PHY831 - Midterm III, Monday November 19th 2012
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;

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

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

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

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

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

For the Ising Hamiltonian with $J > 0$,

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

the mean field Helmholtz free energy is,

$$F_{MF} = N[\frac{1}{2}Jzm^2 - k_BTln(2) - k_BTln(Cosh(\beta Jzm + \beta h))]. \tag{10}$$

The Helmholtz free energy within van der Waals theory is,

$$F_{vdW} = -k_BTln(Z) = -k_BTln\left(\frac{(V-bN)^N}{N!\lambda^{3N}}\right) - a\frac{N^2}{V} \tag{11}$$

where $a = -\frac{1}{2}\int_{\sigma}^{\infty} u(r)4\pi r^2 dr$; $\quad b = 2\pi\sigma^3/3$.

The BCS pairing Hamiltonian is,

$$H_{pair} - \mu N = \sum_{\vec{k}\sigma}(\epsilon_{\vec{k}\sigma} - \mu)\ a^{\dagger}_{\vec{k}\sigma} a_{\vec{k}\sigma} + \sum_{\vec{k}\vec{l}} V_{\vec{k}\vec{l}}\ a^{\dagger}_{\vec{k}\uparrow} a^{\dagger}_{-\vec{k},\downarrow} a_{-\vec{l}\downarrow} a_{\vec{l}\uparrow}, \tag{12}$$

The Bogolubov-Valatin transformation reduces the mean field form of the BCS Hamiltonian to the free Fermion form,

$$H_{MF} - \mu N = \sum_{\vec{k}}(\epsilon_{\vec{k}} - \mu - E_{\vec{k}} + \Delta_{\vec{k}} b^*_{\vec{k}}) + \sum_{\vec{k},\sigma} E_{\vec{k}} \gamma^{\dagger}_{\vec{k}\sigma}\gamma_{\vec{k}\sigma} \tag{13}$$

where $E_{\vec{k}}$ is the quasiparticle spectrum, and the first term is the condensation energy.

1. (10 points)
Consider the Hamiltonian of the ferromagnetic Ising model with co-ordination number z (i.e. Eqs. (9)), where $S_i = \pm 1$ and the sum is over the nearest neighbors of a square lattice.
(i) Derive the high temperature series expansion for the free energy of the model with $h = 0$ to order t^8, where $t = tanh(\beta J)$.
(ii) Now write down the free energy of this model within the mean field approximation (see Eq. (10)) at temperatures $T > T_c$. Are the results of (i) and (ii) the same at high temperatures? Explain any similarities or differences.

Solutions
(i) Using Eq. (9), the partition function of the Ising model on a square lattice

$$Z = \sum_{\{S_i=\pm1\}} \prod_{<ij>} (cosh(K) + S_i S_j sinh(K)) = \sum_{\{S_i=\pm1\}} (cosh(K))^{2N} \prod_{<ij>} (1 + S_i S_j t) \tag{14}$$

where $t = tanh(K)$. Expanding to order t^8 (ignoring non-extensive terms by invoking the linked cluster theorem) gives,

$$Z = 2^N (cosh(K))^{2N} [1 + Nt^4 + 2Nt^6 + \frac{9}{2} Nt^8 + ...] \tag{15}$$

so the Helmholtz free energy is,

$$-\frac{\beta F}{N} = ln(2) + 2ln(Cosh(K)) + t^4 + 2t^6 + \frac{9}{2} t^8 + ... \tag{16}$$

(ii) For $T > T_c$, the magnetization within mean field theory is $m = 0$ in zero field, so the free energy from Eq. (10) reduces to

$$-\frac{\beta F}{N} = ln(2) \tag{17}$$

Clearly the high temperature series expansion does a better job of describing cluster fluctuations at high temperature, while the mean field theory ignores these fluctuations. A systematic analysis of the phase behavior using series expansions is usually more accurate than mean field theory however it is more difficult and in some cases restricted in its ability to access all phases occuring in a system.

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2. (10 points)
(i) The virial expansion for an interacting particle system is given by,

$$\frac{Pv}{k_B T} = \sum_{l=1} a_l(T) (\frac{\lambda^3}{v})^{l-1}; \qquad or; \qquad \frac{P}{k_B T} = \rho + B_2 \rho^2 + B_3 \rho^3 + ... \tag{18}$$

where $v = 1/\rho = V/N$. Consider an interacting classical gas with an attractive pair potential $u(r) = -c/r^s$ for $r > \sigma$ and with a repulsive hard core at short distances, i.e. $u(r) = \infty$ for $r < \sigma$. Here c is a positive constant. Considering cases where $s > 3$ find the second virial coefficient, B_2, for this system. Hint, the cluster integrals are given by,

$$b_l = \frac{1}{V \lambda^{3l-3} l!} [Sum\ over\ contributions\ from\ connected (linked)\ diagrams] \tag{19}$$

and $a_2(T) = -b_2$. You can carry out the integral considering only the lowest order term in an expansion in $\beta = 1/(k_B T)$.
(ii) Find the second virial coefficient of the van der Waals equation, for the the pair interaction of (i), using the expressions for a and b given after Eq. (11). Is B_2 for the van der Waals case the same as the result from the cluster expansion you found above? Explain why or why not.

Solutions
(i) From the definition we have,

$$b_2 = \frac{1}{2V\lambda^3} \int f_{12} d^3r_1 d^3r_2 = \frac{1}{2\lambda^3} \int (e^{-\beta u(r)} - 1) 4\pi r^2\ dr \tag{20}$$

so that,

$$b_2 = \frac{1}{2\lambda^3}[-\frac{4\pi}{3}\sigma^3 + \int_\sigma^\infty (e^{\beta c/r^s} - 1)4\pi r^2\ dr] \tag{21}$$

The integral is evaluated by expanding the exponential,

$$\int_\sigma^\infty (e^{\beta c/r^s} - 1)4\pi r^2\ dr = 4\pi \sum_{l=1}^{\infty} \frac{(\beta c)^l}{l!} \int_\sigma^\infty \frac{dr}{r^{ls-2}} = 4\pi \sum_{l=1}^{\infty} \frac{(\beta c)^l}{l!} \frac{-\sigma^{3-sl}}{3-sl} \tag{22}$$

where the condition $s > 3$ ensures that the upper limit does not contribute to the integral. We then have,

$$B_2 = \lambda^3 a_2 = -\lambda^3 b_2 = \frac{2\pi}{3}\sigma^3 - \frac{4\pi}{2} \sum_{l=1}^{\infty} \frac{(\beta c)^l}{l!} \frac{\sigma^{3-sl}}{sl-3} \tag{23}$$

The question suggests only taking the leading term, i.e. just $l = 1$ in the sum, which gives,

$$B_2 \approx \frac{2\pi\sigma^3}{3}[1 - \frac{3}{s-3}\frac{\beta c}{\sigma^s}] \tag{24}$$

(ii) From the free energy for the van der Waals gas, we find,

$$P = -\frac{\partial F}{\partial V} = \frac{k_B T}{v-b} - \frac{a}{v^2} \tag{25}$$

Expanding to find the second virial coefficient, we find,

$$\frac{P}{k_B T} = \rho(1 + b\rho) - \frac{a}{k_B T}\rho^2 \tag{26}$$

If we take just the first term in the expansion of $e^{\beta u(r)} - 1 \approx \beta u(r)$, we find

$$a = \frac{1}{2}\int_\sigma^\infty u(r)4\pi r^2 dr \approx \frac{k_B T}{2}\int_\sigma^\infty [e^{\beta u(r)} - 1] \tag{27}$$

We thus find that the second virial coefficient in van der Waals theory is the same as the second virial coefficient of the interacting gas, to leading order in an expansion in $1/(k_B T)$. Van der Waals theory takes into account only pair interactions and so does the second virial coefficient so it is not surprising they are similar. From this analysis a more accurate expression for attraction parameter, a, in the van der Waals gas equation can be found by carrying out the integral over interactions to higher order, as in part (i).

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3. (10 points)

(i) The Bogolubov-Valatin transformation reduces the mean field form of the BCS Hamiltonian to the free Fermion form,

$$H_{MF} - \mu N = \sum_{\vec{k}}(\epsilon_{\vec{k}} - \mu - E_{\vec{k}} + \Delta_{\vec{k}} b^*_{\vec{k}}) + \sum_{\vec{k}} E_{\vec{k}}(\gamma^\dagger_{\vec{k}\uparrow}\gamma_{\vec{k}\uparrow} + \gamma^\dagger_{\vec{k}\downarrow}\gamma_{\vec{k}\downarrow}). \tag{28}$$

where the quasiparticle dispersion relation is given by,

$$E_{\vec{k}} = [(\epsilon_{\vec{k}} - \mu)^2 + |\Delta_{\vec{k}}|^2]^{1/2} \tag{29}$$

For the case of an isotropic gap, find an expression for the density of quasiparticle states as a function of energy. Make a plot of your result. Also find and plot the density of states of the free Fermion gas as a function of energy and compare the two cases.

(ii) Within BCS theory, the gap equation is given by,

$$\Delta_{\vec{k}} = -\sum_{\vec{l}} V_{\vec{k}\vec{l}} \frac{\Delta_{\vec{l}}}{2E_{\vec{l}}} \tag{30}$$

Making the isotropic approximation, and assuming that the attractive potential is $-V$ on the energy interval $E_F - \hbar\omega_c < \epsilon < E_F + \hbar\omega_c$, from this expression derive the equation,

$$\Delta(0) \approx 2\hbar\omega_c Exp[\frac{-1}{N(\epsilon_F)V}] \tag{31}$$

Explain the assumptions and approximations that you make in going from Eq. (30) to Eq. (31).

Solutions

In the special case of an angle independent gap $\Delta_{\vec{k}} = \Delta$, and assuming a constant pairing potential $-V$ in a band near the Fermi surface of width $\hbar\omega_c$, Eq. (30) reduces to,

$$1 = \frac{N(\epsilon_F)V}{2} \int_{\epsilon_F-\hbar\omega_c}^{\epsilon_F+\hbar\omega_c} \frac{d\epsilon}{((\epsilon-\epsilon_F)^2+|\Delta|^2)^{1/2}} = N(\epsilon_F)V \int_0^{\hbar\omega_c/\Delta} \frac{dx}{(1+x^2)^{1/2}} = N(\epsilon_F)V \ Sinh^{-1}(\frac{\hbar\omega_c}{\Delta}) \tag{32}$$

From (32), we take the weak coupling limit $\hbar\omega_c/\Delta >> 1$ to find the BCS gap *at zero temperature*,

$$\Delta = 2\hbar\omega_c Exp[\frac{-1}{N(\epsilon_F)V}] \tag{33}$$

The *density of states* for the excitations is very important as it is measured in tunnelling. The density of states is found from,

$$D(E)dE = N(\epsilon)d\epsilon \approx N(\epsilon_F)d\epsilon \tag{34}$$

Since,

$$dE = \frac{2(\epsilon-\mu)d\epsilon}{2((\epsilon-\mu)^2+\Delta^2))^{1/2}}, \tag{35}$$

we have,

$$D(E) = \frac{N(\epsilon_F)((\epsilon-\mu)^2+\Delta^2))^{1/2}}{\epsilon-\mu} = \frac{N(\epsilon_F)E}{(E^2-\Delta^2)^{1/2}} \tag{36}$$

This density of state applies for $E > |\Delta|$, while the density of states is zero otherwise.

The density of state for the non-interacting gas is found using,

$$\epsilon_k = \frac{\hbar^2k^2}{2m}; \qquad N(k) = (\frac{L}{2\pi})^3 4\pi k^2 \tag{37}$$

Using

$$N(k)dk = n(\epsilon)d\epsilon \quad so \quad n(\epsilon) = N(k)/(\partial\epsilon/\partial k) \tag{38}$$

we find,

$$n(\epsilon) = \frac{\hbar V}{\pi^2\sqrt{2m}}\epsilon^{1/2} \tag{39}$$