be or Mg be metals rather than insulators?

In insulators, the valence (VB) band is filled and the conductance band (CB) is empty. In metals, CB is partially filled. Divalent elements such as Be or Mg can be metals only if VB & CB overlap, resulting in incompletely filled bands. Semiconductors have the same band structure as insulators, but with a smaller gap.

c) Please describe the nature of sp^3 hybridization in materials such as diamond or Si where each atom is surrounded by 4 other atoms of the same type.

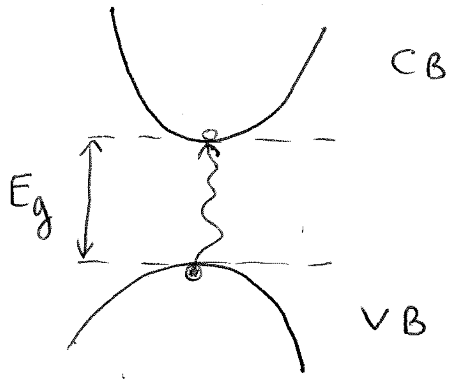
In these materials, covalent bonds are formed in a tetrahedral arrangement. For example, an isolated C atom has $2s^2 2p^2$. Since $\underbrace{E_{2s}}_{\text{only slightly lower}} \simeq E_{2p}$, one of the 2s $\bar{e}$'s can get excited into the 2p state:

$$2s^2 2p^2 \rightsquigarrow 2s^1 2p^3 .$$

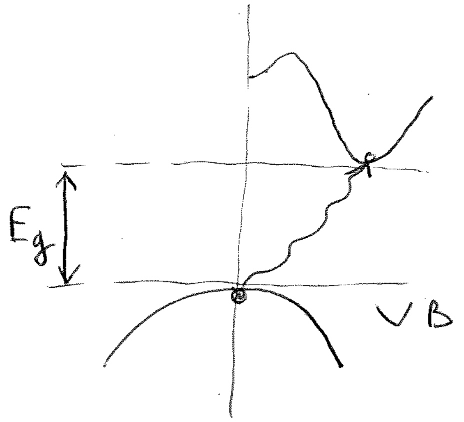
Now, linear combinations of 1 s-orbital & 3 p-orbitals can form in a tetrahedral arrangement. This mixing of s & p states is called sp^3 hybridization.

4. a) Please sketch the band structure of direct and indirect gap semiconductors. Describe how the fundamental absorption process (photon absorption causing electron transitions from valence to conduction band) can occur in these two classes of materials, and what elementary absorption events are involved. For a direct gap semiconductor with E_g = 1 eV, estimate the absorption edge (the minimum photon frequency below which the fundamental transition is impossible). Estimate the momentum carried by a photon with the frequency at the absorption edge.

Direct gap



Indirect gap



$$\begin{cases} E_f = E_i + h\nu \\ \vec{k}_f = \vec{k}_i + \vec{q}_\phi \end{cases}$$

$\vec{q}_\phi \approx 0$ for a photon $\Rightarrow \vec{k}_f = \vec{k}_i$

optical or IR

Fundamental absorption can be mediated by a photon alone in direct gap sc. In indirect gap sc, phonon absorption is necessary to provide momentum (photon provides most energy in both cases). If $E_g = 1\,eV$,

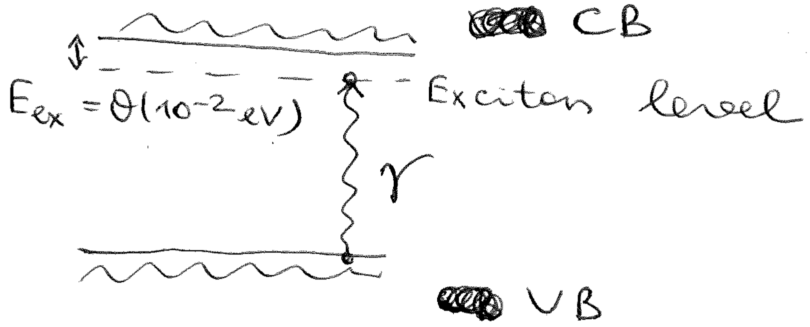
abs. edge → $\nu_0 = \frac{E_g}{h} \approx 2.42 \times 10^{14}\ s^{-1}$.

$\lambda = \frac{c}{\nu} \approx 1.24\ \mu m$ optical wavelength

Finally, $\underset{\approx \hbar k}{p} = \frac{h}{\lambda} \approx 5.34 \times 10^{-28}\ \frac{kg \cdot m}{s}$

b) Please describe how exciton states are formed, and sketch the exciton level on the band structure diagram. Show photon absorption involving the exciton level, and explain why it can obscure the fundamental edge.

Exciton states are weakly bound $\bar{e}$-hole states.



Photon absorption into the exciton level is very close to the fundamental edge because exciton formation energies are $\mathcal{O}(10^{-2})$ eV. Thus exciton absorption can make detecting the fundamental edge more difficult.

5. a) Write down the Schrodinger equation for an electron in a 1D periodic potential. Use Fourier series expansions of the potential energy and the wavefunction to derive the central equation. Carefully explain which values of the wavevector k are permitted by the periodic boundary conditions, and what further restrictions on the values of k are imposed by the periodicity of the potential.

(1D) periodic potential:

$U(x)=U(x+a)$, where a is lattice constant.

$U(x) = \sum_G U_G e^{iGx}$, where G are reciprocal lattice vectors.

SE: $H\Psi = E\Psi$, or

$$\left(\frac{p^2}{2m} + \sum_G U_G e^{iGx}\right)\Psi(x) = E\Psi(x)$$

Use $\Psi(x) = \sum_k C(k)\, e^{ikx}$, where $k = \frac{2\pi}{L} n$, $n \in \mathbb{Z}$ is set by periodic BCs. Then

$$\frac{\hbar^2}{2m}\sum_k k^2 C(k)\, e^{ikx} + \sum_{G,k} U_G C(k)\, e^{i(k+G)x} =$$

$$= E \sum_k C(k)\, e^{ikx}, \text{ or}$$

central eq'n $\Big[$ $(\lambda_k - E)\, C(k) + \sum_G U_G C(k-G) = 0$, where

$$\lambda_k = \frac{\hbar^2 k^2}{2m}$$

Note that only $C(k-G)$, $\overbrace{\forall k}^{\text{permitted by periodic BCs}}$ are relevant. This allows us to rewrite $\Psi(x)$ as a sum over G, not k - a much smaller set! (see next page)

b) Use the Fourier series expansion of the wavefunction to derive the Bloch theorem (i.e., show that the wavefunction can be written as a product of a free electron phase factor and $u_k(x)$, which has the periodicity of the lattice).

$\Psi(x)$ in a periodic potential is thus given by

$$\Psi_k(x) = \sum_G C(k-G)\, e^{i(k-G)x}.$$

↑ labeled by wavenumber

Then
$$\Psi_k(x) = \underbrace{\left(\sum_G C(k-G)\, e^{-iGx}\right)}_{\equiv\, u_k(x)} e^{ikx}.$$

Indeed,
$$u_k(x+\overset{\forall \text{ direct lattice vector}}{\underset{\downarrow}{T}}) = \sum_G C(k-G)\, e^{-iG(x+T)} =$$

$$= \underbrace{e^{-iGT}}_{\substack{= \\ 1 \text{ by} \\ \text{construction}}} \underbrace{\sum_G C(k-G)\, e^{-iGx}}_{u_k(x)} = \underset{\text{periodic}}{u_k(x)}.$$

So,
$$\underline{\underline{\Psi_k(x) = u_k(x)\, e^{ikx}.}}$$

Bloch theorem