



FACULTY OF SCIENCE
FAKULTEIT NATUURWETENSKAPPE

DEPARTMENT OF PHYSICS
DEPARTEMENT FISIKA

APK

PHY003B

STATISTICAL AND SOLID STATE PHYSICS

DATE: 09th November 2019

SESSION: 08:30 – 11:30

INTERNAL MODERATOR

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EXTERNAL MODERATOR

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DURATION 3 HOURS

THIS PAPER CONSISTS OF 12 PAGES INCLUDING THIS COVER

Instructions

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

For each question, 15 marks or more counts for 100 %

Total 120 marks (60 marks per section) is a 100 %

Section A : STATISTICAL MECHANICS

QUESTION A1 [18 marks available, but 15 or more is 100 %]

Consider a system of two independent particles occupying three single-particle states with energies E_1 , E_2 and E_3 . Assuming the two particles are indistinguishable:

(a) List all the two-particle microstates by sketching the energy-level occupation diagrams. (3)

(b) Write down the two-particle partition function Z_2 and show that it is not equal to $(Z_1)^2/2!$, where Z_1 is the single-particle partition function. (6)

(c) However, show that $Z_2 = (Z_1)^2/2!$ in the classical approximation. (4)

(d) Write down the expression for the average energy \bar{E} in the limit $T \rightarrow \infty$. (5)

QUESTION A2 [16 marks available, but 15 or more is 100 %]

(a) What is the criterion for validity of the classical regime of an ideal gas in terms of inter-particle spacing l and particle de-Broglie wavelength

$$\lambda_{dB} = \frac{h}{\sqrt{3mk_B T}} ? \quad (2)$$

(b) Show how we arrive at this by considering the condition for the mean number of particles \bar{n}_s in translational energy state ε_s^{tr} and the Boltzmann probability distribution $P_s = \frac{\exp(-\beta\varepsilon_s^{tr})}{Z_1^{tr}}$ in a gas of N particles, where $\beta = 1/k_B T$.

Recall the partition function for a single particle $Z_1^{tr} = V \left(\frac{2\pi mk_B T}{h^2} \right)^{3/2}$,

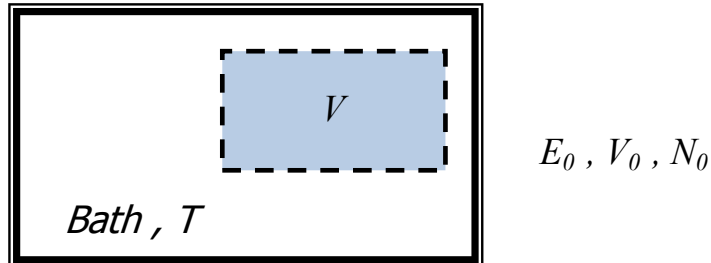
$p = h/\lambda$, where p specifies momentum and the average translation energy per particle is $\bar{\varepsilon}_s^{tr} = \frac{3}{2} k_B T$. (8)

(c) The expression for the average translational (kinetic) energy is obtained from $\bar{E}_{tr} = E_{tr} = - \left(\frac{\partial \ln Z_{tr}}{\partial \beta} \right)$. Use this to find the average translational energy of N indistinguishable particles of a classical gas, using

$$Z_{tr} = \frac{1}{N!} [Z_1^{tr}]^N \text{ and } N! = \left(\frac{N}{e} \right)^N. \quad (6)$$

QUESTION A3 [15]

Consider a system of fixed volume V in contact with a heat bath, which can exchange particles and energy with the heat bath. If the system has N particles it can possess a sequence of energies (microstates) states $E_{N1} \leq E_{N2} \leq E_{N3} \leq \dots$



The total energy, volume and number of particles of the composite system is fixed at E_0 , V_0 and N_0 , respectively.

(i) Write down the probability that the total energy E_0 is partitioned between the bath and system as $E_0 - E_{Nr}$ and E_{Nr} , respectively, in terms of statistical weights of microstates. (3)

(ii) Formulate the statistical weight in terms of entropy S . Justify why you can make an appropriate Taylor series expansion of S_{Bath} and use this to find an expression for statistical weight of microstates of the bath in terms of T , system energy E_{Nr} and the chemical potential $\mu = -\frac{\partial E_{bath}}{\partial N_0}$. (9)

(iii) Show that the probability of the system being in energy state E_{Nr} when it has N particles is given by the Gibbs (grand canonical) distribution

$$P_{Nr} = \frac{\exp \left[-\beta (E_{Nr} - \mu N) \right]}{\mathbf{Z}} . \quad (3)$$

The grand partition function is

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

and $N = \sum_i n_i$ and $E_{Nr} = \sum_i n_i \varepsilon_i$ when the subscript i refers to *single particle energy states* ε_i . The derivation is similar to what you did for the Boltzmann distribution. Explain the reasoning of each of your steps in the derivations.

QUESTION A4 [19 marks available, but 15 or more is 100 %]

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) Use this to derive an expression for the partition function Z_{ph} of photons in a cavity at temperature T and show that

$$\ln(Z_{ph}) = -\sum_{i=1}^{\infty} \ln(1 - e^{-\beta \varepsilon_i}). \quad (9)$$

- (b) Derive Planck's result for the mean occupation number of the single-particle energy level ε_i , namely that:

$$\bar{n}_i = -\frac{1}{\beta} \frac{\partial \ln(Z_{ph})}{\partial \varepsilon_i} = \frac{1}{e^{\beta \varepsilon_i} - 1} \quad \text{where } \beta = 1/k_B T. \quad (4)$$

- (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 $f(p)dp = \frac{V \times 2 \times 4\pi p^2 dp}{h^3}$. First use this to find the density of photon frequency states and then show that the number of photons in the frequency interval ω to $\omega + d\omega$ is :

$$dN(\omega, T) = V \frac{\omega^2 d\omega}{\pi^2 c^3 (\exp(\beta \hbar \omega) - 1)} \quad (6)$$

QUESTION A5 [17 marks available, but 15 or more is 100 %]

For the case of conduction electrons in a block of metal of volume V , the number of momentum states between p and $p + dp$ is:

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

- (i) Explain (but do not derive) how this density of momentum states expression arises. (3)

The energy dispersion relation and Fermi-Dirac distribution, respectively, are formulated as:

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

- (ii) Use this to show that we arrive at the following expression for the total number of conduction electrons in volume V :

$$N = \left[\frac{4\pi V}{h^3} (2m)^{3/2} \int_0^\infty \frac{\varepsilon^{1/2} d\varepsilon}{\exp[\beta(\varepsilon - \mu)] + 1} \right]. \quad (6)$$

- (iii) Explain what is the Fermi energy E_F , especially with reference to the single-particle energy level occupancy diagram as $T \rightarrow 0$ K. At this extremum of temperature show that the expression for E_F in terms of the conduction electron number density N/V is:

$$E_F = \frac{h^2}{2m} \left(\frac{3}{8\pi} \frac{N}{V} \right)^{2/3}. \quad (6)$$

- (iv) Show how your single-particle energy level occupancy diagram is modified at finite temperatures. (2)

Explain and justify all steps in your derivations above.

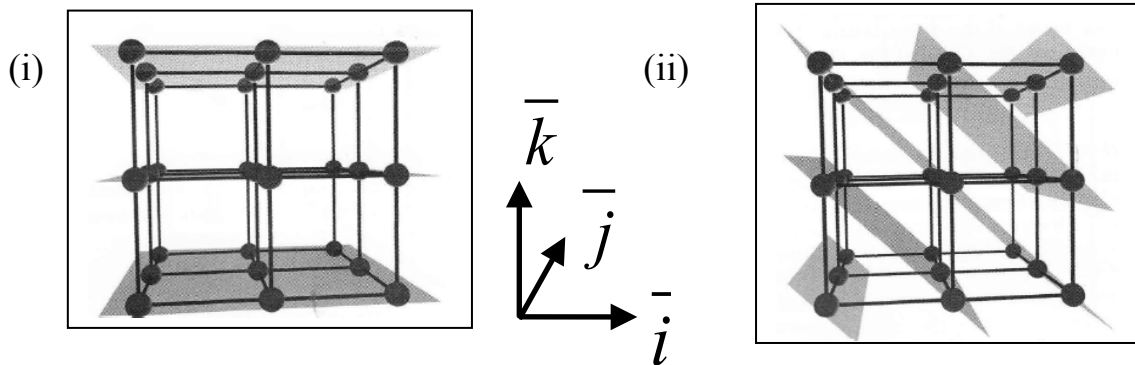
Section B : SOLID STATE PHYSICS

QUESTION B1 [19 marks available, but 15 or more is 100 %]

(a) Distinguish between these three terms: Bravais lattice, basis and crystal structure. Use a diagram to illustrate your answer. List any two classes of Bravais lattices other than that of the cubic lattices.

(7)

(b) A simple cubic lattice with unit cell length a is shown below. Obtain the Miller indices (h,k,l) for the following diffraction planes and calculate the spacing between the planes $d = a / \sqrt{(h^2 + k^2 + l^2)}$:



(6)

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

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

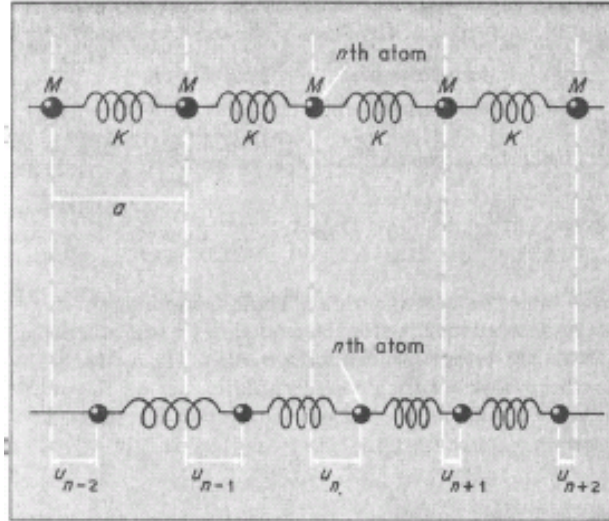
(i) The structure factor impacts on the scattered intensity. Explain, with the aid of diagrams, how and why this arises.

(ii) Explain what the form factor represents.

(6)

QUESTION B2 [20 marks available, but 15 or more is 100 %]

Consider a one-dimensional chain of identical atoms of mass M coupled with nearest – neighbour interactions with a “spring constant” K as in the diagram below , where $u_n, u_{n\pm 1}, u_{n\pm 2}$ indicate displacements of the $n^{\text{th}}, n\pm 1, n\pm 2$ atoms from their equilibrium positions.



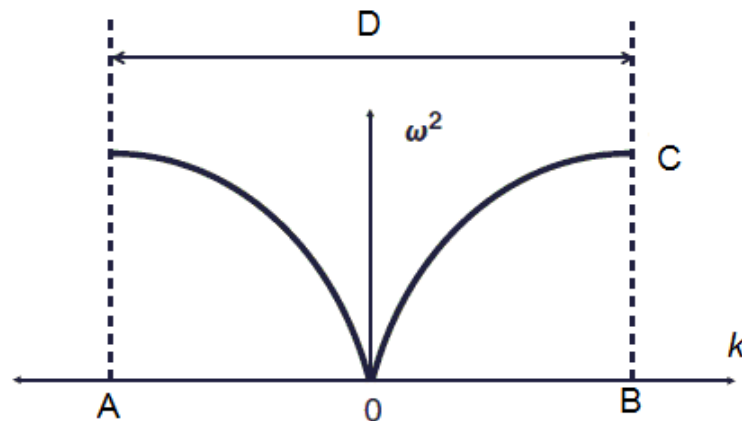
- (a) The following dispersion relation is obtained for this monoatomic chain:

$$\omega^2 = 4 \frac{K}{M} \sin^2 \left(\frac{1}{2} ka \right).$$

Describe how we arrive at this equation. There is no need to for a detailed derivation.

(5)

- (b) The plotted dispersion relation is as follows:



Question B2(b) continued

Answer the following questions on the dispersion curve:

- (i) What are the k values for A and B ? What is the term used for the region D extending from A to B ? (3)
- (ii) Where is the long wavelength limit in the plot ? What is the group velocity as a function of K and M of the density wave in this limit ? (4)
- (iii) What is the value of C ? What is the group velocity of the density wave at A or B ? (2)
- (iv) Explain why A or B correspond to the shortest wavelength that can be sustained in the medium. (2)
- (v) Show that the Bragg condition ($2d\sin\theta = n\lambda$) is satisfied at A or B by indicating the meaning of d , θ , n and λ in the present context, and explain how this relates to the second part of (iii) above. (4)

QUESTION B3 [18 marks available, but 15 or more is 100 %]

The single particle energies of a harmonic oscillator (phonon) mode of vibration is given by $\varepsilon_n = (n + \frac{1}{2})\hbar\omega$.

(a) Set up the partition function Z_1 and show that it can be written as

$$Z_1 = \frac{\exp(-x/2)}{1 - \exp(-x)} \quad \text{where} \quad x = \hbar\omega/k_B T. \quad (4)$$

(b) Using $\bar{\varepsilon} = -\frac{\partial \ln Z_1}{\partial \beta}$, show that

$$\bar{\varepsilon} = \frac{1}{2}\hbar\omega + \frac{\hbar\omega}{\exp(\hbar\omega/k_B T) - 1}.$$

What is this average energy of the oscillator in the high temperature limit ? (7)

(c) Denote $\theta = \frac{\hbar\omega}{k_B}$, then show that the heat capacity in the low temperature limit is

$$C_V = k_B \left(\frac{\theta}{T} \right)^2 \exp(-\theta/T). \quad (5)$$

(d) Briefly comment on why this is considered an Einstein model of lattice vibrations in a solid and how it differs from the Debye model. (2)

QUESTION B4 [16 marks available, but 15 or more is 100 %]

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 :

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

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) Use an appropriate travelling wave solution for the electron and 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.

(9)

- (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.

(5)

- (c) From what you have sketched in (a), an energy gap is opened up at $k = \pm\pi/a$. Briefly explain why this is the case for this periodic linear chain.

(2)

QUESTION B5 [18 marks available, but 15 or more is 100 %]

- (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.

(8)

- (ii) Doping as mentioned above has the effect of introducing hydrogenic type atoms into the host Si lattice. Explain what is meant by this and calculate the Bohr radius in this case using the information below. Also calculate typical ionization energies for donor impurities in Si. The dielectric constant of Si is $\epsilon_r = 12$ and the effective mass m_e is one-tenth of the bare electron mass m .

(8)

- (iii) Based on your calculations in (ii) comment on the effect of room temperature, 300 K, on the electrical properties of doped Si.

(2)

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

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

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

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