THE UNIVERSITY OF NEW SOUTH WALES

SCHOOL OF PHYSICS FINAL EXAMINATION JUNE 2012

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
$$W_B = N! \prod_{i=1}^n \frac{g_j^{N_j}}{N_j!} \qquad \frac{N_j}{g_j} = \frac{N}{Z} e^{-\varepsilon_j/kT} \qquad Z = \sum_{i=1}^n g_j e^{-\varepsilon_j/kT}$$

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
$$W_{FD} = \prod_{j=1}^{n} \frac{g_{j}!}{N_{j}!(g_{j} - N_{j})!} \qquad \frac{N_{j}}{g_{j}} = \frac{1}{e^{(\epsilon_{j} - \mu)/kT} + 1}$$

Bose-Einstein
$$W_{BE} = \prod_{j=1}^{n} \frac{(N_j + g_j - 1)!}{N_j! (g_j - 1)!} \qquad \frac{N_j}{g_j} = \frac{1}{e^{(\varepsilon_j - \mu)/kT} - 1}$$

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

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

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

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

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

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

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

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

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

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

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

QUESTION 1 (20 marks)

- (a) Consider a system in which the allowed energy levels $0, \varepsilon, 2\varepsilon, 3\varepsilon, 4\varepsilon, \ldots$ are nondegenerate $(g_j = 1)$. If the system has 3 distinguishable particles and a total energy of $U = 5\varepsilon$, tabulate the possible distributions of the particles among the energy levels and calculate the thermodynamic weight of each macrostate.
- (b) Explain how this tabulation changes if the particles are indistinguishable bosons.
- (c) Construct the same table of macrostates and thermodynamic weights for indistinguishable fermions.
- (d) Calculate the average occupancy of each energy level for the fermion system.
- (e) How many ways can the energy of the fermion system be decreased to a total energy of 4ε by changing the energy level of one fermion? Justify your answer.
- (f) Construct the table of macrostates for 3 fermions with energy $U = 4\varepsilon$.
- (g) How many macrostates are possible for 3 fermions with energy 3ε ? Calculate the average occupancy of each energy level in the system with energy 3ε .
- (h) Comment on the temperature and chemical potential μ of the system of 3 fermions with energy 3ε .

QUESTION 2 (20 marks)

(a) For a system with discrete energy levels in contact with a heat reservoir derive the canonical probability distribution

$$p_j = \frac{g_j e^{-E_j/kT}}{Z}$$

and obtain an expression for the canonical partition function Z.

(b) For a classical system of N particles in three dimensions with a continuum of energy levels show that the kinetic contribution to the canonical partition function is given by

$$Z_K = \int d\mathbf{p}_1 ... \int d\mathbf{p}_N \exp(-\beta H) = (2\pi mkT)^{3N/2},$$

where
$$H = \sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{2m}$$
.

(c) Calculate the average internal energy from the derivative of the partition function

$$\langle U \rangle = -\left(\frac{\partial \ln Z(N, V, T)}{\partial \beta}\right)_V$$

(d) If the average square of the energy is given by

$$\langle U^2 \rangle = \int d\mathbf{p}_1 ... \int d\mathbf{p}_N H^2 \exp(-\beta H)$$

show formally that

$$\frac{\partial^2}{\partial \beta^2} \ln(Z) = \langle U^2 \rangle - \langle U \rangle^2$$

(e) Using the partition function from part (b) calculate the mean square fluctuation $\langle \Delta U^2 \rangle = \langle U^2 \rangle - \langle U \rangle^2$.

QUESTION 3 (20 marks)

(a) Use Boltzmann statistics to calculate the partition function of the quantum harmonic oscillator with energy levels $\varepsilon_j = (j + \frac{1}{2})hv$, j = 0,1,2,...

$$Z = \left(\frac{e^{-\theta/2T}}{1 - e^{-\theta/T}}\right),\,$$

where $\theta = hv/k$ is the characteristic temperature.

(b) Why can Boltzmann statistics be used for indistinguishable oscillators?

(c) Show that the Boltzmann entropy for a system of N oscillators is $S = -k \sum_{j} N_{j} \ln \left(\frac{N_{j}}{N} \right)$.

(d) Using the Boltzmann distribution show that the Boltzmann entropy becomes

$$S = \frac{U}{T} + kN \ln Z.$$

(e) Using $U = NkT^2 \left(\frac{\partial}{\partial T} \ln Z\right)_V$ calculate the internal energy. Find the limiting behaviour of $U/Nk\theta$ as $T \to 0$ and $T \to \infty$. Graph the energy $U/Nk\theta$ as a function of T.

(f) Find the entropy and determine the limiting behavior as $T \rightarrow 0$.

QUESTION 4 (20 marks)

PART A.

(a) A dipole with magnetic moment μ in an external magnetic field **B** will experience a torque **N** given by

$$\mathbf{N} = \mu \times \mathbf{B}$$
.

The magnetic potential energy ε is the work done to rotate the dipole from its zero energy position $\theta = \frac{\pi}{2}$

$$\varepsilon = \int_{\pi/2}^{\theta} Nd\theta'$$

Show that $\varepsilon = -\mu \cdot \mathbf{B} = -\mu_z B$.

(b) The magnetic energy of an atom in quantum state m is $\varepsilon_m = -g\mu_B Bm$ where quantum number m is within the range $-J \le m \le J$. Here g is the Landé g-factor and $\mu_B = e\hbar/2m_e$ is the Bohr magneton. Each atom is in a localized position within a crystal and thus the atoms are distinguishable. Using Boltzmann statistics the probability of state m is

$$P_m = \frac{N_m}{N} = \frac{\exp(-\varepsilon_m/kT)}{Z}.$$

Write down the partition function for this system and show that the mean z-component of the magnetic moment is

$$\overline{\mu}_z = \sum_{m=-1}^{J} \mu_z P_m = \frac{1}{Z} \sum_{m=-1}^{J} g \mu_B m \exp(g \mu_B B m / kT)$$

(c) Show that $\overline{\mu}_z$ can be written as the derivative of the logarithm of the partition function.

PART B.

(a) A Bose gas at low temperature ($T < T_B$, where T_B is the Bose temperature) has an internal energy of

$$U = 0.77NkT \left(\frac{T}{T_B}\right)^{3/2}$$

where $T_B = \frac{h^2}{2\pi mk} \left(\frac{N}{2.612V}\right)^{2/3}$ determine the heat capacity at constant volume.

(b) As the result for the heat capacity is correct at zero temperature, calculate the entropy using

$$S = \int_{0}^{T} \frac{C_{V}}{T'} dT'.$$

(c) Thus show that the Helmholtz function is given by

$$F = -0.51NkT \left(\frac{T}{T_B}\right)^{3/2}.$$

(d) Hence show that $P = \frac{2U}{3V}$.

QUESTION 5 (20 marks)

(a) For a system of fermions where the density of states is given by

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

Show that the Fermi energy at T = 0 is given by

$$\varepsilon_F = \mu(0) = \frac{h^2}{2m} \left(\frac{3N}{8\pi V}\right)^{2/3}$$

(b) The internal energy of a fermion gas is

$$U = 4\pi V \left(\frac{2m}{h^2}\right)^{3/2} \int_0^\infty \frac{\varepsilon^{3/2} d\varepsilon}{e^{(\varepsilon - \mu)/kT} + 1}$$

Explain the interplay between the numerator and denominator of the integrand in determining the value of the internal energy.

(c) The fermionic contribution to the internal energy is

$$U \approx \frac{3}{5} N \varepsilon_F \left(1 + \frac{5\pi^2}{12} \left(\frac{T}{T_F} \right)^2 - \dots \right)$$

Find an expression for the heat capacity.

(d) Integrate the entropy from $TdS = C_V dT$ to obtain the entropy, and hence, the Helmholtz function.

$$F = NkT_F \left[\frac{3}{5} - \frac{\pi^2}{4} \left(\frac{T}{T_F} \right)^2 + \dots \right],$$

where the Fermi temperature is $T_F = \frac{h^2}{2mk} \left(\frac{3N}{8\pi V}\right)^{2/3}$.

(e) Calculate the fermionic contribution to the pressure for a gas of electrons.

(f) If a white dwarf star consists of alpha particles and a degenerate electron gas find the electronic contribution to the internal energy. If the gravitational potential energy $U_{grav} = -b/R$ where R is the radius of the star, explain how a minimum energy results in a stable radius for the star.