



FACULTY OF SCIENCE
FAKULTEIT NATUURWETENSKAPPE

DEPARTMENT OF PHYSICS
DEPARTEMENT FISIKA

APK

PHY003B

STATISTICAL AND SOLID STATE PHYSICS

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INTERNAL MODERATOR

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DURATION 3 HOURS

MARKS 120

THIS PAPER CONSISTS OF 11 PAGES INCLUDING THIS COVER

Instructions

**ANSWER ANY FOUR OUT OF
FIVE QUESTIONS FROM EACH SECTION
(eight questions in total)**

Section A : STATISTICAL MECHANICS**QUESTION A1** [15]

Consider a system of fixed volume and fixed number of particles placed in a heat bath at temperature T . The probability to be in a state r is given by the Boltzmann distribution

$$p_r = \frac{1}{Z} e^{-\beta E_r}, \quad Z = \sum_r e^{-\beta E_r}, \quad \beta = \frac{1}{k_B T}$$

The mean energy \bar{E} of the system in the heat bath is given by $\bar{E} = -\frac{\partial \ln(Z)}{\partial \beta}$.

A system consists of N weakly interacting subsystems and each subsystem possesses only two energy levels of energies zero and ε , each of which is non-degenerate.

- (a) Make use of the Boltzmann distribution above to calculate the average energy of each subsystem.
- (b) Hence show that the heat capacity of the combined system is given by the well-known Schottky anomaly :

$$C = \frac{Nk_B y^2 e^y}{(e^y + 1)^2} \quad \text{where } y = \frac{\varepsilon}{k_B T}.$$

- (c) Consider the behaviour of C in the low and high temperature limits and plot C as a function of y .

QUESTION A2 [15]

One possible means of obtaining fusion energy is to implode spherical capsules containing heavy hydrogen by irradiating them with high power lasers. For fusion to occur the implosion core needs to reach electron temperatures of the order of ~ 1 keV (~ 10 million K) and the electron density needs to be of the order of 10^{33} m^{-3} . Do we need to use Fermi-Dirac (quantum) statistics to describe the electrons, or are Maxwell-Boltzmann (classical regime) statistics sufficient? Give two sets of explanations supported by calculations to justify your answer. Recall that the classical regime requires that the energy levels are sparsely occupied.

[Hints : Take care of using MKS units in the calculations, also calculate the Fermi energy and use the figure provided below as a guide]

Planck's constant $h = 6.626 \times 10^{-34} \text{ J.s} = 4.136 \times 10^{-15} \text{ eV.s}$

Molar gas constant $R = 8.314 \text{ J.K}^{-1}.\text{mol}^{-1}$

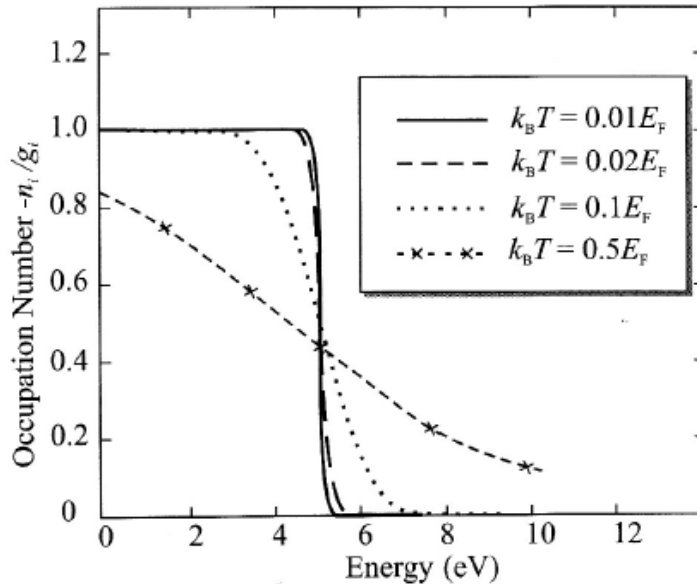
Boltzmann's constant $k_B = 8.617 \times 10^{-5} \text{ eV/K}$

Electron mass $m_e = 9.11 \times 10^{-31} \text{ kg}$

$1 \text{ eV} = 1.602 \times 10^{-19} \text{ J}$

de-Broglie wavelength $\lambda_{\text{dB}} = \frac{h}{\sqrt{3mk_B T}}$

$$E_F = \frac{\hbar^2}{2m} \left(\frac{3\pi^2 N}{V} \right)^{2/3}$$



QUESTION A3 [15]

Depart from the partition function for a perfect quantal gas

$$Z(T, V, N) = \sum_{n_1, n_2, \dots} \exp\{-\beta \sum_r n_r \varepsilon_r\} ,$$

where the summation refers to all possible sets $\{n_1, n_2, n_3, \dots\}$ of the occupancies of single-particle energy states $\{\varepsilon_1, \varepsilon_2, \varepsilon_3, \dots\}$.

- (a) Derive an expression for the partition function Z_{ph} and an expression for the mean occupation number \bar{n}_i for photons radiated in a Blackbody cavity at temperature T .
- (b) Furthermore assume the relation $\bar{n}_i = -\frac{1}{\beta} \frac{\partial \ln(Z_{ph})}{\partial \varepsilon_i}$ to find Planck's result for the mean occupation number

$$\bar{n}_i = \frac{1}{e^{\beta \varepsilon_i} - 1}$$

in terms of $(\beta = 1/k_B T)$ and ε_i . Fully motivate the physics behind your calculations, especially in obtaining Z_{ph} .

- (c) A photon has energy and momentum $\varepsilon = \hbar\omega$ and $p = \varepsilon/c$, respectively. The general expression for the density of momentum states is
- $$f(p) dp = \frac{V 2 \times 4\pi p^2 dp}{h^3} .$$
- Describe qualitatively, the steps you would follow, to arrive at Planck's radiation law for the energy density in the cavity :

$$U(\omega, T) d\omega = \frac{\hbar \omega^3 d\omega}{\pi^2 c^3 (\exp(\beta \hbar \omega) - 1)} .$$

Note , that a detailed derivation of this equation is NOT required.

QUESTION A4 [15]

If a system of chemical potential μ , possesses a sequence of energy states $E_{N1} \leq E_{N2} \leq E_{N3} \leq \dots$ for any given number of particles N , the Gibbs (grand canonical) distribution is given by

$$P_{Nr} = \frac{\exp \left[-\beta (E_{Nr} - \mu N) \right]}{\mathbf{Z}},$$

where P_{Nr} is the probability that the system is in energy state E_{Nr} and the number of particles N can vary due to exchange with the “bath”.

The grand canonical partition function is $\mathbf{Z} = \sum_{N=0}^{\infty} \sum_{r=1}^{\infty} \exp \left[-\beta (E_{Nr} - \mu N) \right]$,

where $N = \sum_i n_i$ and $E_{Nr} = \sum_i n_i \varepsilon_i$ and the subscript i refers to single particle energy states ε_i . Applying the Gibbs formalism to a perfect quantum gas factorizes the Gibbs grand canonical partition function and probability distribution as follows :

$$\mathbf{Z} = \prod_{i=0}^{\infty} z_i, \quad P_{Nr} = \prod_{i=0}^{\infty} p_i(n_i),$$

where
$$z_i = \sum_{n_i} e^{-\beta(\varepsilon_i - \mu)n_i} \quad \text{and} \quad p_i(n_i) = \frac{e^{-\beta(\varepsilon_i - \mu)n_i}}{z_i}.$$

- Assume these results and through appropriate reasoning find expressions for z_i (“single-level partition function”), for both Fermi-Dirac and Bose-Einstein statistics.
- Using the following relation for the mean occupation number of the i -th single particle state given by :

$$\overline{n_i} = \frac{1}{\beta} \left(\frac{\partial \ln z_i}{\partial \mu} \right)_{T,V},$$

derive furthermore an expression for $\overline{n_i}$ for both Fermi-Dirac and Bose-Einstein quantal gases (i.e., the distribution function expressed in terms of ε_i , μ and β).

- Consider the permitted μ values for the two cases and briefly (perhaps by way of a diagram) indicate the behaviour of these expressions in the limit $T \rightarrow 0$ K if the single particle state of lowest energy is ε_0 .

QUESTION A5 [20 marks available, but 15 or more is 100 %]

For a Bose gas the number of momentum states between p and $p + dp$ is :

$$f(p)dp = \frac{V 4\pi p^2 dp}{h^3}.$$

The dispersion relation and Bose-Einstein distribution, respectively, are :

$$\varepsilon = \frac{p^2}{2m}; \quad \bar{n}_\varepsilon = \frac{1}{\exp[\beta(\varepsilon - \mu)] - 1}.$$

- (a) Suppose the Bose gas has N particles. Derive and explain why the following expression is an indication of the number of bosons in the excited energy states $\varepsilon > 0$, if the ground state is considered as $\varepsilon = 0$:

$$N_{exc} = \left[\frac{2\pi V}{h^3} (2m)^{3/2} \int_0^\infty \frac{\varepsilon^{1/2} d\varepsilon}{\exp[\beta(\varepsilon - \mu)] - 1} \right].$$

- (b) Now below the Bose-Einstein temperature T_C when some particles have condensed into the ground state, $\mu \rightarrow 0$. The internal energy E of the system is due to those particles in the excited state.

Show that
$$E = \left[\frac{2\pi V}{h^3} (2m)^{3/2} (k_B T)^{5/2} \times 1.78 \right], \text{ i.e., } E \propto T^{5/2}.$$

[Hint : Use the density of energy states $f(\varepsilon)d\varepsilon$ obtained from $f(p)dp$ above, similar to finding N_{exc}]

- (c) Using $\frac{N}{V} = \left(\frac{2\pi m k_B T_C}{h^2} \right)^{3/2} \times 2.61$ derived in class from the definition of T_C above, show that the heat capacity of the Bose gas at $T < T_C$ is

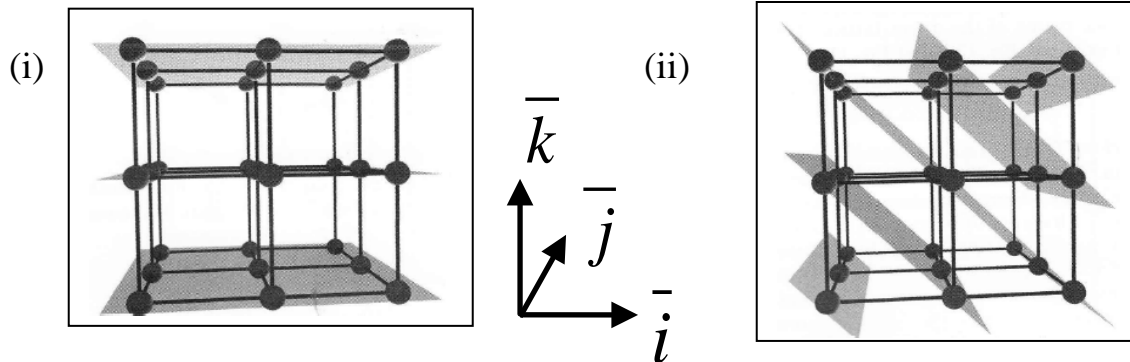
$$C_V = \frac{2}{\sqrt{\pi}} \frac{1.78}{2.61} \frac{5}{2} N k_B \left(\frac{T}{T_C} \right)^{3/2}.$$

It is given that
$$\int_0^\infty \frac{x^{3/2}}{e^x - 1} dx = 1.78$$

Section B : SOLID STATE PHYSICS

QUESTION B1 [15]

- (a) A simple cubic lattice with unit cell length a is shown below. Obtain the Miller indices for the following diffraction planes and calculate the spacing between the planes :



- (b) Consider a basis specified by vectors $\mathbf{r}_1, \mathbf{r}_2 \dots \mathbf{r}_n$ relative to some space lattice. The reciprocal lattice of the underlying space lattice is \mathbf{G} . The structure factor is defined by

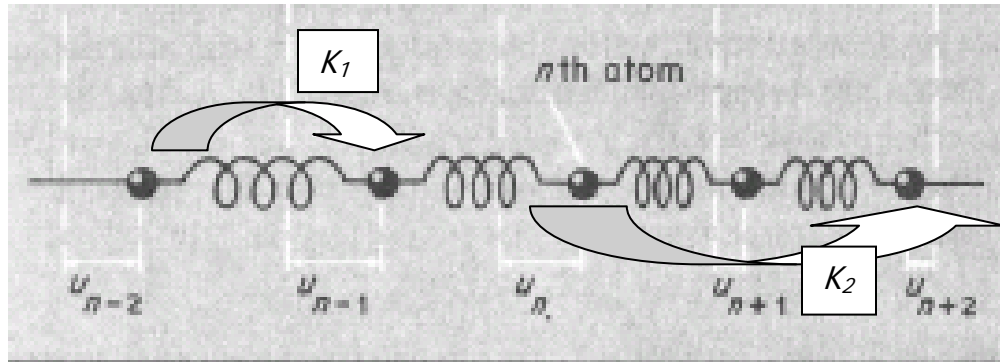
$$S(\vec{G}) = \sum_j f_j(\vec{G}) e^{i\vec{G} \cdot \vec{r}_j} \text{ where } f_j(\vec{G}) \text{ is the form factor.}$$

- (i) Explain what the form factor represents.
- (ii) The structure factor impacts on the scattered intensity. Explain, with the aid of diagrams, how and why this arises.
- (iii) The fcc lattice may be considered as a simple cubic lattice with unit cell length a and basis vectors $\mathbf{r}_1 = (0,0,0)a$ $\mathbf{r}_2 = (\frac{1}{2}, \frac{1}{2}, 0)a$ $\mathbf{r}_3 = (\frac{1}{2}, 0, \frac{1}{2})a$ $\mathbf{r}_4 = (0, \frac{1}{2}, \frac{1}{2})a$. Write out the expression for the reciprocal lattice points \mathbf{G} in terms of the Miller indices (h,k,l) and the conventional unit vectors.
- (iv) Then write out the expression for the structure factor. Consider what is its value when the indices (h,k,l) are all even or all odd. Then consider the case when the indices are a mixture of odd and even values. What can you then conclude about the effect of the structure factor on the resultant x-ray diffraction pattern for an fcc metal like Cu.

Useful information : $e^{in\pi}$ is 1 if n is even and -1 if n is odd.

QUESTION B2 [15]

Lattice vibrations are considered for a linear chain of identical masses M separated by a distance a from each other. Each mass is connected to its first and second nearest-neighbours effectively by springs of spring constants K_1 and K_2 , respectively, as sketched below. Longer range interactions are neglected.



The atoms are separated by a distance a at equilibrium. Write down the equation of motion for the n -th atom in terms of displacements U_n , U_{n-1} , U_{n-2} , U_{n+1} , U_{n+2} of the atoms from their equilibrium positions. Use a solution $U_n = A \exp[i(kx_n^0 - \omega t)]$ with $x_n^0 = na$ the equilibrium position of the n^{th} atom and derive the following dispersion relation for this chain:

$$\omega^2 M = E K_1 (1 - \cos F ka) + G K_2 (1 - \cos H ka).$$

The numerical values of E, F, G and H should follow from your calculation.

Information :

$$\frac{e^{i\theta} + e^{-i\theta}}{2} = \cos(\theta)$$

$$\frac{e^{i\theta} - e^{-i\theta}}{2i} = \sin(\theta)$$

QUESTION B3 [15]

The energy of lattice vibrations in a crystal is given by

$$E = \int_0^{\infty} \left(\frac{1}{2} \hbar \omega + \frac{\hbar \omega}{e^{\hbar \omega / k_B T} - 1} \right) g(\omega) d\omega$$

and the density of energy or frequency states in three-dimensions is given as

$$g(\omega) = \frac{V k^2}{2\pi^2} \frac{dk}{d\omega},$$

where k is the wave vector.

- (a) Discuss the behaviour of the phonon system at low temperatures and show, with motivation, that

$$g(\omega) = \frac{V \omega^2}{2\pi^2} \left(\frac{1}{v_L^3} + \frac{2}{v_T^3} \right)$$

where subscripts L and T refer to longitudinal and transverse acoustic modes.

- (b) Using this expression for $g(\omega)$ show that the heat capacity at low temperatures is given by

$$C = \frac{2V}{15} \pi^2 k_B \left(\frac{1}{v_L^3} + \frac{2}{v_T^3} \right) \left(\frac{k_B T}{\hbar} \right)^3$$

Note that in the expressions for E and C , k_B is Boltzmann's constant.

It is given that $\int_0^{\infty} \frac{x^3 dx}{e^x - 1} = \frac{\pi^4}{15}$.

QUESTION B4**[15]**

The following equation relates to the probability amplitudes $c_n(t)$, c_{n-1} and c_{n+1} associated with an extra electron at the positions of covalently bonded atoms n , $n-1$ and $n+1$, respectively, on a linear chain with lattice spacing a :

$$i\hbar \frac{dc_n(t)}{dt} = Bc_n - Ac_{n-1} - Ac_{n+1} \quad .$$

Where $|c_n(t)|^2$ is the probability of finding the electron in an energy level (stationary state) B on atom n . A is the coupling (overlap integral) involving the orbitals on neighbouring atoms.

- (a) Using an appropriate travelling wave solution for the electron, show that it leads to a dispersion relation $\varepsilon = B - 2A \cos(ka)$. Sketch the dispersion relation ε versus k for $A > 0$. Explain what is the bandwidth and rationalize how it has evolved from the energy levels B of isolated atoms.
- (b) Furthermore show that near the bottom of the band the dispersion relation is parabolic and highlight what is the effective mass of carriers in the band. Indicate why we refer to this as the tight-binding approximation.
- (c) From what you have sketched in (a), an energy gap is opened up at $k = \pi/a$. Briefly explain why this is the case for this periodic linear chain.

QUESTION B5 [15]

- (i) Explain what it means to add donor impurities to a semiconductor like Si and give an example of such donor impurities. Then explain what it means to add acceptor impurities to Si and give an example of such acceptors. Draw a fully labelled E versus k dispersion diagram for the doped semiconductor to illustrate what is the effect of the above mentioned doping.
- (ii) Doping as mentioned above has the effect of introducing hydrogenic type atoms into the host Si lattice. Explain what is meant by this. Using the information below, calculate typical ionization energies for donor impurities if the dielectric constant of Si is $\epsilon_r = 12$ and the effective mass m_e is one-tenth of the bare electron mass m .
- (iii) Based on your calculations in (ii) comment on the effect of room temperature, 300 K, on the electrical properties of doped Si.

For a hydrogenic-type atom the energy level scheme and radii of Bohr orbits are given by

$$E_n = \frac{m_e e^4}{2\epsilon_r^2 \hbar^2 n^2} \left(\frac{1}{4\pi\epsilon_0} \right)^2$$

$$r_n = \frac{\epsilon_r \hbar^2 n^2 (4\pi\epsilon_0)}{m_e e^2}$$

where for the ground state, $n = 1$, in hydrogen

$$E_1 = -13.6 \text{ eV} \text{ and } r_1 = 0.53 \text{ \AA}$$

$$k_B = 8.62 \times 10^{-5} \text{ eV / K}$$

(END OF PAPER)