THE UNIVERSITY OF NEW SOUTH WALES

SCHOOL OF PHYSICS

EXAMINATION - AUGUST 2011

PHYS4103 - PHYS IV (HONOURS)

UNIT B Statistical Mechanics

Time Allowed – 3 hours

Total number of questions - 5

Answer ALL questions

Not all questions are of equal value

Candidates may bring their own calculators.

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

QUESTION 1. 15 Marks

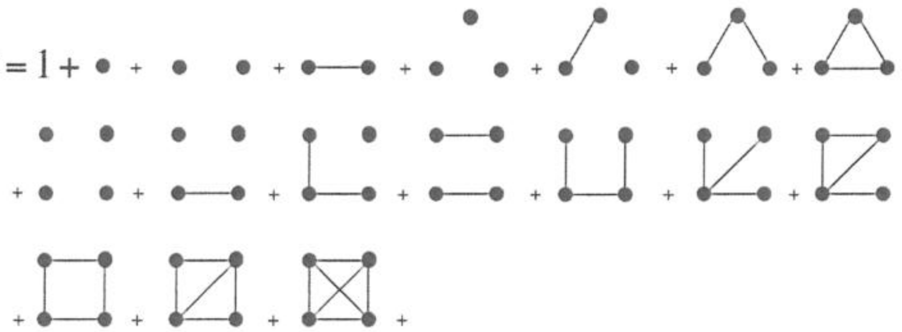
a) The graphical expansion for the grand partition function Ξ can be written in words as

$$\Xi = 1 + \text{the sum of all distinct simple graphs consisting of black } z_1 - \text{circles, some or no } f - \text{bonds,}$$

$= e^{(\bullet)}$

or graphically as

$\Xi = 1 +$



$F+1 = e^{G}$

Write down the theorem that allows us to write the $\log \Xi$ in terms of connected graphs.

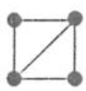
b) Find the graphical expansion for $\log \Xi$ (to the same level as the expansion for Ξ given above).

c) The K-particle grand canonical distribution function can be written as a K^{th} order functional derivative

$$\rho_K(1,\ldots,K) = \frac{1}{\Xi}\left(\prod_{i=1}^{K} z_1(i)\right)\frac{\delta^K \Xi}{\delta z_1(1)..\delta z_1(K)}$$

where the graphical interpretation of the functional derivative of a graph Γ is

$$\frac{\delta^n \Gamma}{\delta\gamma(1)\ldots\delta\gamma(n)} = \text{the sum of all distinct graphs obtained from } \Gamma \text{ by changing } n \text{ black } \gamma - \textit{circles} \text{ to } \textit{white } 1 - \textit{circles} \text{ and labeling them } 1,..n.$$

Find the functional derivative of the graph  with respect to $z_1(1)$.

d) If the initial graph  has symmetry number 4, what are the symmetry numbers of the resultant graph (or graphs)?

e) If the Ursell cluster functions are defined as

$$u_K(1,\ldots,K) = \left(\prod_{i=1}^{K} z_1(i)\right)\frac{\delta^K \log \Xi}{\delta z_1(1)..\delta z_1(K)}$$

and $\mu_1(1) = \rho_1(1)$, find the relationship between $\rho_K(1,\ldots,K)$ and $u_K(1,\ldots,K)$ for $K = 2$ and $K = 3$.

f) Derive the graphical expansion for $\rho_1(1)$ including all graphs with three or less black circles.

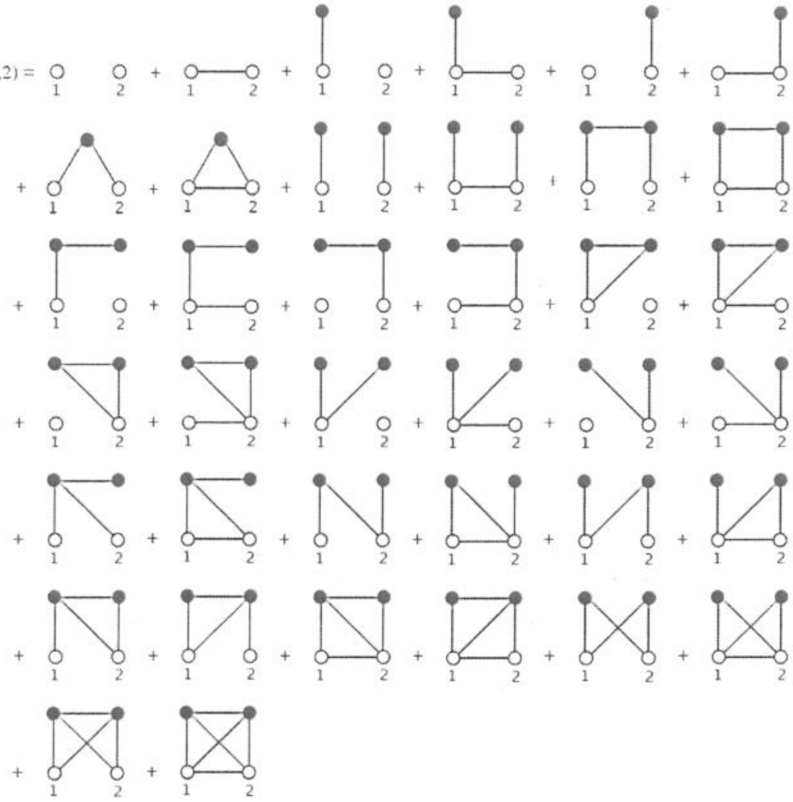
g) The graphical expansion for the 2-particle distribution function $\rho_2(1,2)$ can be written as

$\rho_2(1,2) =$ the sum of all distinct simple graphs consisting of
2 white z_1 – circles labeled 1 and 2 and some or no black
z_1 – circles, some or no f – bonds, such that there is
at least one path from each black circle to a white circle

The graphs with up to two black circles are shown below.

Write down the definition of an articulation circle and give an example.

$\rho_2(1,2) =$



h) What is the role of the circle replacement theorem in the expansion of $\rho_2(1,2)$.

i) Determine which graphs in the expansion for $\rho_2(1,2)$ above remain after the circle replacement theorem is applied.

QUESTION 2. 15 Marks

a) Write down the definition of the correlation functions $g_2(1,2)$ and $h_2(1,2)$ in terms of $\rho_2(1,2)$.

b) From the result of part a), or otherwise, obtain the graphical expansion for $h_2(1,2)$.

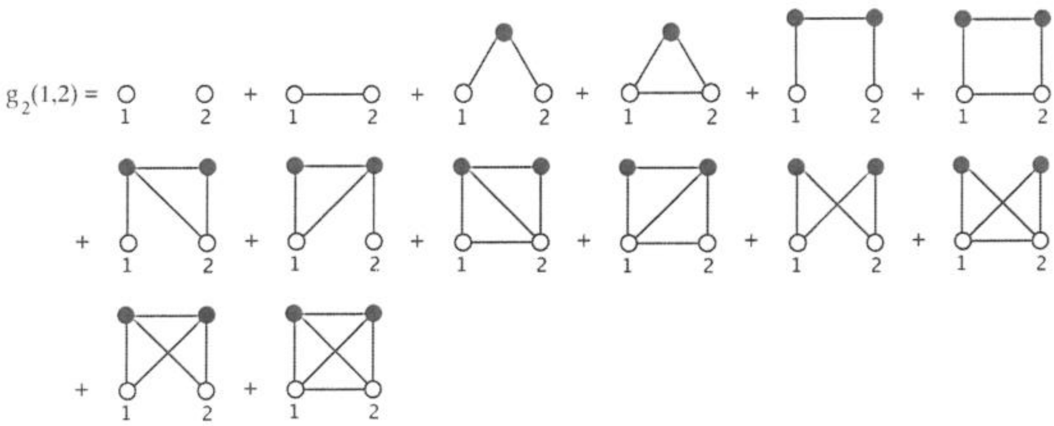
c) Define a nodal circle and identify all the nodal circles in the expansion for $\rho_2(1,2)$ given above.

d) The Ornstein-Zernike equation can be written as

$$h_2(1,2) = c_2(1,2) + t_2(1,2) = c_2(1,2) + \int d3\rho_1(3)c_2(1,3)h_2(3,2).$$

Explain the meaning of the new functions $c_2(1,2)$ and $t_2(1,2)$, and the physical interpretation of the Ornstein-Zernike equation.

e) The graphical expansion of $g_2(1,2)$ to second order in density is given by



Write down the graphical expansion for $c_2(1,2)$ and $t_2(1,2)$.

f) The Percus-Yevick equation can be derived by noticing that all the graphs in $g_2(1,2)$ occur with and without an $f_2(1,2)$ bond. Thus $e_2(1,2) = f_2(1,2) + 1 = \exp[-\beta\phi_2(1,2)]$ can be factored out of the expansion of $g_2(1,2)$ to obtain

$$g_2(1,2) = e_2(1,2)\{1 + t_2(1,2) + E_2(1,2)\}$$

What is the term $E_2(1,2)$ in this expression? Write down the graphical expansion for $E_2(1,2)$.

g) Derive the Percus-Yevick approximation for $c_2(1,2)$. That is, show that

$$c_2(1,2) = \{1 - \exp(\beta\phi_2(1,2))\} g_2(1,2).$$

h) Taking the natural logarithm of both sides of

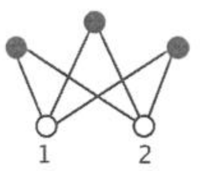
$$g_2(1,2) = e_2(1,2)\{1 + t_2(1,2) + E_2(1,2)\}$$

show that

$$\log[g_2(1,2)] + \beta\phi_2(1,2) = t_2(1,2) + B_2(1,2)$$

and hence derive the hypernetted chain approximation.

i) Does the following graph contribute to the hypernetted chain approximation for $c_2(1,2)$? If so, write down the exact contribution as an integral.



QUESTION 3. 20 Marks

a) Show that the partition function for the one-dimensional Tonks gas is

$$Z(L,N,T) = \frac{1}{N!}\int_0^L dx_1 \ldots \int_0^L dx_N \exp\left(-\beta \sum_{1\le i<j\le N} \phi\left(\left|x_i - x_j\right|\right)\right)$$
$$= \frac{\left(L-(N-1)a\right)^N}{N!}$$

where

$$\phi(x) = \begin{cases} \infty & \text{if } |x| < a \\ 0 & \text{if } |x| > a \end{cases}.$$

b) Find the free energy per particle for the Tonks gas, given that

$$-\frac{\psi}{kT} = \lim_{\substack{N,L\to\infty \\ v=L/N \text{ fixed}}} \frac{\ln Z(L,N,T)}{N}.$$

c) What does this say about the phase transition in the Tonks gas?

d) Draw the phase diagram of the liquid-gas transition for a fluid. Explain the behaviour of typical isotherms above and below the critical temperature T_c. Compare this with the magnetization as a function of magnetic field for isotherms above and below the Curie temperature.

e) Describe the terms in the Hamiltonian for the one-dimensional Ising chain

$$E\{\mu\} = -J\sum_{i=1}^{N} \mu_i \mu_{i+1} - H\sum_{i=1}^{N} \mu_i ,$$

and describe the boundary conditions.

f) For the one-dimensional Ising chain in an external magnetic field the partition function is

$$Z_N = \sum_{\mu_1=\pm1,\ldots\mu_N=\pm1} \exp\left(v\sum_{i=1}^{N} \mu_i\mu_{i+1} + B\sum_{i=1}^{N} \mu_i\right)$$

Show that the partition function can be written as a product of transfer matrices where

$$L(\mu_i,\mu_{i+1}) = \exp\left[\nu\mu_i\mu_{i+1} + \frac{B}{2}(\mu_i + \mu_{i+1})\right].$$

g) Evaluate the partition function in terms of the eigenvalues of the transfer matrix. Note if L has eigenvalues λ_1 and λ_2 then L^N has eigenvalues λ_1^N and λ_2^N.

h) When the external field is zero, find the largest eigenvalue.

i) In two-dimensions the Ising model on a square lattice has energy

$$E\{\mu\} = -J\sum_{i=1}^{m-1}\sum_{j=1}^{n}\mu_{i,j}\mu_{i+1,j} - J\sum_{i=1}^{m}\sum_{j=1}^{n}\mu_{i,j}\mu_{i,j+1} - H\sum_{i=1}^{m}\sum_{j=1}^{n}\mu_{i,j}$$

where $\mu_{i,n+1} = \mu_{i,1}$. Explain the geometry of the model and the meaning of the sums over i and j.

j) Show that if $\sigma_j = (\mu_{1,j},\mu_{2,j},\ldots,\mu_{m,j})$,

$$V_1(\sigma_j) = -J\sum_{i=1}^{m-1}\mu_{i,j}\mu_{i+1,j} - H\sum_{i=1}^{m}\mu_{i,j}$$

and

$$V_2(\sigma_j,\sigma_{j+1}) = -J\sum_{i=1}^{m}\mu_{i,j}\mu_{i,j+1}$$

that the partition function can be written as

$$\begin{aligned} Z_{n,m} &= \sum_{\mu}\exp(-\beta E\{\mu\}) = \sum_{\sigma_1,\ldots,\sigma_n}\exp\left(-\beta\sum_{j=1}^{n}\left[V_1(\sigma_j) + V_2(\sigma_j,\sigma_{j+1})\right]\right) \\ &= \sum_{\sigma_1,\ldots,\sigma_n} L(\sigma_1,\sigma_2)L(\sigma_2,\sigma_3)\ldots L(\sigma_{n-1},\sigma_n)L(\sigma_n,\sigma_1) \\ &= \sum_{\sigma_1} L^n(\sigma_1,\sigma_1) \end{aligned}$$

What is the physical nature of these transfer matrices.

k) What is needed to obtain the solution for the two-dimensional Ising model?

QUESTION 4.   15 Marks

The displacement of a Brownian particle in time t is given by

$$\mathbf{r}(t) - \mathbf{r}_0 = \int_0^t ds\mathbf{v}(s)$$

a) Form the mean square displacement as the integral of the velocity autocorrelation function $Z(t) = \langle \mathbf{v}(t) \cdot \mathbf{v}(0) \rangle$.

b) Show that the mean square displacement grows linearly in time and that the coefficient of the linear dependence is proportion to the infinite time integral of the velocity autocorrelation function.

c) Draw and discuss the time dependence of the velocity autocorrelation function.

d) The Liouville equation is given by

$$\frac{df}{dt} = -f\frac{\partial}{\partial \Gamma} \cdot \dot{\Gamma},$$

What are f, Γ and $\dot{\Gamma}$? What does this equation describe? Explain the different physical situations in which the Boltzmann equation and the Liouville equation apply.

e) If the equations of motion are Newtonian (or Hamiltonian) what can be said about f?

f) If the equations of motion for each particle are

$$\dot{\mathbf{q}}_i = \frac{1}{m}\mathbf{p}_i \qquad \dot{\mathbf{p}}_i = \mathbf{F}_i - \alpha\mathbf{p}_i,$$

with the value of α is chosen so that the kinetic energy is fixed at the value $K(\mathbf{p}_1,\ldots,\mathbf{p}_N) = K_0$, where

$$K(\mathbf{p}_1,\ldots,\mathbf{p}_N) = \sum_{i=1}^{N} \frac{1}{2m}\mathbf{p}_i \cdot \mathbf{p}_i,$$

show that by requiring the rate of change of the kinetic energy equal to zero $\dot{K}(\mathbf{p}_1,\ldots,\mathbf{p}_N) = 0$ at all time, that the explicit expression for α is given by

$$\alpha = \frac{\sum_{i=1}^{N} \frac{1}{m} \mathbf{p}_i \cdot \mathbf{F}_i}{\sum_{i=1}^{N} \frac{1}{m} p_i^2}$$

where $\mathbf{F}_i$ is the total force on particle i.

g) The rate of change of the total potential energy $\Phi(\mathbf{q}_1,\ldots,\mathbf{q}_N)$, is given by

$$\dot{\Phi} = \sum_{i=1}^{N} \frac{\partial \Phi}{\partial \mathbf{q}_i} \cdot \dot{\mathbf{q}}_i = -\sum_{i=1}^{N} \mathbf{F}_i \cdot \dot{\mathbf{q}}_i$$

Find the explicit form for f as a function of $\mathbf{q}_1,\ldots,\mathbf{q}_N,\mathbf{p}_1,\ldots,\mathbf{p}_N$. You can assume that fixed value of the kinetic energy is related to the temperature by $3N/2K_0 = \beta = (kT)^{-1}$.

QUESTION 5.   15 Marks

The Boltzmann equation gives the probability of finding a particle at position $\mathbf{r}$ and velocity $\mathbf{v}$ at time t, and is given by

$$\frac{\partial f}{\partial t} + \mathbf{v}\cdot\frac{\partial f}{\partial \mathbf{r}} + \frac{\mathbf{F}^{ext}}{m}\cdot\frac{\partial f}{\partial \mathbf{v}} = \int d\mathbf{v}_1 \int bdb \int d\varepsilon |\mathbf{v}_1 - \mathbf{v}| (f' f_1' - f_1 f)$$

where $f_1 = f(\mathbf{v}_1, t)$ and $f_1' = f(\mathbf{v}_1', t)$.

a) Show that if there are no external forces and the distribution does not depend on position $\mathbf{r}$, the Boltzmann H function is non-increasing, where

$$H(t) = \int d\mathbf{v} f(\mathbf{v},t) \ln f(\mathbf{v},t).$$

b) The relaxation time Boltzmann equation or BGK equation is obtained by replacing the collision term on the right-hand side by

$$-\nu(f - f_L)$$

where ν is the collision frequency and f_L is the local distribution function. For a system without an external field, but with a spatial dependence in the distribution function consider the time evolution of an entropy density defined by

$$s(\mathbf{r},t) = -k\int d\mathbf{v} f(\mathbf{r},\mathbf{v},t) \ln f(\mathbf{r},\mathbf{v},t).$$

Find the equation of motion for the local entropy $s(\mathbf{r},t)$.

c) If the fluid is stationary $\int d\mathbf{v}\mathbf{v}f = 0$, and both distributions are normalized so that $\int d\mathbf{v}(f - f_L) = 0$, show that

$$\frac{\partial s}{\partial t} + \frac{\partial}{\partial \mathbf{r}}\cdot \mathbf{J}_S = \nu k \int d\mathbf{v}(f - f_L)\ln f$$

where $\mathbf{J}_S = -k\int d\mathbf{v}\mathbf{v} f \ln f$ is the entropy current.

d) What is the physical interpretation of each of the terms in this equation.

e) Show that if $f(\mathbf{v},\mathbf{r}) = f_0(\mathbf{v})\exp(-\beta\phi(\mathbf{r}))$ where $f_0(\mathbf{v})$ is Maxwell's distribution and the force $\mathbf{F} = -\frac{\partial\phi}{\partial\mathbf{r}}$ then

$$\left(\mathbf{v}\cdot\frac{\partial}{\partial\mathbf{r}} + \frac{\mathbf{F}}{m}\cdot\frac{\partial}{\partial\mathbf{v}}\right) f(\mathbf{v},\mathbf{r}) = 0.$$

Explain why this implies that $f(\mathbf{v},\mathbf{r})$ is a time independent solution to Boltzmann's equation.

f) For an ensemble of equilibrium systems with a field turned on at time $t = 0$, linear response theory gives the response of some arbitrary phase variable B as

$$\langle B(t)\rangle = \langle B(0)\rangle - \beta F_e \int_0^t ds \langle B(s)J(\Gamma)\rangle_0$$

where the dissipation function $J(\Gamma)$ is determined by the form of the equations of motion. If

$$\begin{aligned}\dot{\mathbf{q}}_i &= \tfrac{1}{m}\mathbf{p}_i + \mathbf{C}_i F_e \\ \dot{\mathbf{p}}_i &= \mathbf{F}_i + \mathbf{D}_i F_e\end{aligned} \qquad \text{then} \qquad J(\Gamma) = \sum_{i=1}^{N}\left(\mathbf{C}_i\cdot\mathbf{F}_i - \mathbf{D}_i\cdot\tfrac{1}{m}\mathbf{p}_i\right)$$

Determine the dissipation function for a colour field where the equations of motion are

$$\begin{aligned}\dot{\mathbf{q}}_i &= \tfrac{1}{m}\mathbf{p}_i \\ \dot{\mathbf{p}}_i &= \mathbf{F}_i + \hat{\mathbf{x}}c_i F\end{aligned}$$

g) If $J(\Gamma)$, is the dissipation function write down an expression for its nonequilibrium average $\langle J(t)\rangle$.

h) Calculate the equilibrium average $\langle J(0)\rangle$.

i) How would you expect the pressure to respond to the application of a colour field. What would you do to determine normal stress effects, such as $\left\langle P_{xx}(t) - P_{yy}(t)\right\rangle$, for this system.