PHY831 - Midterm III, Monday November 14th 2011

Answer all questions. Time for midterm - 50 minutes

Name:

Formulae that might be helpful

$$\int \frac{dx}{(1+x^2)^{1/2}} = Sinh^{-1}(x) \tag{1}$$

$$\int_{-\infty}^{\infty} dx\ e^{-ax^2+bx} = (\frac{\pi}{a})^{1/2} e^{\frac{b^2}{4a}}; \qquad \int_0^{\infty} dx\ x^n e^{-ax^2} = \frac{1}{2a^{(n+1)/2}} \Gamma(\frac{n+1}{2}) \tag{2}$$

$$\int_0^{\infty} \frac{x^{s-1}dx}{e^x - 1} = \Gamma(s)\zeta(s), \tag{3}$$

where $\Gamma(s) = (s-1)!$ for s a positive integer, and $\zeta(2) = \frac{\pi^2}{6}$, $\zeta(3) = 1.202...$, $\zeta(4) = \pi^4/90$.

Response functions are defined as follows;

$$C_V = \left(\frac{\partial Q}{\partial T}\right)_{V,N} = \left(\frac{\partial U}{\partial S}\right)_{V,N} \left(\frac{\partial S}{\partial T}\right)_{V,N} = T\left(\frac{\partial S}{\partial T}\right)_{V,N}, \tag{4}$$

$$C_P = \left(\frac{\partial H}{\partial T}\right)_{P,N} = \left(\frac{\partial H}{\partial S}\right)_{P,N} \left(\frac{\partial S}{\partial T}\right)_{P,N} = T\left(\frac{\partial S}{\partial T}\right)_{P,N}, \tag{5}$$

$$\kappa_S = -\frac{1}{V}\left(\frac{\partial V}{\partial P}\right)_{S,N} = -\left(\frac{\partial lnV}{\partial P}\right)_{S,N}, \tag{6}$$

$$\kappa_T = -\frac{1}{V}\left(\frac{\partial V}{\partial P}\right)_{T,N} = -\left(\frac{\partial lnV}{\partial P}\right)_{T,N}, \tag{7}$$

$$\alpha_P = \frac{1}{V}\left(\frac{\partial V}{\partial T}\right)_{P,N} = \left(\frac{\partial lnV}{\partial T}\right)_{P,N}, \tag{8}$$

1. (10 points) The Hamiltonian of the spin half, ferromagnetic ($J > 0$) Ising model with co-ordination number z is given by,

$$H = -J \sum_{<ij>} S_i S_j - h \sum_i S_i \tag{9}$$

(i) Derive the mean field expression for the Helmholtz free energy of this model. (ii) Derive the mean field equation for the magnetization per spin (m) of the model, and show that near the critical point $m \propto (T_c - T)^{1/2}$.
(iii) Derive the high temperature series expansion for the model with $h = 0$ to order t^8, where $t = tanh(\beta J)$. Now we explore the predictions of mean field theory for the case of an Ising ferromagnet.

(i) Using the mean field approximation $S_i = m + (S_i - m)$, and keeping leading order terms in the fluctuations, we find,

$$H_{MF} = -\sum_{<i>} S_i(Jzm + h) + J\frac{z}{2}Nm^2 \tag{10}$$

where z is the co-ordination number of the lattice. The partition function for a ferromagnet is then,

$$Z_{MF} = \sum_{\{S_i\}} e^{\beta \sum_i [S_i(Jzm+h)] - \beta J \frac{z}{2} N m^2} = e^{-\frac{1}{2}\beta J z N m^2}[2Cosh(\beta Jzm + \beta h)]^N \tag{11}$$

and the mean field Helmholtz free energy is,

$$F_{MF} = N[\frac{1}{2}Jzm^2 - k_B T ln(2) - k_B T ln(Cosh(\beta Jzm + \beta h))] \tag{12}$$

(ii) The mean field equation is given by,

$$m =< S_i >= \frac{1}{Z}\sum_{\{S_i\}} S_i e^{-\beta H_{MF}} = Tanh(\beta Jzm + \beta h) \tag{13}$$

The order parameter is expected to behave as, $m \approx (T_c - T)^\beta$. Using the expansion $Tanh(y) = y - \frac{1}{3}y^3 + O(y^5)$; (13)

and considering the case $h = 0$, gives,

$$m \approx \beta Jzm - \frac{1}{3}(\beta Jzm)^3 + O(m^5) \tag{14}$$

with solutions,

$$m = 0, \quad m = \pm\left(3\frac{(\beta Jz - 1)}{(\beta Jz)^3}\right)^{1/2} \approx (T_c - T)^\beta \tag{15}$$

where $k_B T_c = Jz$, and $\beta_e = 1/2$ is the mean field order parameter critical exponent for the ferromagnetic Ising model.

(iii) To develop the high temperature expansion, we write the partition function as,

$$Z = \sum_{S_i=\pm1} \prod_{<ij>} e^{KS_iS_j} = (Cosh(K))^{zN/2} \sum_{S_i=\pm1} \prod_{<ij>} (1 + tS_iS_j) \tag{16}$$

When we take the sum of the spin values $S_i = \pm 1$, the only terms that survive in the expansion of the product are terms where the spin operators S_i are raised to an even power. We can represent this graphically, by placing a bond for each spin pair S_iS_j. Terms with n spin pairs are then represented by n edges in the square lattice. All possible placement of edges appear in the product, but only those cases where the spins appear as even powers are finite. The first "graph" or "diagram" that is finite is a square () that appears with weight t^4, with one factor of t for each edge. The number of ways of placing this diagram on a square lattice is N where N is the number of sites in the lattice. The next finite term is a rectangle with 6 sites with six edges, so it is of order t^6, and it has degeneracy $2N$. The next term is of eighth order with eight edges. This case is more interesting as there are four connected diagrams that must be considered, in addition to the disconnected diagrams. The degeneracy for the connected diagrams is $9N$, while the disconnected diagrams have degeneracy $N(N-9/2)$. For the 2-D Ising model this procedure can be carried to infinite order leading to the exact solution (see LL). To order t^8, the partition function is,

$$-\beta F = ln(Z) = \frac{zN}{2} ln(Cosh(K)) + Nln(2) + ln[1 + Nt^4 + 2Nt^6 + N(N + \frac{9}{2})t^8 + 0(t^{10})] \tag{17}$$

Expanding the logarithm and dropping terms that are not extensive (using the linked cluster theorem), gives,

$$-\beta F = \frac{zN}{2} ln(Cosh(K)) + Nln(2) + N[t^4 + 2t^6 + \frac{9}{2}t^8 + ...] \tag{18}$$

Note that the higher order terms in the expansion of the logarithm are not needed (linked cluster theorem) as they lead to non-extensive terms.

2. (10 points) (i) Derive the Helmholtz free energy of the interacting classical gas within the van der Waals approximation, and qualitatively discuss the need for the Maxwell construction. (ii) Derive the van der Waals equation of state for this system and explain why the the behavior on the critical isotherm is expected to be of the form, $\delta v \propto \delta p^{1/3}$. (iii) The virial expansion is given by,

$$\frac{Pv}{k_B T} = \sum_{l=1} a_l(T)(\frac{\lambda^3}{v})^{l-1}; \tag{19}$$

For the interacting classical gas with pair potential $u(r) = u_0 e^{-\alpha r}$, where α is a constant, find the virial expansion up to order $l = 2$. Hint, the cluster integrals are given by,

$$b_l = \frac{1}{V\lambda^{3l-3} l!}[Sum\ over\ contributions\ from\ connected(linked)\ diagrams] \tag{20}$$

and $a_2(T) = -b_2$.

(i) The canonical partition function for a classical particle system is given by (see part 2, Eq. (7)),

$$Z = \frac{1}{N! h^{3N}} \int d^3q_1 ... d^3q_N \int d^3p_1 .... d^3p_n e^{-\beta H}. \tag{21}$$

Recall that the partition function of the ideal classical gas is given by,

$$Z = \frac{V^N}{N!\lambda^N}; \quad where \quad \lambda = \left(\frac{h^2}{2\pi m k_B T}\right)^{1/2} \tag{22}$$

For particle systems with central force pair interactions, the partition function is,

$$Z = \frac{1}{N!\lambda^{3N}} \int d^3r_1 ... d^3r_N e^{-\beta \sum_{i>j} u(|\vec{r}_i - \vec{r}_j|)}. \tag{23}$$

To account for the hard core repulsion and the attractive part of the interation, we make the replacement $V \to V - Nb$, where $b = 4\pi\sigma^3/3$, which takes into account the reduction in the volume available to the particles. This is a mean field approximation as it treats the average effect of the hard core repulsions but not their fluctuations. The attractive contribution is also treated within mean field using the approximation,

$$\int d^3r_1 ... d^3r_N e^{-\beta \sum_{i>j} u(|\vec{r}_i - \vec{r}_j|)} \to I^N \tag{24}$$

where

$$I = Exp[-\beta \frac{N}{V} \int_\sigma u(r) 4\pi r^2 dr] = Exp[\beta a \frac{N}{V}] \tag{25}$$

where $a = -\int u(r) 4\pi r^2 dr$. The canonical partition function is then,

$$Z = \frac{q^N}{N!\lambda^{3N}}; \quad \text{where} \quad q = (V - Nb)e^{aN/(V k_B T)} \tag{26}$$

and the Helmholtz free energy is given by,

$$F = -k_B T ln(Z) = -k_B T ln\left(\frac{(V-bN)^N}{N!\lambda^{3N}}\right) - a\frac{N^2}{V} \tag{27}$$

(ii) The van der Waals equation of state if found from the free energy using,

$$P = -\left(\frac{\partial F}{\partial V}\right)_{T,N} = \frac{Nk_BT}{V-Nb} - \frac{N^2 a}{V^2} \tag{28}$$

The isothermal compressibility is given by,

$$\kappa_T = -\left(V(\frac{\partial P}{\partial V})_T\right)^{-1}; \tag{29}$$

where

$$(\frac{\partial P}{\partial V})_T(V_c) = \frac{1}{Nb^2}\left[\frac{8a}{27b} - T\right] \approx |T-T_c| \quad T \geq T_c \tag{30}$$

comparing () and (), we find that $\gamma = 1$. Calculation of the order parameter behavior is more tedious. We first write,

$$\delta t = 1 - \frac{T}{T_c}; \qquad \delta p = \frac{P}{P_c} - 1; \qquad \delta v = \frac{V}{V_c} - 1 \tag{31}$$

In these variables, the equation of state is,

$$\delta p = \frac{8(1-\delta t)}{2+3\delta v} - \frac{3}{(1+\delta v)^2} - 1 \tag{32}$$

Expanding to third order in δv yields,

$$\delta p = -4\delta t + 6\delta t\delta v + 9\delta t(\delta v)^2 - \frac{3}{2}(\delta v)^3 \tag{33}$$

At T_c, $\delta t = 0$, so we find,

$$P - P_c \approx a(v - v_c)^3 \tag{34}$$

so that $\delta = 3$.

(iii) We have,

$$b_2 = \frac{1}{2\lambda^3}\int_0^\infty 4\pi r^2\left(e^{-\beta u_0[exp(-\alpha r)]} - 1\right) \tag{35}$$

This is not integrable, however the pair potential is rapidly decaying at large r, so we carry out a Taylor expansion,

$$b_2 = \frac{1}{2\lambda^3}\int_0^\infty 4\pi r^2\left(e^{-\beta u_0[exp(-\alpha r)]} - 1\right) = \frac{2\pi}{\lambda^3}\sum_{k=1}^{\infty}\frac{(-\beta u_0)^k}{k!}I_k \tag{36}$$

where the integral I_k is given by,

$$I_k = \int_0^\infty r^2 e^{-\alpha r k} dr = \frac{1}{k^2}\frac{\partial^2}{\partial\alpha^2}\int_0^\infty e^{-\alpha r k}dk = \frac{1}{k^2}\frac{\partial^2}{\partial\alpha^2}(\frac{1}{\alpha k}) = \frac{1}{k^3}\frac{2}{\alpha^3} \tag{37}$$

The second virial coefficient is then,

$$a_2 = -b_2 = -\frac{4\pi}{\alpha^3\lambda^3}\sum_{k=1}^{\infty}\frac{(-\beta u_0)^k}{k!k^3} \tag{38}$$

If we take just the leading order term $k = 1$, we find,

$$a_2 = -b_2 = \frac{4\pi\beta u_0}{\alpha^3\lambda^3} \tag{39}$$

The virial expansion is then Eq. (19), with $a_1(T) = 1$, $a_2(T) = -b_2$. Note that the pressure is increased over the ideal gas value if u_0 is positive (repulsive pair interactions), while the pressure is decreased over the ideal gas value if u_0 is negative (attractive pair interactions).

3. (10 points) (i) Write down the BCS pairing Hamiltonian and the mean field approximation that is used to reduce it to a solvable form. (ii) Within BCS theory, the gap equation is given by,

$$\Delta_{\vec{k}} = -\sum_{\vec{l}} V_{\vec{k}\vec{l}} \frac{\Delta_{\vec{l}}}{2E_{\vec{l}}} \tag{40}$$

From this expression derive the equation,

$$\Delta(0) \approx 2\hbar\omega_c Exp[\frac{-1}{N(\epsilon_F)V}] \tag{41}$$

Explain the assumptions and approximations that you make in going from Eq. (12) to Eq. (13). (iii) Plot the behavior of the superconducting gap as a function of temperature, and give a formula for its scaling behavior near the superconducting phase transition.

(i) The pairing Hamiltonian is given by,

$$H_{pair} - \mu N = \sum_{\vec{k}\sigma}(\epsilon_{\vec{k}\sigma} - \mu)\ a^\dagger_{\vec{k}\sigma} a_{\vec{k}\sigma} + \sum_{\vec{k}\vec{l}} V_{\vec{k}\vec{l}}\ a^\dagger_{\vec{k}\uparrow} a^\dagger_{-\vec{k},\downarrow} a_{-\vec{l}\downarrow} a_{\vec{l}\uparrow}, \tag{42}$$

where $N = \sum_{\vec{k}\sigma} n_{\vec{k}\sigma}$ is the number of electrons in the Fermi sea. We introduce the averages,

$$b_{\vec{k}} =< a_{-\vec{k}\downarrow} a_{\vec{k}\uparrow} >, \quad \text{and} \quad b^*_{\vec{k}} =< a^\dagger_{\vec{k}\uparrow} a^\dagger_{-\vec{k}\downarrow} > . \tag{43}$$

where $b^*_{\vec{k}}$ is the average number of pairs in the system at wavevector $\vec{k}$. We carry out a mean field expansion in the fluctuations by writing,

$$a_{-\vec{l}\downarrow} a_{\vec{l}\uparrow} = b_l + (a_{-\vec{l}\downarrow} a_{\vec{l}\uparrow} - b_l); \qquad a^\dagger_{\vec{k}\uparrow} a^\dagger_{-\vec{k}\downarrow} = b^*_k + (a^\dagger_{\vec{k}\uparrow} a^\dagger_{-\vec{k}\downarrow} - b^*_k) \tag{44}$$

and keeping terms to leading order in the fluctuations.

(ii) Starting with the "gap equation"

$$\Delta_{\vec{k}} = -\sum_{\vec{l}} V_{\vec{k}\vec{l}} \frac{\Delta_{\vec{l}}}{2E_{\vec{l}}} \tag{45}$$

with the quasiparticle excitations having the energy spectrum,

$$E_{\vec{k}} = ((\epsilon_{\vec{k}} - \mu)^2 + |\Delta_{\vec{k}}|^2)^{1/2} \tag{46}$$

We take an angle independent gap $\Delta_{\vec{k}} = \Delta$, and assume a constant pairing potential $-V$ in a band near the Fermi surface of width $\hbar\omega_c$, so that Eq. (42) reduces to,

$$1 = \frac{N(\epsilon_F)V}{2} \int_{\epsilon_F - \hbar\omega_c}^{\epsilon_F + \hbar\omega_c} \frac{d\epsilon}{((\epsilon - \epsilon_F)^2 + |\Delta|^2)^{1/2}} = N(\epsilon_F)V \int_0^{\hbar\omega_c/\Delta} \frac{dx}{(1 + x^2)^{1/2}} = N(\epsilon_F)V\ Sinh^{-1}(\frac{\hbar\omega_c}{\Delta}) \tag{47}$$

or,

$$Sinh(\frac{1}{N(\epsilon_F)V}) = \frac{\hbar\omega_c}{\Delta} = \frac{1}{2}[e^{\frac{1}{N(\epsilon_F)V}} - e^{-\frac{1}{N(\epsilon_F)V}}] \tag{48}$$

In the weak coupling limit $\hbar\omega_c/\Delta >> 1,\ N(\epsilon_F)V << 1$ so that the BCS gap *at zero temperature* is well approximated by,

$$\Delta = 2\hbar\omega_c Exp[\frac{-1}{N(\epsilon_F)V}] \tag{49}$$

Note that, following convention, $N(\epsilon_F)$ is the density of states *for one electron spin*, whereas the density of states quoted in most other applications is a factor of two larger.

(iii) Near the superconducting transition, the gap behaves as the order parameter in a mean field model, so that,

$$\Delta \approx |T - T_c|^{1/2} \tag{50}$$