THE UNIVERSITY OF NEW SOUTH WALES

SCHOOL OF PHYSICS

FINAL EXAMINATION

JUNE 2010

PHYS3020

Statistical Physics

Time Allowed – 2 hours

Total number of questions - 5

Answer ALL questions

All questions ARE of equal value

Students are required to 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

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 $W_{FD} = \prod_{j=1}^{n}\frac{g_j!}{N_j!\left(g_j - N_j\right)!}$ $\frac{N_j}{g_j} = \frac{1}{e^{(\varepsilon_j-\mu)/kT}+1}$

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

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

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

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

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) Show that the thermodynamic weight for Maxwell-Boltzmann statistics is bounded above by Bose-Einstein statistics and below by Fermi-Dirac statistics. Thus show that

$$W_{BE} > W_{MB} > W_{FD}.$$

(b) In the dilute gas limit $g_j >> N_j$ the thermodynamic weight is given by Maxwell-Boltzmann statistics W_{MB} and the distribution is the same as the Boltzmann distribution . Calculate the entropy and the Helmholtz function.

(c) Consider a system in which the allowed (nondegenerate $g_j = 1$) energy levels are $0, \varepsilon, 2\varepsilon, 3\varepsilon, ...$ The system has 4 distinguishable (localized) particles and total energy $U = 6\varepsilon$. Tabulate the nine possible distributions of the four particles among the energy levels.

(d) Evaluate w_k for each of the macrostates, calculate $W = \sum_k w_k$ and the probability of each macrostate p_k

(e) Calculate the average occupancy $\overline{N}_j = \sum_k p_k N_{jk}$ for energy levels 3ε and 4ε.

(f) If energy level 3ε is removed, find the occupancy of energy level 4ε.

(g) Determine the macrostates and their thermodynamic weights for a system of four bosons with total energy $U = 6\varepsilon$ with energy levels $0, \varepsilon, 2\varepsilon, 3\varepsilon, ...$

(h) Determine the macrostates and their thermodynamic weights for a system of four fermions with total energy $U = 6\varepsilon$ with energy levels $0, \varepsilon, 2\varepsilon, 3\varepsilon, ...$

QUESTION 2 (20 marks)

The partition function for a single particle in a system with energy levels ε_j, with degeneracies g_j, is given by

$$Z = \sum_{j=1}^{n} g_j e^{-\varepsilon_j/kT}$$

(a) If the density of states function is given by $g(\varepsilon)d\varepsilon = \left(4\sqrt{2}\pi V/h^3\right)m^{3/2}\varepsilon^{1/2}d\varepsilon$, approximate the sum in the partition function by an integral and derive the result

$$Z = \left(\frac{2\pi mkT}{h^2}\right)^{3/2} V$$

(b) Calculate the internal energy and pressure for this system.

(c) For an N particle monatomic ideal gas system which satisfies the Maxwell-Boltzmann distribution use the thermodynamic weight to show that the entropy is given by

$$S = \frac{U}{T} + Nk\left\{1 - \ln\left(\frac{N}{Z}\right)\right\}.$$

(d) If the ideal gas partition function is

$$Z_{gas} = \left(\frac{2\pi mkT}{h^2}\right)^{3/2} V$$

determine the entropy as function of temperature and volume. Thus determine the additive constant in the entropy S_0.

(e) Derive the heat capacity of the ideal gas.

(f) In what way does the heat capacity of the ideal gas differ from the experimental results.

QUESTION 3 (20 marks)

(a) For a classical system of N particles with Hamiltonian

$$H = \sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{2m} + \Phi(\mathbf{q}_1, \ldots, \mathbf{q}_N)$$

show that the canonical partition function is given by

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

(b) For an ideal gas the potential is equal to zero everywhere (except at collisions). Ignoring collisions, find the classical canonical partition function for the ideal gas.

(c) Show that the average internal energy is obtained from the following derivative of the partition function

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

(d) Show that a measure of the average fluctuation in the internal energy $\Delta U = U - \langle U \rangle$ can be estimated by calculating the mean square fluctuation $\langle \Delta U^2 \rangle = \langle U^2 \rangle - \langle U \rangle^2$. Why not average $U - \langle U \rangle$?

(e) Show that the heat capacity at constant volume is related to a second derivative of the partition function by

$$C_V = \frac{1}{kT^2} \left(\frac{\partial^2 \ln Z}{\partial \beta^2} \right)_V.$$

QUESTION 4 (20 marks)

(a) For photons there is no restriction on the total number of particles so the partition function is independent of N. For an oscillator with non-degenerate energy levels $\varepsilon_j = jh\nu$, show that the partition function z is given by

$$z = \frac{1}{\left(1 - e^{-h\nu/kT}\right)},$$

so that $\ln z = -\ln\left(1 - e^{-h\nu/kT}\right)$.

(b) The number of single particle (photon) states in a volume V in the frequency range ν to $\nu + d\nu$ is

$$g(\nu)d\nu = \frac{8\pi V}{c^3}\nu^2 d\nu$$

Therefore, the partition function Z of the photon gas is the sum over states given by

$$\ln Z = \int_0^\infty d\nu g(\nu)\ln z$$

Changing to dimensionless variable $x \equiv h\nu/kT$ show that integration by parts leads to

$$\ln Z = \frac{8\pi V}{3}\left(\frac{kT}{hc}\right)^3 \int_0^\infty \frac{x^3 dx}{e^x - 1}$$

(c) Evaluate the standard integral to obtain a final expression for $\ln Z$.

(d) Use the result of part (c) to find the total energy density (energy per unit volume) of the photon gas. Expression the result in the form

$$\frac{U}{V} = aT^4$$

find an explicit expression for the constant a.

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) Show that

$$\tfrac{2}{3}\mu(0)^{3/2} = \int_0^\infty \frac{\varepsilon^{1/2}d\varepsilon}{e^{(\varepsilon-\mu)/kT}+1}$$

(d) Integrating by parts gives

$$\int_0^\infty \frac{\varepsilon^{1/2}d\varepsilon}{e^{(\varepsilon-\mu)/kT}+1} = \int_0^\infty \varepsilon^{1/2}f(\varepsilon)d\varepsilon = -\int_0^\infty \tfrac{2}{3}\varepsilon^{3/2}\frac{df(\varepsilon)}{d\varepsilon}d\varepsilon.$$

Expanding $\frac{2}{3}\varepsilon^{3/2}$ in a Taylor series about $\varepsilon=\mu$ to obtain

$$\tfrac{2}{3}\varepsilon^{3/2} \approx \tfrac{2}{3}\mu^{3/2} + \mu^{1/2}(\varepsilon-\mu) + \tfrac{1}{4}\mu^{-1/2}(\varepsilon-\mu)^2 + \ldots,$$

show that $$\mu = \mu(0)\left(1+\frac{\pi^2}{8}\left(\frac{kT}{\mu}\right)^2 + ..\right)^{-2/3}.$$

(e) Hence show that $\mu \approx \mu(0)\left(1-\frac{\pi^2}{12}\left(\frac{kT}{\mu(0)}\right)^2 + ..\right).$