THE UNIVERSITY OF QUEENSLAND
DEPARTMENT OF PHYSICS

Second Semester Examination, November 2001

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 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) In Shannon’s theory of information the entropy, $S_i$, is defined as

$$S_i = -\sum_s P(s) \ln P(s)$$

where the sum is over all microstates accessible to the system and $P(s)$ is the probability of the system being in microstate $s$.
(i) Show that for an isolated system the fundamental assumption of statistical mechanics implies that the above expression reduces to Boltzmann’s expression for the entropy if we multiply Shannon’s expression by Boltzmann’s constant $k_B$.
(ii) For a system in thermal equilibrium with a reservoir at temperature $T$,

$$P(s) = \frac{1}{Z} \exp\left(-\frac{E(s)}{k_BT}\right)$$

where $Z$ is the partition function. Show that in this case Shannon’s expression is consistent with the thermodynamic identity, $F = U - TS$.

2. The rotational kinetic energy of diatomic molecules can be written

$$KE = \frac{\tilde{L}^2}{2I}$$

where $\tilde{L}$ is the orbital angular momenta and $I$ is the moment of inertia about the axis of rotation. The rotational motion is then quantized; and the energy levels of an heteronuclear diatomic molecule such as carbon monoxide are of the form

$$E_l = l(l+1)E_0,$$

where $l$ is any positive integer or zero: $l = 0, 1, 2, \ldots$ and $E_0 = \hbar^2/2I$. The degeneracy of each rotational level is $g(l) = 2l + 1$.
(a) Write down the partition function $Z_R(T)$ for the rotational states of one molecule in thermal equilibrium at a temperature $T$.
(b) Evaluate $Z_R(T)$ approximately for $k_BT \gg E_0$, by converting the sum over $l$’s into an integral.
(c) Evaluate $Z_R(T)$ approximately for $k_B T \ll E_0$, by truncating the sum after the second term.
(d) Give expressions for the internal energy $U$ and the heat capacity $C_V$, as functions of $T$, in both the high and low temperature limits. Relate your results to the equipartition theorem.
(e) Sketch the temperature dependence of $C_V(T)$.

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.
- superfluidity and Bose-Einstein condensation
- protein denaturation or unzipping DNA
- neutron stars
- cooling by adiabatic demagnetisation
- entropic elasticity
- the cosmic microwave background
- black hole thermodynamics
- fermion-boson transmutation in one dimension
- the ultracentrifuge
- phonons and the heat capacity of crystals

PART B

4.
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 a system of non-interacting fermions of spin-1/2 with magnetic moment $\mu$ and at a temperature $T$ much less than the Fermi temperature $T_F$.

(a) Derive an expression for the magnetic susceptibility in terms of the density of states at the Fermi energy.

(b) Contrast the temperature dependence of your result to that of the Curie-Weiss law for localised magnetic moments. Give a simple physical explanation for the difference.

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) 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

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

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

$$<r^2(t)> = \frac{6k_B T t}{\mu}$$

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

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

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

\[ \ln N! \simeq N \ln N - N \quad N \gg 1 \]

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

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

\[ TdS = dU + PdV \]

\[ F = U - TS \]

\[ PV = nRT = N k_B T \quad C_V(T) = \frac{3}{2} N k_B \]

\[ \mu = -k_B T \ln \left( \frac{V}{N v_Q} \right) \quad v_Q = \left( \frac{h}{\sqrt{2\pi m k_B T}} \right)^3 \]

\[ Z = \exp(-\beta F) = \sum_s \exp(-\beta \varepsilon_s) \quad \beta \equiv \frac{1}{k_B T} \]

\[ P(s) = \frac{1}{Z} \exp(-\beta \varepsilon_s) \]

\[ U = -\frac{\partial \ln Z}{\partial \beta} \]

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

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

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

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

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

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