THE UNIVERSITY OF NEW SOUTH WALES

SCHOOL OF PHYSICS

FINAL EXAMINATION

JUNE 2015

PHYS3021 Statistical and Solid State Physics - PAPER 1

PHYS3020 Statistical Physics

Time Allowed – 2 hours

Total number of questions - 5

Answer ALL questions

All questions ARE of equal value

This exam is worth 35% of the final grade for PHYS3021 students

This exam is worth 70% of the final grade for PHYS3020 students

Candidates must supply their own university approved calculator.

Answers must be written in ink. Except where they are expressly required, pencils may only be used for drawing, sketching or graphical work.

This paper may be retained by the candidate

FORMULA SHEET

Boltzmann Entropy $S = k\ln W$

Statistics and Distributions

Boltzmann	$W_B = N!\prod_{j=1}^{n}\frac{g_j^{N_j}}{N_j!}$	$\frac{N_j}{g_j} = \frac{N}{Z}e^{-\varepsilon_j/kT}$	$Z = \sum_{j=1}^{n} g_j e^{-\varepsilon_j/kT}$
Maxwell-Boltzmann	$W_{MB} = \prod_{j=1}^{n}\frac{g_j^{N_j}}{N_j!}$	$\frac{N_j}{g_j} = \frac{N}{Z}e^{-\varepsilon_j/kT}$	$Z = \sum_{j=1}^{n} g_j e^{-\varepsilon_j/kT}$
Fermi-Dirac	$W_{FD} = \prod_{j=1}^{n}\frac{g_j!}{N_j!(g_j - N_j)!}$		$\frac{N_j}{g_j} = \frac{1}{e^{(\varepsilon_j-\mu)/kT}+1}$
Bose-Einstein	$W_{BE} = \prod_{j=1}^{n}\frac{(N_j + g_j - 1)!}{N_j!(g_j - 1)!}$		$\frac{N_j}{g_j} = \frac{1}{e^{(\varepsilon_j-\mu)/kT}-1}$

Microcanonical $$f_{mc}(q,p) = \frac{\delta(H(q,p) - E)}{\int dqdp\,\delta(H(q,p) - E)}$$

Canonical $$f_C(q,p) = \frac{\exp(-\beta H(q,p))}{Z(N,V,T)} \qquad Z(N,V,T) = \int dqdp \exp(-\beta H(q,p))$$

Grand-canonical $$f_G(q,p) = \frac{\exp(\beta(\mu N - H))}{\Xi(\mu,V,T)} \qquad \Xi(\mu,V,T) = \sum_{N=0}^{\infty} z^N Z(N,V,T)$$

Thermodynamic Potentials

Internal energy	U	$dU = TdS - PdV$
Enthalpy	$H = U + PV$	$dH = TdS + VdP$
Helmholtz function	$F = U - TS$	$dF = -SdT - PdV$
Gibbs function	$G = U - TS + PV$	$dG = -SdT + VdP$

Statistical Mechanics Canonical Ensemble

Internal energy $U = kT^2\left(\frac{\partial \ln Z}{\partial T}\right)_V$ Pressure $P = kT\left(\frac{\partial \ln Z}{\partial V}\right)_T$

Mathematical identities

$$\ln N! \approx N \ln N - N \qquad \int_0^\infty \frac{x^3 dx}{e^x - 1} = \frac{\pi^4}{15} \qquad \frac{x}{5} = 1 - e^{-x} \;\Rightarrow\; x = 4.96$$

$$1 + y + y^2 + \ldots = \frac{1}{1-y} \qquad \int_{-\infty}^{\infty} dx e^{-x^2/\alpha} = \sqrt{\pi\alpha} \qquad \int_0^\infty d\varepsilon \varepsilon^{1/2} e^{-\varepsilon/\alpha} = \frac{\alpha}{2}\sqrt{\pi\alpha}$$

$$\sinh(x) = \frac{e^x - e^{-x}}{2} \qquad \frac{d}{dx}\sinh(x) = \cosh(x) \qquad \operatorname{csch}(x) = \frac{1}{\sinh(x)}$$

$$\cosh(x) = \frac{e^x + e^{-x}}{2} \qquad \frac{d}{dx}\cosh(x) = \sinh(x) \qquad \operatorname{sech}(x) = \frac{1}{\cosh(x)}$$

$$\tanh(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}} \qquad \tanh(x) = \frac{\sinh(x)}{\cosh(x)} \qquad \frac{d}{dx}\tanh(x) = \operatorname{sech}^2(x)$$

$$\coth(x) = \frac{e^x + e^{-x}}{e^x - e^{-x}} \qquad \coth(x) = \frac{\cosh(x)}{\sinh(x)} \qquad \frac{d}{dx}\coth(x) = -\operatorname{csch}^2(x)$$

$$\int_{-\infty}^{\infty} \frac{e^y dy}{\left(e^y + 1\right)^2} = 1 \qquad \int_{-\infty}^{\infty} \frac{y^2 e^y dy}{\left(e^y + 1\right)^2} = \frac{\pi^2}{3}$$

QUESTION 1 (20 marks)

(a) A system of three distinguishable particles has allowed energy levels 0, ε, 2ε, 3ε, ..., and has total energy $U = 4\varepsilon$. Assume the degeneracy $g = 1$ for each level. Tabulate all the possible distributions of the particles among the allowed energy levels. Calculate the thermodynamic weight of each macrostate and the average occupation number of each of the energy levels 0, ε, 2ε, 3ε, ... (6 marks).

(b) Tabulate the possible distributions if the particles are indistinguishable bosons. Determine the average occupation number of each level (3 marks).

(c) Tabulate the possible distributions if the particles are indistinguishable fermions and the energy levels are nondegenerate. Determine the average occupation number of each level (3 marks).

(d) Consider the dilute gas limit ($N_j << g_j$) for both Bose-Einstein and Fermi-Dirac statistics. Derive the Maxwell-Boltzmann thermodynamic probability (4 marks):

$$W_{MB} = \prod_j \frac{g_j^{N_j}}{N_j!}$$

How does this differ from the Boltzmann distribution? (2 marks)

(e) If $x = (\varepsilon_j - \mu)/(k_B T)$, sketch N_j/g_j versus x for Bose-Einstein, Fermi-Dirac and Maxwell-Boltzmann statistics (2 marks).

QUESTION 2 (20 marks)

In the Einstein model, all the vibrational modes of a solid are assumed to have the same frequency ω_E.

(a) What is the name given to these vibrational modes? (1 mark)

(b) If the solid is composed of N atoms, what is the total number of vibrational modes N_{tot}? (1 mark)

Each vibrational mode can be modelled as a simple harmonic oscillator with allowed energies $\varepsilon_n = (n + 1/2)\,\hbar\omega_E$, where n is an integer. All modes are identical.

(c) What is the partition function Z_1 for a single mode? (3 marks)

(d) What is the partition function Z for all vibrational modes? (2 marks)

(e) Calculate the internal energy U of the system (3 marks). What value does U tend to as the temperature becomes very large? Why? (3 marks)

(f) Calculate the heat capacity C_V (3 marks). What values does it tend to at high temperatures? (2 marks) How about at low temperatures? (2 marks)

QUESTION 3 (20 marks)

Consider an ion with a spin-1/2 ground state and zero orbital angular momentum. Then the total angular momentum $J = 1/2$ and the Lande g-factor $g = 2$. This ion is placed in an external magnetic field $\boldsymbol{B} \mathbin{//} z$.

(a) The z-component of the magnetic moment, μ_z, has two possible values, $\mu_z = g\,\mu_B\,m$, where m is an integer. What are the two possible values of m? (2 marks)

(b) What are the two possible energies of this ion in the magnetic field? (2 marks)

(c) Determine the partition function Z of the ion and express your answer in terms of the quantity

$$\eta = \frac{2\mu_B B}{k_B T}$$

(4 marks)

(d) Determine the magnetic energy U (4 marks). What happens to U at high temperatures? Why? (2 marks) How about at low temperatures? Why? (2 marks).

(e) Determine the general form of the heat capacity at constant B, C_B, of the ion (4 marks).

QUESTION 4 (20 marks)

For bosons of spin zero the density of states is given by

$$g(\varepsilon)d\varepsilon = \frac{4\pi\sqrt{2}}{h^3} V m^{3/2} \varepsilon^{1/2} d\varepsilon$$

(a) We can assume the ground state energy of the boson system to be zero. What do we expect the bosons to do as the temperature is lowered towards absolute zero? (2 marks)

(b) Is the ground state included in the above expression for $g(\varepsilon)$? (1 mark)

(c) We can write the total number of bosons as the sum of two contributions $N = N_0 + N_{ex}$, where N_0 represents the occupation of the ground state, and N_{ex} the number of bosons in excited states. Write down an expression for N_{ex}. (2 marks)

(d) As the temperature tends towards absolute zero, what values do N_0, ε, and the chemical potential μ tend to? (3 marks) Approximating ε and μ in this way, evaluate N_{ex} explicitly, noting that

$$\int_0^\infty \frac{x^{1/2}dx}{e^x - 1} = \frac{2.612\pi^{1/2}}{2}$$

(6 marks)

(e) Above a certain temperature T_B, all bosons are in excited states. Use your result for N_{ex} to determine T_B. (3 marks)

(f) Determine an expression for the dependence of the fraction of bosons in the ground state, N_0/N, on temperature. (3 marks)

QUESTION 5 (20 marks)

(a) According to the equipartition theorem, if the energy of a system is quadratic in one variable, and if the system exchanges energy with a heat bath, what is the mean thermal energy of the system at temperature T? (2 marks)

(b) Consider a diatomic molecule. What is the contribution to the mean thermal energy due to translational motion? (2 marks)

(c) What is the contribution to the mean thermal energy due to rotational motion? (2 marks) Sketch the molecule and indicate the possible axes of rotation. (2 marks)

(d) What is the contribution to the mean thermal energy due to vibrational motion? (2 marks) Sketch the molecule and indicate the contributions due to vibrational motion. (2 marks)

(e) Let us consider the vibrational degrees of freedom in more detail. These can be modelled as a quantum mechanical rotor with moment of inertia I and energies $\varepsilon_l = l(l+1)\,\hbar^2/(2I)$, each with degeneracy $g_l = 2l+1$. Write down the partition function for the rotor. (2 marks)

(f) For many gases, at ordinary temperatures $T >> \hbar^2/(2Ik_B)$, and we can approximate $x = l(l+1)$ as a continuous variable. By doing this evaluate the partition function explicitly. (4 marks)

(g) What is the mean thermal energy? Does your result agree with the one you found in part (d)? (2 marks)