

The Handbook of Mathematics, Physics and Astronomy Data is provided

KEELE UNIVERSITY

EXAMINATIONS, 2009/10

Level II

Monday 17th May, 16.00-18.00

PHYSICS/ASTROPHYSICS

PHY-20026

STATISTICAL MECHANICS AND SOLID STATE PHYSICS

Candidates should attempt to answer FOUR questions.

NOT TO BE REMOVED FROM THE EXAMINATION HALL

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1. (a) In the context of crystallography, what is meant by
 - i. lattice;
 - ii. primitive unit cell;
 - iii. translation vector;
 - iv. basis;
 - v. reciprocal lattice vector;
 - vi. reciprocal space.

[5]
[5]
[5]
[5]

(b) The simple orthorhombic lattice has primitive translation vectors

$$\mathbf{a} = a \mathbf{i}$$

$$\mathbf{b} = b \mathbf{j}$$

$$\mathbf{c} = c \mathbf{k}$$

where \mathbf{i} , \mathbf{j} and \mathbf{k} are the usual cartesian unit vectors and a , b and c are constants. Determine

- i. the volume of the unit cell; [15]
- ii. the reciprocal lattice vectors; [45]
- iii. the volume of the unit cell in the reciprocal lattice. [10]

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2. (a) Sketch the form of the Fermi-Dirac distribution for (i) a gas at $T = 0$ K. [10]
(ii) a gas at $T > 0$ K. Indicate on your plot the location of the Fermi energy. [10]
- (b) Assuming that the density of states is given by

$$g(E) dE = \frac{V}{2\pi^2} \left(\frac{2m}{\hbar^2} \right)^{2/3} E^{1/2} dE$$

in the usual notation, show that the Fermi energy is given by

$$E_F = \frac{\hbar^2}{2m} (3\pi^2 n)^{2/3}$$

where n is the number of fermions per unit volume. [25]

- (c) Sodium has density 988 kg m^{-3} and unit valency.
- i. Calculate the number of conduction electrons m^{-3} in sodium. [20]
 - ii. Calculate the Fermi energy of the electron gas. [10]
 - iii. Determine whether or not the electrons are relativistic. [20]
 - iv. Estimate the temperature of the *classical* gas for which the mean electron energy would be the same as your answer to part (c) ii. [10]

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3. Consider a system at temperature T containing N particles, of which n_i have energy ϵ_i , and the energy levels are non-degenerate.

(a) Write down expressions for

i. the number of particles n_i with energy ϵ_i [5]

ii. the partition function Z [5]

iii. the internal energy U [10]

(b) Hence show that

$$\frac{\partial \ln Z}{\partial T} = \frac{U}{Nk_B T^2} \quad [30]$$

(c) To a good approximation, the rotational partition function Z_{rot} for diatomic molecules in a gas at temperature T is

$$Z_{\text{rot}} = \frac{2\mathcal{I}k_B T}{\hbar^2}$$

where \mathcal{I} is the moment of inertia of the molecule. Determine the following quantities for the rotational energy of a kg-mole of a diatomic gas.

i. the internal energy [30]

ii. and the specific heat [20]

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4. (a) Describe, without going into mathematical detail, the essential features of the classical, Einstein and Debye theories of the specific heats of solids.
- (b) Explain in each case, with the aid of a suitable sketch and without giving mathematical detail, how each theory describes the temperature-dependence of the specific heat of solids. [20]
- (c) The energy of a simple harmonic, one-dimensional quantum oscillator with frequency ω is given by

$$E_n = (n + \frac{1}{2}) \hbar\omega .$$

Write down an expression for the partition function for the oscillator. [10]

- (d) The internal energy is given by

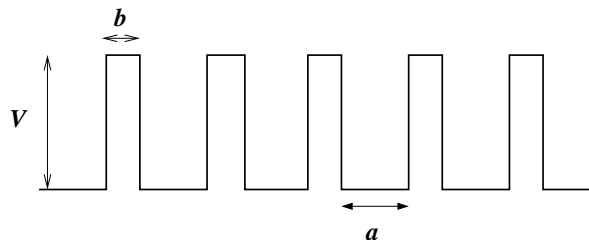
$$U = Nk_B T^2 \frac{\partial \ln Z}{\partial T} = \frac{N\hbar\omega}{2} + \frac{N\hbar\omega}{\exp[\hbar\omega/k_B T] - 1}$$

Determine the specific heat of the one-dimensional harmonic oscillator. [20]

- (e) What is the specific heat of the corresponding two-dimensional harmonic oscillator? [20]

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5. The figure shows part of a periodic one-dimensional step potential, which extends indefinitely in both directions. The potential height and width are V and b respectively, and the separation of the steps is a . An electron with mass m and energy $E < V$ moves in this potential.



- (a) i. In the case that the product bV is vanishingly small, what can be said about the electron? [10]
- ii. Write down an expression for the electron energy, in terms of the electron wavenumber k , for this case. [10]
- iii. Describe and explain the behaviour of the electron, and its energy, in the case that the product bV is very large (but with b still $\ll a$) [20]
- (b) By considering the dependence of electron energy on bV , discuss the relevance of the results from part (a) i-iii to the formation of energy bands in solids. [30]
- (c) Sketch the dispersion relation for a free electron. [15]
- (d) Discuss how the dispersion relation in part (c) is amended in the presence of energy bands. [15]

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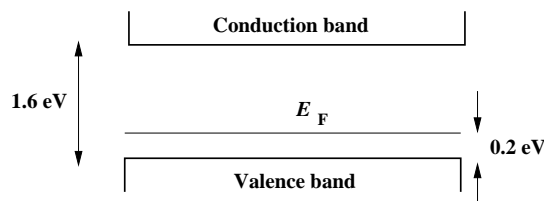
6. (a) The concentrations of conduction electrons (n) and holes (p) in a semiconductor at temperature T are given by

$$n \simeq N_c \exp[-(E_c - E_F)/k_B T]$$

$$p \simeq N_v \exp[-(E_F - E_v)/k_B T]$$

respectively.

- i. State what each of the undefined terms in these expressions means. [15]
 - ii. What are the assumptions that lead to these expressions? [15]
- (b) The figure shows the energy band for a semiconductor, in the region of the band gap.



- i. Would you consider that the semiconductor is an n -type or a p -type? Explain your answer. [10]
- ii. Calculate the probability, at 270 K, that an electron occupies an energy state at the bottom of the conduction band. [15]
- iii. Calculate the probability, also at 270 K, that there is a vacancy in an energy state at the top of the valence band. [15]
- iv. For this semiconductor, the effective masses are $m_e^* = 0.05 m_e$ and $m_h^* = 0.2 m_e$. Calculate the density of states at the top of the valence band and at the bottom of the conduction band at 270 K. [15]
- v. Hence calculate the concentration of holes at the top of the valence band and of electrons at the bottom of the conduction band. [15]

[N.B. You may assume that the probability of occupancy of a state with energy E is

$$f(\epsilon) = \frac{1}{1 + \exp\left[\frac{E - E_F}{k_B T}\right]}$$

and that

$$N_c = N_v = 2 \left(\frac{m^* k_B T}{2\pi \hbar^2} \right)^{3/2} \quad \text{where } m^* \text{ is the effective mass. } \quad]$$