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2.57/2.570 Midterm Exam No. 1

April 4, 2012
11:00 am -12:30 pm

Instructions:

(1) 2.57 students: try all problems
(2) 2.570 students: Problem 1 plus one of two long problems. You can also do both long problems, and one will be considered for bonus points.
(3) Clearly state your assumptions.
(4) Closed book, one sheet of notes allowed.

Unless otherwise noted, assume electron mass equals that of free electron in vacuum.

Constants:

Boltzmann constant $k=1.38\text{x}10^{-23}$ J/K
Electron charge $e=1.6\text{x}10^{-19}$ C
Free electron mass $m=9.1\text{x}10^{-31}$ kg
Planck constant $h=6.6\text{x}10^{-34}$ J.s
Proton mass $M=1.67\text{x}10^{-27}$ kg
Speed of light $c=3\text{x}10^{8}$ m/s

1. Answer the following short questions. Briefly explain your answer **(60 Points)**

(1) (6 points) A bulk semiconductor has a direct band gap of 1 eV. Both electrons and holes have the same effective mass that equals to free electron. If the same semiconductor is made into a thin film of 5 nm, sandwiched between materials with an infinite barrier height, the first quantized energy level of conduction band will move up and that of the valence band will move down. What is the new bandgap of the thin film?

Solution:

Given:

$E_{G,bulk} = 1\,\text{eV}$

$m_e = m_h = 9.1\times10^{-31}$ kg

$d = 5\,\text{nm}$

By sandwiching a thin-film semiconductor between two materials with an infinite barrier height, a 1D quantum well is created. Due to quantization effects, the density of states (recall Example 3.5) will only be nonzero after the first energy level is excited. Therefore, the new bandgap of the thin film can be formulated as,

$$E_{G,film} = E_{G,bulk} + 2\cdot E_1$$

where, the first energy level for the electrons and holes are assumed equal since the effective masses are equal. For a quantum well, the energy levels are,

$$E_n = \frac{1}{2m}\cdot\left(\frac{nh}{2D}\right)^2 \tag{2.42}$$

The first energy level is therefore,

$$E_1 = \frac{1}{2(9.1\times10^{-31}\ \text{kg})}\cdot\left(\frac{(1)(6.636\times10^{-34}\ \text{J}\cdot\text{s})}{2(5\times10^{-9}\ \text{m})}\right)^2\cdot\frac{1}{1.602\times10^{-19}}\frac{\text{eV}}{\text{J}} = 0.0151\,\text{eV}$$

Thus,

$$E_{G,film} = 1 + 2\cdot(0.0151) = \boxed{1.0302\,\text{eV}}$$

(2) (6 points) Typical thermal conductivity of gas changes with T^n. Make your best estimate of the value of n and justify your value.

Solution:

In general we can formulate the thermal conductivity of a gas as follows,

$$k = \frac{C v \Lambda}{3} \qquad (1.35)$$

Each term has its own temperature dependence. Assuming an ideal monatomic gas, the volumetric specific heat, *C*, is

$$C = \frac{3k_b N}{2V} = \frac{3P}{2T} \sim \frac{1}{T} \qquad (4.29 \ \& \ 4.47)$$

The average speed of the molecules, *v*, is,

$$v = \sqrt{\frac{8k_b T}{m}} \sim \sqrt{T} \qquad (p.24)$$

And finally the mean free path, Λ, using a simple kinetic model is,

$$\Lambda = \frac{k_b T}{\pi\sqrt{2} P d^2} \sim T \qquad (1.38)$$

Therefore,

$$k \sim \frac{1}{T} \cdot \sqrt{T} \cdot T = \sqrt{T}$$

Thus,

$$\boxed{n = \frac{1}{2}}$$

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(3) Light at 1 μm wavelength is incident from vacuum towards a semi-infinite medium of refractive index N=2+0.01i at normal incidence. Answer the following two questions:

(3a) (6 points) What is the percentage that the light is absorbed by the medium.

(3b) (6 points) What is the skin depth, i.e., the distance when light intensity drop to e^{-1} inside the medium.

Solution:

Given:

$\lambda = 1\,\mu\text{m}$

$N_1 = 1$

$N_2 = 2 + 0.01i$

$\theta_i = 0^\circ$

(a) Since the media is semi-infinite, the absorptivity is equal to the transmissivity. From the Fresnel coefficients,

$$t = \frac{2N_1}{N_1 + N_2} = \frac{2(1)}{1 + 2 + 0.01i} = 0.6667 - 0.00222i \qquad (5.72\ \&\ 5.74)$$

Thus,

$$\tau = \frac{\mathrm{Re}(N_2^*)}{\mathrm{Re}(N_1^*)}|t|^2 = \frac{\mathrm{Re}(2 - 0.01i)}{\mathrm{Re}(1)}|0.6667 - 0.00222i|^2 = \boxed{0.8889}$$

(b) The skin depth of the material is defined as the inverse of the absorption coefficient,

$$\delta = \frac{1}{\alpha} = \frac{\lambda}{4\pi\kappa} = \frac{1\times10^{-6}m}{4\pi(0.01)} = \boxed{7.96\,\mu\text{m}} \qquad (5.40)$$

(4) Light with TM polarization at 1 μm wavelength is incident from a semi-infinite medium of refractive index N=2 towards an interface. Answer the following two questions:

(4a) (6 points) What is the critical angle of incidence.

(4b) (6 points) For an angle of incidence at 60^o, total internal reflection happens. How far does the electric field penetrate into the vacuum side, i.e., find the distance when the electric field drops to e^{-1} of its value at the interface (at the vacuum side).

Solution:

Given:

$\lambda = 1\,\mu\text{m}$

$N_1 = 2$

$N_2 = 1$

TM polarization

(a) The critical angle is,

$$\theta_c = \sin^{-1}\left(\frac{N_2}{N_1}\right) = \sin^{-1}\left(\frac{1}{2}\right) = \boxed{30^o} \qquad (5.80)$$

(b) The penetration depth for an evanescent TM wave is,

$$\delta = \frac{\lambda}{2\pi N_2 \left|\cos\theta_t\right|} = \frac{1\times10^{-6}\,m}{2\pi(1)\left|\sqrt{1-\left(\frac{2}{1}\sin(60^o)\right)^2}\right|} = \boxed{112.5\text{ nm}} \qquad (5.145)$$

(5) (6 points) An atom has two nondegenerate electronic quantum states with energy at E_1=-1.0 eV and E_2 = -0.97 eV from the vacuum level. At room temperature, the average number of electron count in each atom at the E_1 level is 0.5. What is the average number of electron count at the E_2 level.

Solution:

Given:

$T = 300\,\mathrm{K}$

$E_1 = -1.0\,\mathrm{eV}$

$E_2 = -0.97\,\mathrm{eV}$

$\langle n_1 \rangle = 0.5$

To determine the average number of electrons for the E_2 level, the chemical potential must first be found using the information given for the E_1 level,

$$\langle n_1 \rangle = f(E, T, \mu) = \frac{1}{\exp\left(\dfrac{E_1 - \mu}{k_b T}\right) + 1}$$

Thus,

$$0.5 = \frac{1}{\exp\left(\dfrac{-1.0\,\mathrm{eV} - \mu}{(1.38\times10^{-23}\,\mathrm{J/K})(300\,\mathrm{K})}\right) + 1} \rightarrow \mu = -1.0\,\mathrm{eV}$$

Therefore,

$$\langle n_2 \rangle = \frac{1}{\exp\left(\dfrac{-0.97\,\mathrm{eV} - (-1.0\,\mathrm{eV})}{(1.38\times10^{-23}\,\mathrm{J/K})(300\,\mathrm{K})} \cdot 1.602\times10^{-19}\,\dfrac{\mathrm{J}}{\mathrm{eV}}\right) + 1} = \boxed{0.239}$$

(6) (6 points) At 300K and 10^5 Pa, what is the average number of helium atoms per unit volume and per unit speed interval with a speed at 1000 m/s?

Solution:

Given:

$T = 300\,\mathrm{K}$

$P = 10^5\ \mathrm{Pa}$

$v = 1000\,\mathrm{m/s}$

$m = 4 \cdot m_p = 6.68\times10^{-27}\ \mathrm{kg}$

The average number of atoms traveling at a speed of 1000 m/s can be determined by the product of the total atom density and the Maxwell speed distribution,

$$\left.\frac{N}{V}\right|_v = \frac{N}{V}\cdot f(v)$$

To determine the total atom density, the ideal gas law can be used,

$$\frac{N}{V} = \frac{P}{k_b T} = \frac{\left(10^5\ \mathrm{Pa}\right)}{\left(1.38\times10^{-23}\ \mathrm{J/K}\right)\left(300\,\mathrm{K}\right)} = 2.415\times10^{25}\,\frac{\#}{m^3} \qquad (4.29)$$

The Maxwell speed distribution is the Maxwell distribution integrated over the solid angle,

$$f(v) = 4\pi\left(\frac{m}{2\pi k_b T}\right)^{\frac{3}{2}} v^2 \exp\left(-\frac{mv^2}{2k_b T}\right) \qquad (\text{p.}24)$$

$$f(v) = 4\pi\left(\frac{\left(6.68\times10^{-27}\ \mathrm{kg}\right)}{2\pi\left(1.38\times10^{-23}\ \mathrm{J/K}\right)\left(300\,\mathrm{K}\right)}\right)^{\frac{3}{2}}\left(1000\,\mathrm{m/s}\right)^2 \exp\left(-\frac{\left(6.68\times10^{-27}\ \mathrm{kg}\right)\left(1000\,\mathrm{m/s}\right)^2}{2\left(1.38\times10^{-23}\ \mathrm{J/K}\right)\left(300\,\mathrm{K}\right)}\right)$$

$$f(v) = 0.00073\left[\frac{\mathrm{s}}{\mathrm{m}}\right]$$

Thus,

$$\left.\frac{N}{V}\right|_v = \left(2.415\times10^{25}\,\frac{\#}{\mathrm{m}^3}\right)\cdot\left(0.00073\right) = \boxed{1.7629\times10^{22}\,\frac{\#}{\mathrm{m}^3}\cdot\frac{\mathrm{s}}{\mathrm{m}}}$$

(7) (6 points) Copper has an fcc lattice with a lattice constant of 3.61 Å (one Cu atom per lattice point). What is the lattice specific heat per unit volume at high temperatures.

Solution:
Given:
$a = 3.61\,\text{Å}$
FCC lattice

For an FCC lattice, the number of units per unit cell is equal to $N = 4$. At high temperature, the lattice specific heat will take the following form,

$$C_v = 3k_b \frac{N}{V} \tag{4.46}$$

This is due to 2 degrees of freedom in each coordinate direction (potential energy of the atom bonds and the kinetic energy of the atoms). Based on the given information,

$$C_v = 3\left(1.38\times10^{-23}\text{ J/K}\right)\frac{4}{\left(3.61\times10^{-10}\,\text{m}\right)^3} = \boxed{3.52\times10^{6}\,\frac{\text{J}}{\text{m}^3\text{K}}}$$

(8) (6 points) Electrons in a graphene sheet has a linear dispersion relation $E = c\sqrt{\left(k_x^2 + k_y^2\right)}$, where

$k_x, k_y = \pm\frac{2\pi}{L}, \pm\frac{4\pi}{L}, ..., \frac{\pi}{\mathrm{a}}$ (a the lattice constant). What is the density of states of electrons per unit energy interval and per unit area?

Solution:
Given:
$E = ck$; where $k = \sqrt{k_x^2 + k_y^2}$

The density of states in *k* space for this 2D system is,

$$D(k) = 2 \cdot \frac{2\pi k dk}{\left(\frac{2\pi}{L}\right)^2} \cdot \frac{1}{L^2 dk} = \frac{k}{\pi}$$

To convert to per unit energy interval, the following can be used,

$$D(E) = D(k)\frac{dk}{dE} = \frac{E}{\pi c} \cdot \frac{1}{c} = \boxed{\frac{E}{\pi c^2}}$$

Long Problems:

2. (20 points) **Interband Absorption of Photons.** A direct semiconductor has the following dispersions for the conduction and the valence bands,

$$E_c = E_G + \frac{\hbar^2\left(k_x^2 + k_y^2 + k_z^2\right)}{2m_c} \qquad \text{(for conduction band)}$$

$$E_v = -\frac{\hbar^2\left(k_x^2 + k_y^2 + k_z^2\right)}{2m_v} \qquad \text{(for valence band)}$$

where $k_x, k_y, k_z = \pm\frac{2\pi}{L}, \pm\frac{4\pi}{L}, ..., \frac{\pi}{\mathrm{a}}$; E_G is the bandgap, and m_c and m_v are the effective masses of the conduction and the valence band, respectively. Consider the interband absorption process in which a photon is absorbed, lifting an electron from the valence band to the conduction band. Because photons have very small momentum, we can approximate the absorption as a vertical process, i.e., no momentum change. The absorbed photon energy, E_p, should equal to the energy difference of the electrons and holes at the same wavevector, E_c-E_v. The absorption coefficient of the semiconductor, α, is proportional to the density of states available for such as transition. Show that the absorption coefficient varies as

$$\alpha \propto \sqrt{E_p - E_G}$$

Solution:

Given:

The energy dispersions given are:

$$E_c = E_G + \frac{\hbar^2 k^2}{2m_c} \qquad ;\ k^2 = k_x^2 + k_y^2 + k_z^2$$

$$E_v = -\frac{\hbar^2 k^2}{2m_v}$$

As given in the problem, the energy of an absorbed photon will equal to the energy difference between electrons and holes at the same wave vector *k*. Based on this information, the energy dispersion of this absorbed photon will be,

$$E_p = E_c - E_v = E_G + \frac{\hbar^2 k^2}{2m_c} + \frac{\hbar^2 k^2}{2m_v}$$

Or,

$$E_p - E_G = \frac{\hbar^2}{2}\left(\frac{1}{m_c} + \frac{1}{m_v}\right)k^2 = Ck^2$$

where,

$$C = \frac{\hbar^2}{2}\left(\frac{1}{m_c} + \frac{1}{m_v}\right)$$

Note that the energy dispersion relations given in the problem are taken with respect to the top of the valence band. However, the transition is defined with respect to E_v. By defining the energy dispersion in this form, the reference point is automatically changed. To prove that the absorption coefficient is proportional to the square root of energy, the density of states for this system must be determined. Starting in *k* space for a 3D system,

$$D(k) = 2 \cdot \frac{4\pi k^2 dk}{\left(\frac{2\pi}{L}\right)^3} \cdot \frac{1}{L^3 dk} = \frac{k^2}{\pi^2}$$

Once again, this can be written per unit energy interval by,

$$D(E) = D(k)\frac{dk}{dE} = \frac{\left(E_p - E_G\right)}{C\pi^2} \cdot \frac{1}{2\sqrt{C}} \cdot \frac{1}{\sqrt{E_p - E_G}}$$

$$D(E) = \frac{C^{-\frac{3}{2}}}{2\pi^2} \cdot \sqrt{E_p - E_G}$$

Therefore,

$$\boxed{\alpha \propto D(E) \propto \sqrt{E_p - E_G}}$$

3. (20 points) **Phonon Peak Energy in a Debye Crystal.** A Debye crystal at temperature T has the following dispersion relation

$$\omega = \mathrm{v_D} k = \mathrm{v_D}\sqrt{k_x^2 + k_y^2 + k_z^2} = \frac{2\pi \mathrm{v_D}}{\lambda}$$

where $k_x, k_y, k_z = \pm\frac{2\pi}{L}, \pm\frac{4\pi}{L}, \ldots, \frac{\pi}{\mathrm{a_D}}$, $\mathrm{v_D}$ (=3000 m/s) is the Debye velocity, and $\mathrm{a_D}$ (=2 Å) is the equivalent lattice constant of the Debye crystal. Answer the following questions

(a) (5 points) Derive an expression for the phonon density of states per unit volume and per wavelength interval.

(b) (5 points) Derive an expression for the internal energy per unit volume and per unit wavelength interval, u_λ.

(c) (5 points) Derive a corresponding Wien's law for phonons, i.e., determine the phonon wavelength at which the internal energy u_λ peaks.

(d) (5 points) Based on the answer for (c) and the shortest physically allowed phonon wavelength in the crystal, determine the wavelength at which u_λ peaks at 10 K and 300 K.

Solution:

Given:

$$\omega = \mathrm{v_D} k = \mathrm{v_D}\frac{2\pi}{\lambda}$$

$$\mathrm{v_D} = 3000\ \mathrm{m/s}$$

$$\mathrm{a_D} = 2\ \text{Å}$$

(a) The density of states can once again be derived starting in *k* space,

$$D(k) = 3\cdot\frac{4\pi k^2 dk}{\left(\frac{2\pi}{L}\right)^3}\cdot\frac{1}{L^3 dk} = \frac{3k^2}{2\pi^2}$$

To convert to per wavelength interval,

$$D(\lambda) = D(k)\left|\frac{dk}{d\lambda}\right| = \frac{3}{2\pi^2}\cdot\left(\frac{2\pi}{\lambda}\right)^2\cdot\left|-\frac{2\pi}{\lambda^2}\right|$$

$$\boxed{D(\lambda) = \frac{12\pi}{\lambda^4}}$$

(b) The internal energy of phonons per unit volume per unit and per unit wavelength interval can be written as,

$$u_\lambda = E(\lambda)\cdot f(E(\lambda),T)\cdot D(\lambda)$$

Thus,

$$u_\lambda = \hbar \cdot \left(\frac{2\pi \mathrm{v_D}}{\lambda}\right) \cdot \frac{1}{\exp\left(\frac{\hbar}{k_b T} \cdot \frac{2\pi \mathrm{v_D}}{\lambda}\right) - 1} \cdot \frac{12\pi}{\lambda^4}$$

$$u_\lambda = \frac{24\pi^2 \hbar \mathrm{v_D}}{\lambda^5 \left(\exp\left(\frac{2\pi\hbar \mathrm{v_D}}{k_b} \cdot \frac{1}{\lambda T}\right) - 1\right)}$$

If the following constants are defined,

$$C_1 = 24\pi^2 \hbar \mathrm{v_D}$$

$$C_2 = \frac{2\pi\hbar \mathrm{v_D}}{k_b}$$

The expression for the internal energy becomes,

$$\boxed{u_\lambda = \frac{C_1}{\lambda^5 \left(\exp\left(\frac{C_2}{\lambda T}\right) - 1\right)}}$$

(c) To derive a Wien's law for phonons, the peak position in the internal energy must be found as a function of wavelength. Therefore, the expression for the internal energy from (b) must be differentiated and a critical point must be found,

$$\frac{du_\lambda}{d\lambda} = C_1 \left[-\frac{5}{\lambda^6 \left(\exp\left(\frac{C_2}{\lambda T}\right) - 1\right)} + \frac{\exp\left(\frac{C_2}{\lambda T}\right) \cdot \frac{C_2}{\lambda^2 T}}{\lambda^5 \left(\exp\left(\frac{C_2}{\lambda T}\right) - 1\right)^2} \right] = 0$$

Simplifying leads to,

$$\frac{5(\lambda T)}{C_2} \cdot \left(\exp\left(\frac{C_2}{\lambda T}\right) - 1\right) - \exp\left(\frac{C_2}{\lambda T}\right) = 0$$

Defining $x = \lambda T$, the expression becomes,

$$\frac{5x}{C_2} \cdot \left(\exp\left(\frac{C_2}{x}\right) - 1\right) - \exp\left(\frac{C_2}{x}\right) = 0$$

To solve for *x*, the expression must either be iterated or graphically solved. Based on the given information,

$$C_2 = 1.4426 \times 10^{-7}\ \mathrm{K \cdot m}$$

Using either method will lead to,

$$x = \lambda T = \boxed{0.029\ \mu\mathrm{m} \cdot \mathrm{K}}$$

Alternatively, this value can be deduced by observing that the only difference between this particular case and the photon case is the speed of the particle, i.e. Debye velocity vs. speed of light. Since the Debye velocity is 10^5 smaller, the corresponding Wien's law should also be 10^5 smaller compared to the photon case.

(d) For phonons, the wave vector *k* is limited by the discrete nature of the crystal lattice. Specifically,

$$k_{\max} = \frac{\pi}{a}$$

In terms of wavelength,

$$k_{\max} = \frac{2\pi}{\lambda_{\min}} = \frac{\pi}{a} \rightarrow \lambda_{\min} = 2a = 4\,\text{Å}$$

For $T_1 = 10\,\text{K}$,

$$\lambda_1 = \frac{0.029\,\mu\text{m}\cdot\text{K}}{10\,\text{K}} = \boxed{2.91\,\text{nm}}$$

Since $\lambda_1 > \lambda_{\min}$, the peak given by the phonon Wien's law is observable.

For $T_2 = 300\,\text{K}$,

$$\lambda_2 = \frac{0.029\,\mu\text{m}\cdot\text{K}}{300\,\text{K}} = 0.967\,\text{Å}$$

In this case, $\lambda_2 < \lambda_{\min}$. Therefore the peak value in the internal energy will occur at $\lambda_{\min}$,

$$\lambda_2 = \lambda_{\min} = \boxed{4\,\text{Å}}$$

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