King's College London

UNIVERSITY OF LONDON

This paper is part of an examination of the College counting towards the award of a degree. Examinations are governed by the College Regulations under the authority of the Academic Board.

B.Sc. EXAMINATION

CP3212 Statistical Mechanics

Summer 2003

Time allowed: THREE Hours

Candidates must answer SIX parts of SECTION A, and TWO questions from SECTION B.

The approximate mark for each part of a question is indicated in square brackets.

You must not use your own calculator for this paper. Where necessary, a College calculator will have been supplied.

TURN OVER WHEN INSTRUCTED

Avogadro's number	N_A	$= 6.0221 \times 10^{23}\ \mathrm{mol}^{-1}$
Bohr magneton	μ_B	$= 9.2740 \times 10^{-24}\ \mathrm{J\,T}^{-1}$
Boltzmann's constant	k_B	$= 1.3807 \times 10^{-23}\ \mathrm{J\,K}^{-1}$
Planck constant	h	$= 6.626 \times 10^{-34}\ \mathrm{J\,s}$
Dirac constant	$\hbar$	$= 1.0546 \times 10^{-34}\ \mathrm{J\,s}$
Speed of light in free space	c	$= 2.998 \times 10^{8}\ \mathrm{m\,s}^{-1}$

SECTION A – Answer SIX parts of this section

1.1) Consider an ideal system of 5 non-interacting spin $\frac{1}{2}$ particles in the absence of an external magnetic field. What is the probability that n of the five spins have spin up for each of the cases $n = 0, 1, 2, 3, 4, 5$?

[7 marks]

1.2) Consider an ideal gas of N molecules which is in equilibrium within a container of volume V_0. Denote by n the number of molecules located within any subvolume V of this container. The probability p that a given molecule is located within the subvolume V is then given by $p = \frac{V}{V_0}$.

Find the standard deviation Δn in the number of molecules located within the subvolume.

[7 marks]

1.3) Consider a system of non-interacting particles of mass m confined within a box of edge lengths L_x, L_y, and L_z along the x, y, and z axes respectively. In a general quantum state σ specified by three integer quantum numbers n_x, n_y, and n_z the energy is given by

$$E = \frac{\pi^2\hbar^2}{2m}\left(\frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2} + \frac{n_z^2}{L_z^2}\right).$$

In state σ a particle exerts a force F_x in the x-direction on the wall on which $x = L_x$ and the wall exerts an equal and opposite force on the particle. Show that in a cubic box, at some non-zero temperature, the mean value of the force F_x denoted by $\langle F_x \rangle$ is given by

$$\langle F_x \rangle = \frac{2}{3}\frac{\langle E \rangle}{L_x}$$

where $\langle E \rangle$ is the mean value of E.

[Hint: $F_x = -\frac{\partial E}{\partial L_x}$.]

[7 marks]

1.4) Consider two identical boson particles which are to be placed in four single particle states.Two of these states have energy 0, one has energy ε, and the last has energy 2ε. Calculate the partition function when the system is at temperature T.

[7 marks]

1.5) The energy density emitted by a black body in the wavelength range λ to $\lambda + d\lambda$ is $u(\lambda)\, d\lambda$ where

$$u(\lambda) = \frac{8\pi hc}{\lambda^5 \left(e^{hc/\lambda k_B T} - 1\right)}.$$

Show that to a good approximation $u(\lambda)$ has a maximum at a wavelength λ which is inversely proportional to T.

[7 marks]

1.6) Consider an ideal Fermi gas whose atoms have a mass of $m = 5 \times 10^{-27} kg$, nuclear spin $\frac{1}{2}$, and nuclear magnetic moment $\mu_N = 10^{-26} J\,T^{-1}$. The gas is placed in a magnetic field B so that the spin energy levels are $\pm\mu_N B$. At zero temperature what is the largest density for which the gas can be completely polarised by a magnetic induction field of $10\,T$?

[7 marks]

[Hint: show that the condition for complete polarisation is $2\mu_N B > \frac{\hbar^2 k_{F\uparrow}^2}{2m}$ where $k_{F\uparrow}$ is the Fermi wave vector of the up-spin states.]

1.7) A ferro-electric crystal has a free energy of the form

$$F = \frac{1}{2}\alpha (T - T_c) P^2 + \frac{1}{4} b P^4 + \frac{1}{6} c P^6 + D x P^2 + \frac{1}{2} E x^2$$

where P is the electric polarization and x represents the strain applied to the crystal. Minimize the free energy with respect to x , determine the free energy at the minimum and hence deduce that for

$$b > \frac{2D^2}{E}$$

the system has a second order phase transition.

[7 marks]

1.8) The density of states for a highly relativistic particle in one dimension is constant. Use this to show that the partition function Z at temperature T is proportional to $k_B T$.

[7 marks]

[Hint: Ignore the mass of the particle when it is highly relativistic.]

SECTION B – Answer TWO questions

2) Let $\Omega(N, V, E)$ be the number of microscopic states with N particles in volume V and energy between E and $E + \delta E$. Why is δE usually taken to be non-zero and why are the thermodynamic consequences insensitive to the choice of δE?

[4 marks]

Show that the temperature T satisfies

$$\beta = \left(\frac{\partial \log \Omega}{\partial E}\right)_{N,V}$$

where $\beta = 1/k_B T$ by using the first law of thermodynamics.

[9 marks]

Consider two macroscopic systems A and A' with energies E and E' respectively. As above let $\Omega(N, V, E)$ be the number of states accessible to A and $\Omega'(N', V', E')$ the number accessible to A'. Denote by A^* the combined system of A and A'. A^* is assumed to be isolated and has fixed energy E_0.

What is the basic statistical assumption concerning the microstates accessible to A^*?

[3 marks]

Calculate the number $\Omega^*(E)$ of states of A^* which are compatible with the system A having an energy in the range E and $E + \delta E$.

[3 marks]

Hence calculate the probability $P(E)\, dE$ for A to have an energy in the range E and $E + dE$.

[3 marks]

Assume that $P(E)$ has the form

$$P(E) \propto \exp\left(-\left(E - \langle E\rangle\right)^2 / \left(2k_B T^2 C_V\right)\right)$$

where the symbols have their usual meanings.

Use this to estimate the probability for observing a spontaneous fluctuation in E of the size of $10^{-6}\langle E\rangle$ for 0.001 moles of a monatomic gas.

[8 marks]

3) At low temperature the atoms of a solid vibrate about their equilibrium positions. The phonon gas hamiltonian H can be expressed as

$$H = \sum_{\alpha=1}^{DN} H_\alpha$$

where H_α is the harmonic oscillator hamiltonian with a fundamental frequency ω_α, D is the dimensionality of the lattice and N is the number of particles. Explain why the canonical partition Q for the lattice can be written as

$$Q(\beta, N, V) = \sum_{n_1, n_2, \ldots = 0}^{\infty} \exp\left[-\beta \sum_\alpha \left(\frac{1}{2} + n_\alpha\right) \hbar\omega_\alpha\right]$$

with a suitable interpretation of the symbols.

[12 marks]

[Hint: Recall that the eigenenergy of a harmonic oscillator with frequency ω is $\left(\frac{1}{2} + n\right)\hbar\omega,\ n = 0, 1, 2, \ldots$.]

Show that

$$\log(Q) = -\sum_{\alpha=1}^{DN} \log\left[\exp\left(\frac{\beta\hbar\omega_\alpha}{2}\right) - \exp\left(\frac{-\beta\hbar\omega_\alpha}{2}\right)\right].$$

[6 marks]

The Helmholtz free energy F can be written as

$$\beta F = \int_0^\infty d\omega g(\omega) \log\left[\exp\left(\frac{\beta\hbar\omega}{2}\right) - \exp\left(-\frac{\beta\hbar\omega}{2}\right)\right]$$

where

$g(\omega)\,d\omega =$ the number of phonon states with frequency between ω and $\omega + d\omega$.

For a 3-dimensional solid (D=3) with

$$g(\omega) = \begin{cases} \left(\frac{9N}{\omega_0^3}\right)\omega^2, & \omega < \omega_0 \\ 0, & \omega > \omega_0 \end{cases}$$

show that for $\beta\hbar\omega \gg 1$

$$\beta F = \frac{9N\hbar\omega_0}{8}\beta.$$

[6 marks]

Hence show that the mean energy $\langle E\rangle$ in this limit is $\frac{9N\hbar\omega_0}{8}$.

[6 marks]

4) a) Define the grand canonical partition function Ξ for a system.

[3 marks]

The entropy S is given by

$$S = -k_B \left[-\log \Xi - \beta \langle E \rangle + \beta \mu N \right]$$

where the symbols have their standard meanings.

b) Deduce that

$$\beta p V = \log \Xi$$

where p is the thermodynamic pressure.

[3 marks]

c) For an ideal gas of fermions the grand canonical partition function has the form

$$\Xi = \sum_{n_1, n_2, \ldots, n_j, \ldots = 0}^{1} \exp \left[-\beta \sum_j n_j \left(\varepsilon_j - \mu \right) \right]$$

where n_j are occupation numbers of single particle states of energy ε_j.

Show that the average occupation number is given by

$$\langle n_j \rangle = \frac{1}{e^{\beta(\varepsilon_j - \mu)} + 1}.$$

[6 marks]

d) Structureless fermions of mass m have an energy $\varepsilon = \frac{\hbar^2 k^2}{2m}$. Use the results of b) and c) to prove that

$$\beta p = \frac{1}{\lambda^3} f(z)$$

where $z = \exp(\beta\mu)$, $\lambda = \left(\frac{2\pi\beta\hbar^2}{m} \right)^{\frac{1}{2}}$ and

$$f(z) = \frac{4}{\sqrt{\pi}} \int_0^\infty dx\, x^2 \log \left(1 + z e^{-x^2} \right).$$

[18 marks]

5) In the Ising model N spins s_i $(s_i = \pm 1)$ are arranged on a lattice. In the presence of a magnetic field H the energy of the system in a particular state ν is

$$E_\nu = -\sum_{i=1}^{N} H\mu s_i - \frac{J}{2}\sum_{\langle ij \rangle} s_i s_j$$

where J is a coupling constant, μ is the magnetic dipole moment and the second sum is over nearest neighbour pairs.

a) Describe the mean field approach to calculating the mean magnetization m per particle at temperature T and show that this leads to the formula

$$m = \tanh\left(\beta\mu H + \beta z J m\right)$$

where $\beta = \frac{1}{k_B T}$ and z is the number of nearest neighbours for a lattice site.

[15 marks]

b) Show that

$$\beta = \frac{1}{2Jzm}\log\left(\frac{1+m}{1-m}\right)$$

when $H = 0$.

[5 marks]

c) Use the Taylor expansion for temperatures near $\frac{zJ}{k_B}$ to show that

$$m \propto (T_c - T)^{1/2}$$

where T_c is the critical temperature.

[6 marks]

d) Prove that at zero temperature this theory gives $m = \pm 1$.

[4 marks]