THE UNIVERSITY OF QUEENSLAND
DEPARTMENT OF PHYSICS

Final Examination, June 2002

PHYS 3020: Statistical Mechanics

(SCIENCE)

TIME: TWO AND HALF hours for working.
Ten minutes for perusal before examination begins.

There are SIX (6) questions
Answer TWO (2) questions from Part A and TWO (2) questions from Part B.
Each question and each part of each question is worth equal marks.

Some useful formulae are supplied.

Approved calculators allowed.
PART A

1. (a) In no more than two sentences explain the basic goal of statistical mechanics. (b) Give a precise statement of the fundamental assumption of statistical mechanics. Make sure all the terminology you use is explained. (c) Clearly define the different systems that are respectively described by the microcanonical, canonical, and grand canonical ensembles. (d) For a general ensemble Gibbs introduced the entropy \( S_g \), defined as

\[
S_g = -k_B \sum_s P(s) \ln P(s)
\]

where the sum is over all microstates accessible to the system and \( P(s) \) is the probability of the system being in microstate \( s \). Show that for the microcanonical ensemble the fundamental assumption of statistical mechanics implies that the above expression reduces to Boltzmann’s expression for the entropy. (e) Show that for the canonical ensemble Gibb’s expression for the entropy is consistent with the thermodynamic identity, \( F = U - TS \).

2. A zipper has \( N \) links; each link has a state in which it is closed with energy 0 and a state in which it is open with energy \( E \). We require, however, that the zipper can only unzip from the left end, and that the link number \( s \) can only open if all links to the left (1, 2, 3, ..., \( s - 1 \)) are already open. The last link cannot open. Suppose that there are \( G \) possible orientations for each open link. This means that the state with \( s \) open links is \( G^s \)-fold degenerate. (a) Show that the partition function can be summed in the form

\[
Z = \frac{1 - G^N \exp(-NE/k_BT)}{1 - G \exp(-E/k_BT)}.
\]

(b) Find the probability that \( s \) links are open at a temperature \( T \) and give a general expression for the average number of open links, \( < s > \). (c) In the low and high temperature limits, find the average number of open links, \( < s > \). (d) Sketch \( < s > \) as a function of temperature. (e) What phenomena in physical biochemistry can this model describe?

3. Write as much as possible about how statistical mechanics provides an understanding of any TWO of the following physical phenomena. Be as specific and as quantitative as possible.
The Ising model on the square lattice in a magnetic field $B$ is defined by the Hamiltonian

$$H = -J \sum_{<ij>} S_i S_j + \gamma B \sum_i S_i$$

where $S_i = \pm 1$ is the spin on site $i$ and each spin has a magnetic moment of magnitude $\gamma$.

(a) Use mean-field theory to show that at temperature $T$ and zero magnetic field ($B = 0$) the magnetisation $M(T)$ per site must satisfy

$$M(T) = \gamma \tanh \left( \frac{4JM(T)}{\gamma k_B T} \right)$$

(b) Sketch the temperature dependence of the magnetisation.

(c) Show that the Curie temperature $T_c$ is given by

$$k_B T_c = 4J.$$

(d) Show that at temperatures just below $T_c$ mean-field theory predicts

$$M(T) \sim (T_c - T)^{1/2}$$

leading to a critical exponent $\beta = 1/2$.

(e) The exact solution of the model gives $T_c = 2.27 J/k_B$ and $\beta = 1/8$. Explain the physical origin of the failure of mean-field theory.
5. Consider \( N \) non-interacting non-relativistic identical bosons of mass \( m \) inside a cube of volume \( V \).

(a) Show that the density of states \( g(\epsilon) \) is given by

\[
g(\epsilon) = V \frac{2}{\sqrt{\pi}} \left( \frac{2\pi m}{\hbar^2} \right)^{3/2} \epsilon^{3/2}
\]

(b) Suppose the temperature \( T \) is sufficiently low that a macroscopic number of bosons, \( N_0(T) \), are in the ground state. Argue that the number of bosons in excited states is

\[
N_{ex}(T) = \int_{0}^{\infty} d\epsilon \frac{g(\epsilon)}{\exp(\epsilon/k_B T) - 1}
\]

(c) Evaluate this integral to give a simpler expression for \( N_{ex}(T) \). Sketch \( N_0(T) \) and \( N_{ex}(T) \) as a function of temperature.

(d) Use your results from (c) to show that the transition temperature \( T_c \) for Bose-Einstein condensation is related to the number density by

\[
k_B T_c = 0.527 \left( \frac{\hbar^2}{2\pi m} \right)^{2/3} \left( \frac{N}{V} \right)^{2/3}
\]

(e) Evaluate \( T_c \) for liquid \(^4\)He which has a mass density of 0.145 g/cm\(^3\). Why do you think this value disagrees with the observed superfluid transition temperature, \( T_\lambda = 2.17 \) K?

6. Consider a large spherical particle of mass \( M \) and radius \( a \), such as a pollen particle or a globular protein, immersed in a gas or liquid of viscosity \( \eta \) at temperature \( T \).

Suppose that at time \( t \) the particle is at \( \vec{r}(t) \) and \( \vec{r}(t = 0) = 0 \). The dynamics of the particle are described by the stochastic differential equation, originally proposed by Langevin,

\[
M \frac{d^2 \vec{r}}{dt^2} = -\mu \frac{d\vec{r}}{dt} + \vec{F}(t)
\]

where \( \vec{F}(t) \) is a random force and \( \mu = 6\pi a \eta \) is the coefficient of friction.

(a) Derive a differential equation for \( r^2 \equiv \vec{r} \cdot \vec{r} \) and then average it over all possible configurations of the random force.

(b) Give a clear and precise statement of the equipartition theorem of classical statistical mechanics.

(c) Applying the equipartition theorem to the kinetic energy of the large particle show that \( u(t) \equiv <r^2(t)> \) (where \( <..> \) denotes an average over all possible configurations of the
random force) satisfies the differential equation

\[ M \frac{d^2u}{dt^2} = -\mu \frac{du}{dt} + 6k_B T \]

(d) Solve the above equation for large times \((t \gg \mu/M)\) to show that

\[ \langle r^2(t) \rangle = \frac{6k_B T}{\mu} t \]

(e) Explain how the result from (d) can be the basis of an experimental determination of Avogadro’s number.
Useful formulae

$$\sinh x \equiv \frac{1}{2}(e^x - e^{-x})$$

$$\tanh x = x - \frac{x^3}{3} + \cdots \quad \coth x = \frac{1}{x} + \frac{x}{3} + \cdots$$

$$\sum_{n=0}^{M} x^n = \frac{1 - x^{M+1}}{1 - x}$$

$$\ln N! \approx N \ln N - N \quad N \gg 1$$

$$\int_{-\infty}^{\infty} dx \exp(-ax^2) = \sqrt{\frac{\pi}{a}}$$

$$\int_{0}^{\infty} \frac{x^3}{\exp(x)-1} = \frac{\pi^4}{15}$$

$$\int_{0}^{\infty} dx \frac{\sqrt{x}}{\exp(x)-1} = 2.315$$

$$dxdydz = r^2 \sin \theta dr d\theta d\phi$$

$$TdS = dU + PdV$$

$$F = U - TS$$

$$PV = nRT = Nk_B T \quad C_V(T) = \frac{3}{2} Nk_B$$

$$U = -\vec{M} \cdot \vec{B}$$

$$S(U, V) = k_B \ln g(U, V)$$

$$\mu = -k_B T \ln \left( \frac{V}{Nv_Q} \right) \quad v_Q = \left( \frac{h}{\sqrt{2\pi mk_BT}} \right)^3$$

$$Z = \exp(-\beta F) = \sum_s \exp(-\beta \epsilon_s) \quad \beta \equiv \frac{1}{k_B T}$$

$$P(s) = \frac{1}{Z} \exp(-\beta \epsilon_s)$$

$$U = -\frac{\partial \ln Z}{\partial \beta}$$

$$n_{FD}(\epsilon) = \frac{1}{\exp(\beta(\epsilon - \mu)) + 1}$$
\[ n_{BE}(\epsilon) = \frac{1}{\exp(\beta(\epsilon - \mu)) - 1} \]

\[\epsilon(n_x, n_y, n_z) = \frac{\hbar^2}{8mL^2} (n_x^2 + n_y^2 + n_z^2) \quad n_x = 1, 2, \cdots \]

\[\epsilon(n_x, n_y, n_z) = \frac{\hbar c}{2L} (n_x^2 + n_y^2 + n_z^2)^{1/2} \quad n_x = 1, 2, \cdots \]

\[\sum_{\mathbf{k}} \to \left( \frac{L}{2\pi} \right)^3 \int d^3k \]

\[\rho(E) = \sum_{\alpha} \delta(E - E_{\alpha}) \]

\[E_F = \frac{\hbar^2}{8m} \left( \frac{3N}{\pi V} \right)^{2/3} \quad d = 3 \]

\[U(T = 0) = \frac{3}{5} NE_F \quad PV = \frac{2}{3} U \]