SEMESTER 2 EXAMINATION 2013-2014

QUANTUM PHYSICS OF MATTER

Duration: 120 MINS (2 hours)

This paper contains 8 questions.

Answers to Section A and Section B must be in separate answer books

Answer **all** questions in **Section A** and **only two** questions in **Section B**.

Section A carries 1/3 of the total marks for the exam paper and you should aim to spend about 40 mins on it.

Section B carries 2/3 of the total marks for the exam paper and you should aim to spend about 80 mins on it.

An outline marking scheme is shown in brackets to the right of each question.

A Sheet of Physical Constants is provided with this examination paper.

Only university approved calculators may be used.

A foreign language translation dictionary (paper version) is permitted provided it contains no notes, additions or annotations.

Section A

A1. State which three variables are held fixed for i) the microcanonical ensemble; ii) the canonical ensemble; iii) the grand canonical ensemble. Define the chemical potential μ in terms of internal energy U from the fundamental relation of thermodynamics, and describe what happens when two systems (with the same type of particles) with different chemical potentials come into contact. [5]

A2. Explain the main assumption of the Debye model, and discuss the difference between the Debye frequency and the Einstein frequency. [5]

A3. Write down the Fermi-Dirac and the Bose-Einstein distribution functions for a discrete system, and state the possible values of the occupation numbers (n_k) for both of these distributions. [4]

A4. The statistical average $\langle F \rangle$ of some macroscopic observable $F(p,q)$ of a physical system which is described by Lagrangian variables is defined by

$$\langle F \rangle = \int_{\text{phase-space}} dp\, dq\, \rho(p,q) \cdot F(p,q)\,.$$

Explain what the statistical distribution $\rho(p,q)$ is, and write down its functional form for a microcanonical ensemble of total energy E_0. Explain why the definition of the microcanonical ensemble unambiguously leads to a specific function for $\rho(p,q)$.

[6]

Section B

B1. (a) Define the statistical entropy σ for a particular macrostate of a discrete system. By considering a system made up of two parts, with a number of particles N_A in part A and with a number of particles N_B in part B, show that statistical entropy σ is an extensive quantity. [5]

(b) State whether the number of accessible microstates in an isolated system increases, decreases, or stays the same for i) a reversible process, and for ii) an irreversible process. [2]

(c) Consider two systems A and B, initially isolated from each other and such that each is individually in thermal equilibrium. The two systems are then placed in contact, keeping the number of particles (N_A and N_B) and volumes (V_A and V_B) fixed, while allowing energy to be exchanged (i.e. thermal contact). The two energies E_A and E_B can vary but their sum $E = E_A + E_B$ is conserved since the combined system $A + B$ is isolated. Show that the condition for thermal equilibrium for the combined system $A + B$ is given by $\tau_A = \tau_B$, where τ is statistical temperature and is defined as:

$$\frac{1}{\tau} \equiv \left(\frac{\partial \sigma}{\partial E} \right)_{V,N} .$$

[7]

(d) Before the combined system $A + B$ reaches thermal equilibrium (i.e. the process of thermalisation), by considering its total entropy show that the energy flow is from the system (A or B) with higher statistical temperature to the system (A or B) with lower statistical temperature. [6]

B2. (a) Show that the partition function Z for a classical ideal gas of N constituents each of mass m in volume V at temperature T in a canonical ensemble assumes the following form:

$$Z(T, V, N) = \frac{V^N}{N! \lambda_{\text{th}}(T)^{3N}}, \qquad \lambda_{\text{th}}(T) = \frac{h}{\sqrt{2\pi m k_B T}}.$$ [6]

Hint: The partition function of a system of N constituents with a continuous energy spectrum (e.g. a classical ideal gas) is given by:

$$Z(T, V, N) = \frac{1}{h^{3N}} \frac{1}{N!} \int dq^{3N} \, dp^{3N} \exp\left(-E(p, q)/(k_B T)\right).$$

The energy of an ideal gas assumes the rather simple form:

$$E(p, q) = \sum_{i=1}^{N} \frac{\vec{p}_i^2}{2m}, \qquad \vec{p}_i^2 = (p_i^x)^2 + (p_i^y)^2 + (p_i^z)^2.$$

You might need the following integral:

$$\int_{-\infty}^{\infty} dx \exp\left(-ax^2\right) = \sqrt{\frac{\pi}{a}}, \qquad a > 0.$$

(b) From the results of (a) and making use of $\ln n! = n \ln n - n$ for $n \gg 1$ and

$$F = -k_B T \ln Z \quad \text{and} \quad S = -\left.\frac{\partial F}{\partial T}\right|_{V,N},$$

where F is the free energy and S is the entropy, derive the Sackur-Tetrode equation for an ideal gas:

$$S = k_B N \left[\ln\left(\frac{V}{N} \frac{1}{\lambda_{\text{th}}(T)^3}\right) + \frac{5}{2}\right].$$

The thermal wavelength $\lambda_{\text{th}}(T)$ has been defined above. [8]

(c) Now consider a canonical ensemble of a discrete system. By making use of the relation $F = U - \tau\sigma$ (where τ is statistical temperature and σ is

statistical entropy), derive the following formula for the Gibbs entropy:

$$\sigma = -\sum_i P_i \log P_i.$$

Here P_i is the probability to find the system in a microstate with energy E_i and is defined by:

$$P_i = \frac{e^{-\frac{E_i}{\tau}}}{Z},$$

where Z is the partition function for the discrete system. Then show that in the microcanonical ensemble the Gibbs entropy is equivalent to the Boltzmann definition of entropy.   [6]

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B3. Consider an ideal paramagnet with N magnetic dipole moments. Let $n_\uparrow$ and $n_\downarrow$ be the number of spins parallel and antiparallel to an external magnetic field B, with $N = n_\uparrow + n_\downarrow$. Since interactions are neglected the total energy,

$$E = -mB\Delta N \, , \quad \Delta N \equiv (n_\uparrow - n_\downarrow) \, ,$$

is simply the sum of the N individual energies, where m denotes the magnitude of the magnetic dipole moment.

(a) Define what a macrostate is for this system and derive the general expression for the statistical weight of a macrostate in terms of $N!$, $n_\downarrow!$ and $n_\uparrow!$. [5]

(b) For $N, n_\uparrow, n_\downarrow \gg 1$ show that the entropy S is given in terms of N and ΔN by

$$S(E(\Delta N), N) = \frac{1}{2} k_B \left[(N + \Delta N) \ln \left(\frac{2N}{N + \Delta N} \right) + (N - \Delta N) \ln \left(\frac{2N}{N - \Delta N} \right) \right] \, ,$$

by using Stirling's formula $\ln n! \simeq n(\ln(n) - 1)$ (for $n \gg 1$). [4]

(c) Use the microscopic definition of the temperature to obtain

$$\frac{1}{T} = \left(\frac{k_B}{2mB} \right) \ln \left(\frac{N + \Delta N}{N - \Delta N} \right).$$ [4]

Hint: You may find it useful to use the chain-rule: $\frac{\partial f(\Delta N(E))}{\partial E} = \frac{\partial f(\Delta N)}{\partial \Delta N} \frac{\partial \Delta N}{\partial E}$.

(d) Solve the equation given in part (c) for ΔN to obtain:

$$\frac{\Delta N}{N} = \frac{\exp \left(\frac{2mB}{k_B T} \right) - 1}{\exp \left(\frac{2mB}{k_B T} \right) + 1} \, .$$

[3]

(e) Investigate the entropy obtained in (b) for $\Delta N \to 0$ and deduce the statistical weight through the formula $S = k_B \ln W$. Why does this weight not agree with the one in (a) with $\Delta N = 0$ assumed? [4]

B4. (a) State the equipartition theorem and use it to write down the mean energy for a system of a single classical harmonic oscillator in one dimension with energy given by

$$E = \left(\frac{p^2}{2m} + \frac{kx^2}{2} \right) .$$

Then calculate the heat capacity at constant volume (c_V) for this oscillator.

[4]

(b) Now consider a single quantum harmonic oscillator whose energy levels are given by

$$\varepsilon_n = \hbar \omega \left(n + \frac{1}{2} \right) .$$

Write down the partition function (Z) for this quantum harmonic oscillator, and calculate the mean energy $\langle \varepsilon \rangle$ and the heat capacity c_V. You may use the following results, where τ is statistical temperature and $\beta = 1/\tau$: [8]

$$\sum_{n=0}^{\infty} r^n = \frac{1}{1-r} \quad (r < 1) \quad \text{and} \quad \langle \varepsilon \rangle = -\frac{\partial}{\partial \beta} \ln Z .$$

(c) Evaluate the values of $\langle \varepsilon \rangle$ and c_V for the quantum harmonic oscillator in the limit of very large τ. Compare with the corresponding values for the classical harmonic oscillator, and explain the physical reasons for any agreement or disagreement.

[5]

(d) The statistical entropy σ of the single quantum harmonic oscillator is given by:

$$\sigma = \frac{\beta \hbar \omega}{e^{\beta \hbar \omega} - 1} - \ln[1 - e^{-\beta \hbar \omega}] .$$

Evaluate the value of σ as $\tau \to 0$ and comment on whether or not this agrees with the third law of thermodynamics.

[3]

END OF PAPER