Solutions to problems for Part 3

Assigned problems and sample quiz problems

Sample Quiz Problems

Quiz Problem 1. Draw the phase diagram of the Ising Ferromagnet in an applied magnetic field. Indicate the critical point. Plot the magnetization as a function of the applied field for three temperatures \( T < T_c, T = T_c, T > T_c \).

Quiz Problem 2. Plot the behavior of the magnetization of the Ising ferromagnet as a function of the temperature, for three applied field cases: \( h < 0, h = 0, h > 0 \). Indicate the critical point.

Quiz Problem 3. Write down the definition of the critical exponents \( \alpha, \beta, \gamma, \delta, \eta \) and \( \nu \). What values do these exponents take within mean field theory.

Solution.

\[ C_V \sim t^{-\alpha}; \quad m \sim t^\beta; \quad \chi \sim t^{-\gamma}; \quad m(T_c) \sim h^{1/\delta}; \quad c(r) \sim e^{-r/\xi}/r^{d-2+\eta} \]  

where \( \xi = t^{-\nu} \), and \( t = |T - T_c| \). Within mean field theory \( \alpha = 0, \beta = 1/2, \gamma = 1, \delta = 3, \eta = 0, \nu = 1/2 \)

Quiz Problem 4. Write down the mean field equation for the Ising ferromagnet in an applied field, on a lattice with co-ordination number \( z \) and exchange constant \( J \). From this equation find the critical exponent \( \delta \) for the Ising ferromagnet within mean field theory.

Solution.

\[ m = \tanh(\beta J zm + \beta h) \sim (\beta J zm + \beta h) - \frac{1}{3}(\beta J zm + \beta h)^3 \]  

at the critical point \( \beta J z = 1 \), so \( m \sim h^{1/3} \) and hence \( \delta = 3 \).

Quiz Problem 5. Write down the scaling hypothesis for the magnetization, susceptibility, free energy and correlation function. From these relations, find the Fisher, Widom and Rushbrooke critical exponent relations. Also write down the hyperscaling relation.

Solution

We assume that the correlation length is the key quantity in the scaling theory so that the scaling behavior is of the form,

\[ F(T, h) = t^{2-\alpha} F_s(h \xi^y); \quad M(T, h) = t^{\beta} M_s(h \xi^y); \quad \chi(T, h) = t^{-\gamma} \chi_s(h \xi^y); \quad C(r) = r^{-\nu} C_s(r/\xi, h \xi^y) \]  

where \( t = |T - T_c| \), and \( y > 0 \). We also define \( \xi^y = t^{-\Delta} \), so that \( \nu y = \Delta \), where \( \Delta \) is the gap exponent. We also have \( p = d - 2 + \eta \), and \( \xi = t^{-\nu} \). The scaling functions have the property that as their argument \( x = h \xi^y = h/t^{\Delta} \) goes to zero, the scaling functions must approach a constant. Moreover the scaling assumption states that for \( h < \xi^{-y} \) the scaling functions are constant. Moreover, as \( x \to \infty \), the scaling functions go to zero. First consider the behavior of the magnetization when we are at the critical point, so that,

\[ M(t = 0, h \neq 0) \sim t^{\beta} M_s(x \to \infty) \sim h^{1/\delta}; \quad \text{so that} \quad M_s(x) \sim x^k \]  

where,

\[ t^{\beta} x^k = t^{\beta} \left( \frac{h}{t^{\Delta}} \right)^k = h^{1/\delta}; \quad \text{so that} \quad k = 1/\delta; \quad \text{and} \quad \Delta = \beta \delta \]
Now consider the relation between the magnetization and the susceptibility, 
\[ M \sim \int_0^\Delta \chi dh \sim t^{-\gamma} t^\Delta \sim t^\beta; \]  
so that \( \beta = \Delta - \gamma \) \hspace{1cm} (6)

In a similar manner, 
\[ F \sim \int_0^\Delta M dh \sim t^\beta t^\Delta \sim t^{2-\alpha}; \]  
so that \( \beta + \Delta = 2 - \alpha \) \hspace{1cm} (7)

Finally, consider the scaling of the correlation function in the case where \( h \xi^y \) is zero, so that \( C_s \) is a constant for \( r < \xi \) and zero otherwise. We then have, 
\[ \chi \sim \int d^3r \sim \int_\xi^\xi drr^{-p}C_s(r/\xi, h\xi^y) \sim \xi^{d-(d-2+\eta)} \sim t^{-\gamma}; \]  
so that \( \gamma = \nu(2-\eta) \) \hspace{1cm} (8)

These exponent relations are usually written in the form,
\[ \Delta = \beta + \gamma; \quad \gamma = \nu(2-\eta) \quad (Fisher); \quad \alpha + 2\beta + \gamma = 2 \quad (Rushbrooke); \quad \gamma = \beta(\delta - 1) \quad (Widom) \]  
(9)

Since we have added the “gap” exponent \( \Delta \), there are seven exponents in the problem. We have four exponent relations so that only three exponents are independent. Josephson introduced another relation, called the hyperscaling relation. He introduced the hypothesis that the singular part of the free energy scales as \( 1/\xi^d \). This implies that,
\[ f_{\text{sing}} \approx \xi^{-d} \approx t^{2-\alpha}; \]  
so that \( dv = 2 - \alpha \) \quad (Josephson, or hyperscaling relation) \hspace{1cm} (10)

The hyperscaling relation is considered the most likely of the scaling relations to fail and for example is known to fail in some heterogeneous models such as the Spin glass model.

**Quiz Problem 6.** Find the domain wall energy for the Ising (\( O(1) \) model) and for the \( O(2) \) model. From these expressions find the lower critical dimension for these two problems.

**Solution**

We consider the ground state energy of a domain wall. The \( O(1) \) model is the Ising case so the spin is either up or down, while \( O(2) \) corresponds to a spin vector that has unit length and can take any angle \( 0 < \theta < 2\pi \). A ferromagnetic interaction favors all the spins pointing in the same direction for both models. For both cases, a domain wall created by setting the spins on one side of a hypercubic system in the up direction, while the spins on the opposite size are in the down direction. The interface between the up and down domains that this boundary condition creates is called the domain wall. For an Ising system we found that in the ground state,
\[ E_{\text{Ising}}^{DW} = 2JL^{d-1} \]  
(11)

For the \( O(2) \) case, the domain wall energy is,
\[ E_{\text{continuous}}^{DW} \approx \frac{\pi}{2} JL^{d-2} \]  
(12)

The lower energy of domain walls in systems with an order parameter that can take a continuum of values, like the \( O(2) \) model is due to the possibility of a wide domain wall that changes smoothly between the boundary states. In the Ising case the domain wall is abrupt and this costs more energy. For the \( O(2) \) case, the Hamiltonian is,
\[ H = -J \sum_{<ij>} \vec{S}_i \cdot \vec{S}_j = -J \sum_{<ij>} |S|^2 \cos(\theta_{ij}) \]  
(13)

where \( \vec{S}_i \) is a unit vector with angle \( \theta_i \) to the z axis, and \( \theta_{ij} = \theta_j - \theta_i \). To find the domain wall energy we consider the direction perpendicular to the domain wall and notice that the lowest energy domain wall is formed by making a wide domain wall with small differences in energy between spins. Since the domain wall corresponds to changing the
spin orientation from up to down, the angle must rotate by $\pi$. If the width of the domain wall is $L$, the angle between adjacent spins is $\pi/L$. The energy cost of the domain wall is then,

$$E_{DW}^{O(2)} = L^{d-1} J \sum_{i=1}^{L} \left( 1 - \cos \left( \frac{\pi}{L} \right) \right) = L^{d-1} J L \frac{1}{2} \left( \frac{\pi}{L} \right)^2 = \frac{\pi}{2} J L^{d-2} \quad (14)$$

The lower critical dimension is the dimension below which the domain wall energy is finite, while above the lower critical dimension the energy of a domain grows with the length of the domain wall. From the above we find that for the Ising system $d_{lc} = 1 + \epsilon$, while for the $O(2)$ model $d_{lc} = 2 + \epsilon$, where $\epsilon$ is small and positive.

**Quiz Problem 7.** Write down the van der Waals equation of state. Draw the $P,v$ phase diagram of the van der Waals gas and indicate the critical point.

**Solution.**

$$P = \frac{k_b T}{v - b} - \frac{a}{v^2} \quad (15)$$

**Quiz Problem 8.** Make plots of the van der Waals equation of state isotherms, for $T > T_c$, $T < T_c$ and for $T = T_c$. For the case $T < T_c$ explain why the non-convex part of the curve cannot occur at equilibrium and the Maxwell construction to obtain a physical $P,v$ isotherm.

**Quiz Problem 9.** Write down the Landau free energy for the Ising and fluid-gas phase transitions. Explain the correspondences between the quantities in the magnetic and classical gas problems.

**Solution.**

$$F = a(T - T_c)y^2 + by^4 + cy \quad (16)$$

For the Ising model $y = m, c = h$, for the van der Waals gas, $y = v_g - v_l, c = P - P_c$.

**Quiz Problem 10.** Derive the Helmholtz free energy of the van der Waals gas and explain the physical meaning of the parameters $a$ and $b$. Using your free energy explain the Maxwell construction.

**Solution**

See lecture notes.

**Quiz Problem 11.** Write down the Gibb’s free energy of the van der Waals gas. Explain the conditions under which co-existence is expected to occur.

**Solution**

See lecture notes

**Quiz Problem 12.** Explain the meaning of the upper critical dimension and lower critical dimension in the theory of critical phenomena.

**Solution**

Below the lower critical dimension, there is no traditional phase transition to an ordered phase at finite temperature. It should be noted however that at the critical dimension special transitions may occur, for example in the case of the $O(2)$ model the Kosterlitz-Thouless transition occurs in two dimensions and this is a special phase transition that is different that the phase transitions of the model above the lower critical dimensions.

Above the upper critical dimension, the critical phenomena is correctly described by mean field critical exponents. Between the upper and lower critical dimensions, critical exponents and the nature of the transition (continuous or discontinuous) may change.
Quiz Problem 13. State the universality hypothesis in the theory of critical phenomena and using it explain why the liquid gas phase transition is in the same universality class as the Ising model.

Solution
The universality hypothesis refers to continuous phase transitions where the correlation length diverges so that fluctuations occur on all length scales. The universality hypothesis states that the critical exponents describing continuous phase transitions depend on only three things:

(i) The spatial dimension
(ii) The order parameter symmetry
(iii) The range of the interactions

This predicts for example that systems described by very different physics, such as the liquid-gas transition and Ising magnetic phase transition, should be described by the same critical exponents.

Quiz Problem 14. Explain the importance of the “linked-cluster” theorems in perturbation theory of many particle systems.

Solution.
Linked cluster theorems state that averages of observables can be described by sums of linked diagrams, and that non-extensive contributions from disconnected diagrams must cancel when the diagrams are summed to all orders.

Quiz Problem 15. Draw the high temperature series expansion diagrams to order \( t^8 \) (where \( t = \tanh(\beta J) \)) for the square lattice, nearest neighbor, spin half Ising ferromagnet partition function. What is the degeneracy of each of these diagrams? Write down the expansion for the Helmholtz free energy and give a physical reason why only the terms of order \( N \) are kept.

Solution.
See Lecture Notes

Quiz Problem 16. Draw the low temperature series expansion diagrams to order \( s^8 \) (where \( s = \exp[-2\beta J] \)) for the square lattice, nearest neighbor, spin half Ising ferromagnet partition function. What is the degeneracy of each of these diagrams? Write down the expansion for the Helmholtz free energy and give a physical reason why only the terms of order \( N \) are kept.

Solution.
See Lecture Notes

Quiz Problem 17. Write down the mathematical form of the virial expansion for many particle systems and explain why it is important. What physical properties can be extracted from the second virial coefficient?

Solution
The virial expansion is given by,

\[
P_{k_B T} = \rho + B_2 \rho^2 + B_3 \rho^3 + \ldots
\]  

(17)

where \( \rho = N/V \) is small. Keeping only the leading order term on the right hand side of this equation leads to the ideal gas law. The first correction to the ideal gas law is due to the prefactor \( B_2 \), which is called the second virial coefficient. The second virial coefficient for a particle system described by central force pair potential is given by,

\[
B_2 = -\int dR \ R^2 (e^{-\beta u(r)} - 1)
\]  

(18)

From this expression we can see that the second virial coefficient is related to the interatomic potential. If we measure \( B_2 \) as a function of temperature it is possible to extract a lot of information about \( u(r) \).
Quiz Problem 18. Explain the meaning of second quantization. Discuss the way that it can be used in position space and in the basis of single particle wavefunctions. Write down the commutation relations for Bose and Fermi second quantized creation and annihilation operators.

Solution.
Second quantization is a formulation of quantum mechanics and of quantum field theory that is expressed in terms of creation and annihilation operators. In many body quantum physics creation and annihilation operators create and destroy particles in many body basis sets constructed from single particle wave functions. In the case of Fermions a many body basis function is a determinant, while for Bosons it is a permanent. The commutation relations for Fermions and Bosons are similar, except that for fermions we have anticommutators and for Bosons we have commutators. In many body quantum mechanics we have,

\[
[a_i, a_j^\dagger] = \delta_{ij}; \quad \text{for bosons; and } \{a_i, a_j^\dagger\} = \delta_{ij}; \quad \text{for fermions};
\]

while for quantum fields, we have,

\[
[\psi(x), \psi^\dagger(x')] = \delta(x - x'); \quad \text{for bosons; and } \{\psi(x), \psi^\dagger(x')\} = \delta(x - x'); \quad \text{for fermions};
\]

These days, new theories are often formulated using creation and annihilation operators rather than the Heisenberg or Schrödinger formulations of quantum theory.

Quiz Problem 19. Write down the Hamiltonian for BCS theory, and the decoupling scheme used to reduce it to a solvable form. Explain the physical reasoning for the decoupling scheme that is chosen.

Solution.
In the s-wave BCS theory a singlet state is assumed, so that,

\[
H_{\text{pair}} - \mu N = \sum_{k\sigma} (\epsilon_{k\sigma} - \mu) a_{k\sigma}^\dagger a_{k\sigma} + \sum_{kl\sigma} V_{kl} a_{k\uparrow}^\dagger a_{l\downarrow}^\dagger a_{-l\downarrow} a_{-k\uparrow},
\]

where \( N = \sum_{k\sigma} n_{k\sigma} \) is the number of electrons in the Fermi sea. We carry out an expansion in the fluctuations,

\[
a_{-l\downarrow} a_{l\uparrow} = b_l \quad (a_{-l\downarrow} a_{l\uparrow} - b_l); \quad a_{k\uparrow}^\dagger a_{-k\downarrow}^\dagger = b_k^* \quad (a_{k\uparrow}^\dagger a_{-k\downarrow} - b_k^*)
\]

The mean field Hamiltonian keeps only the leading order term in the fluctuations so that,

\[
H_{\text{MF}} - \mu N = \sum_{k\sigma} (\epsilon_{k\sigma} - \mu) a_{k\sigma}^\dagger a_{k\sigma} + \sum_{kl\sigma} V_{kl} (a_{k\uparrow}^\dagger a_{-k\downarrow}^\dagger b_l + b_k^* a_{-l\downarrow} a_{l\uparrow} - b_k^* b_l)
\]

This is the Hamiltonian that leads to the BSC solution.

Quiz Problem 20. Consider the inverse Bogoliubov-Valatin transformation,

\[
\gamma_{k\sigma} = u_k^* a_{k\sigma}^\dagger - \sigma v_k^* a_{-k\sigma}^\dagger.
\]

Show that if the operators \( a, a^\dagger \) obey standard fermion anti-commutator relations, then the operators \( \gamma, \gamma^\dagger \) also obey these relations, provided,

\[
|u_k|^2 + |v_k|^2 = 1
\]

Solution The anticommutator,

\[
\{\gamma_{k\sigma}, \gamma_{l\alpha}\} = \{u_k^* a_{k\sigma}^\dagger - \sigma v_k^* a_{-k\sigma}^\dagger, u_l^* a_{l\alpha} - \sigma v_l^* a_{-l\alpha}^\dagger\}.
\]
Expanding the anticommutator gives,

\[
\{ \gamma_{\vec{k}\sigma}, \gamma_{\vec{l}\alpha} \} = (u_{k}^{*} a_{\vec{k}\sigma} - \sigma v_{\vec{k}} a_{\vec{l} - \sigma}) (u_{l}^{*} a_{\vec{l}\alpha} - \alpha v_{\vec{l}} a_{\vec{l} - \alpha}) + (u_{k}^{*} a_{\vec{l}\alpha} - \alpha v_{\vec{k}} a_{\vec{l} - \alpha}) (u_{l}^{*} a_{\vec{k}\sigma} - \sigma v_{\vec{l}} a_{\vec{l} - \sigma})
\]

which reduces to,

\[
\{ \gamma_{\vec{k}\sigma}, \gamma_{\vec{l}\alpha} \} = u_{k}^{*} u_{l}^{*} \{ a_{\vec{k}\sigma}, a_{\vec{l}\alpha} \} + \sigma \alpha v_{\vec{k}} v_{\vec{l}} \{ a_{\vec{k} - \sigma}, a_{\vec{l} - \alpha} \} - \alpha u_{k}^{*} v_{\vec{l}} a_{\vec{l}, a_{\vec{l} - \alpha}} - \sigma u_{k}^{*} u_{l}^{*} \{ a_{\vec{k} - \sigma}, a_{\vec{l} - \alpha} \}
\]

The first two anticommutators are zero. The second two anticommutators are finite when the conditions \( \delta(k, -l) \delta(\sigma, -\alpha) \) hold. However when this condition holds, the two commutators are equal and opposite, so they sum to zero. Taking the adjoint of Eq. (15) shows that \( \{ \gamma_{\vec{k}\sigma}, \gamma_{\vec{l}\alpha} \} = 0 \). Now consider,

\[
\{ \gamma_{\vec{k}\sigma}, \gamma_{\vec{l}\alpha}^{\dag} \} = (u_{k}^{*} a_{\vec{k}\sigma} - \sigma v_{\vec{k}} a_{\vec{l} - \sigma}) (u_{l}^{*} a_{\vec{l}\alpha} - \alpha v_{\vec{l}} a_{\vec{l} - \alpha}) + (u_{k}^{*} a_{\vec{l}\alpha} - \alpha v_{\vec{k}} a_{\vec{l} - \alpha}) (u_{l}^{*} a_{\vec{k}\sigma} - \sigma v_{\vec{l}} a_{\vec{l} - \sigma})
\]

which reduces to

\[
\{ \gamma_{\vec{k}\sigma}, \gamma_{\vec{l}\alpha}^{\dag} \} = u_{k}^{*} u_{l}^{*} \{ a_{\vec{k}\sigma}, a_{\vec{l}\alpha}^{\dag} \} + \sigma \alpha v_{\vec{k}} v_{\vec{l}} \{ a_{\vec{k} - \sigma}, a_{\vec{l} - \alpha}^{\dag} \} - \alpha u_{k}^{*} v_{\vec{l}} a_{\vec{l}, a_{\vec{l} - \alpha}} - \sigma u_{k}^{*} u_{l}^{*} \{ a_{\vec{k} - \sigma}, a_{\vec{l} - \alpha}^{\dag} \} = 0
\]

This anticommutator thus requires Eq. (12) in order for the \( \gamma \) operators to obey Fermion anticommutator relations.

**Quiz Problem 21.** Given that the energy of quasiparticle excitations from the BCS ground state have the spectrum,

\[
E = [ (\epsilon - \epsilon_{F})^2 + |\Delta|^2 ]^{1/2},
\]

where \( \Delta \) is the superconducting gap and \( E_{F} \) is the Fermi energy, show that the quasiparticle density of states if given by,

\[
D(E) = \frac{N(\epsilon_{F}) E}{(E^2 - \Delta^2)^{1/2}}
\]

**Solution** We use the relation,

\[
N(\epsilon_{F}) d\epsilon = D(E) dE; \quad \text{and} \quad dE = \frac{\epsilon - \epsilon_{F}}{[(\epsilon - \epsilon_{F})^2 + \Delta^2]^{1/2}} d\epsilon
\]

to find,

\[
D(E) = \frac{N(\epsilon_{F}) [(\epsilon - \epsilon_{F})^2 + \Delta^2]^{1/2}}{\epsilon - \epsilon_{F}}
\]

and using,

\[
(\epsilon - \epsilon_{F})^2 = E^2 - |\Delta|^2
\]

yields,

\[
D(E) = \frac{N(\epsilon_{F}) E}{[E^2 - |\Delta|^2]^{1/2}}
\]

**Quiz Problem 22.** Describe the physical meaning of the superconducting gap, and the way in which BCS theory describes it.

**Solution**

The superconducting gap is the energy required to generate a quasiparticle excitation from the superconducting ground state. In BCS theory, the quasiparticles behave like non-interacting fermions and the energy required to generate a quasiparticle is at least \( 2\Delta(T) \).
Quiz Problem 23. Given the general solutions to the BCS mean field theory

\[ \Delta_k = -\sum_l V_{kl} \frac{\Delta_l}{2E_l} \quad E_k = ((\epsilon_k - \mu)^2 + |\Delta_k|^2)^{1/2} \tag{38} \]

Describe the assumptions that are made in deducing that,

\[ 1 = N(\epsilon_F) \frac{V}{2} \int_{\epsilon_F - \hbar \omega_c}^{\epsilon_F + \hbar \omega_c} \frac{d\epsilon}{((\epsilon - \epsilon_F)^2 + |\Delta|^2)^{1/2}} = \]

\[ N(\epsilon_F) V \int_0^{\hbar \omega_c / \Delta} \frac{dx}{(1 + x^2)^{1/2}} = N(\epsilon_F) V \sinh^{-1} \left( \frac{\hbar \omega_c}{\Delta} \right) \tag{39} \]

and hence,

\[ \Delta = 2\hbar \omega_c \exp \left( \frac{-1}{N(\epsilon_F) V} \right) \tag{40} \]

Solution

We assume an isotropic gap, and that the attractive coupling between electrons is constant \(-V\), over the range \(\epsilon_F - \hbar \omega_c < \epsilon < \epsilon_F + \hbar \omega_c\). The density of states is assumed constant with value \(N(\epsilon_F)\).

Assigned problems

Assigned Problem 1. From Eq. (18) of the notes, derive the Landau form Eq. (44). Explain the approximations that are made. Plot \(F_L\) as a function if \(m\) for \(T > T_c\) and \(T < T_c\) for \(h = 0\) and for \(h \neq 0\). Explain the concept of spontaneous symmetry breaking (SSB) using your graphs.

Solution.

Equation (18) is,

\[ -f_R = -\frac{\beta F_{MF}}{N} + \ln(2) = -\frac{1}{2} J z m^2 + \ln(Cosh(\beta J zm + \beta h)) \]

\[ \approx -\frac{1}{2} \beta J zm^2 + \frac{1}{2} (\beta J zm + h)^2 - \frac{1}{12} (\beta J zm + h)^4 + O(m^6) \tag{41} \]

where we used the expansion of \(\log(cosh(x))\) for small \(x\). Now we use the fact that \(k_B T_c = J z\) and expanding in \(h\) to linear order we find,

\[ f_L = a(T - T_c)m^2 + bm^4 + hm \tag{42} \]

where constant prefactors in the term \(hm\) are absorbed into \(f_L\), \(a\) and \(b\).

Assigned Problem 2. Consider the Ising ferromagnet in zero field, in the case where the spin can take three values \(S_i = 0, \pm 1\). a) Find equations for the mean field free energy and magnetization. b) Find the critical temperature and the behavior near the critical point. Are the critical exponents \((\beta, \gamma, \alpha, \delta)\) the same as for the case \(S = \pm 1\)? Is the critical point at higher or lower temperature than the spin \(\pm 1\) case? c) Is the free energy for the the spin \(0, \pm 1\) case higher or lower than the free energy of the \(\pm 1\) case? Why? d) Carry out an expansion of the free energy to fourth order in the magnetization. Does this free energy have the Landau form expected for an Ising ferromagnet?

Solution. The partition function and Helmholtz free energy are,

\[ Z = [1 + 2Cosh(\beta J zm)]^N; \quad F = -k_B TN ln[1 + 2Cosh(\beta J zm)] \tag{43} \]
The mean field equation is,

$$m = \frac{2\sinh(\beta Jz m)}{1 + 2\cosh(\beta Jz m)} \approx \frac{2}{3} \beta Jz m - \frac{1}{3} (\beta Jz m)^3 + ...$$  \hspace{1cm} (44)

The critical point is at $\beta Jz = 3/2$, so the critical temperature is at $k_B T_c = 2Jz/3$ which is lower than that for spin 1/2 due to the additional entropy of the spin one system. The critical exponents $\beta$ and $\delta$ are clearly the same as for the spin 1/2 case. The free energy is lower for the spin 1 case due to the higher entropy.

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**Assigned Problem 3.** By using $b = \xi$ show that Eqs. (58) reduces to Eqs. (50).

**Assigned Problem 4.** Consider the Landau free energy,

$$F = a(T - T_c) m^2 + bm^4 + cm^6$$  \hspace{1cm} (45)

where $c(T) > 0$ as required for stability. Sketch the possible behaviors for $a(T), b(T)$ positive and negative, and show that the system undergoes a first order transition at some value $T_c$. Find the value of $a(T_c)$ and the discontinuity in $m$ at the transition.

**Solution.**
The mean field equation is,

$$\frac{\delta F}{\delta m} = am + bm^3 + cm^5 = 0;$$ \hspace{1cm} (46)

Note that in general we do a variation with respect to $m$, so when we add fluctuations later, we need to use the Euler-Lagrange equation. Here the variation is the same as a partial derivative with respect to $m$. Solving the mean field equation, we find five solutions.

$$m = 0, \quad m = \pm m_{\pm}; \quad m_{\pm}^2 = \frac{-b \pm (b^2 - 4ac)^{1/2}}{2c}$$ \hspace{1cm} (47)

Though there are always five solutions, only the real solutions are physical. Analysis of the behavior of the model reduces to identifying the real solutions, and finding which real solution has the lowest free energy. We can understand the nature of the solutions by looking at the second derivative,

$$\frac{\partial^2 F}{\partial m^2} = a + 3bm^2 + 5cm^4,$$ \hspace{1cm} (48)

which enables us to distinguish between maxima and minima. We also use the fact that $F$ is symmetric in $m$ and that at large $m$, because $c$ is positive, $F$ is large and positive for large $|m|$. Finally, without loss of generality, we can divide through by $c$, or equivalently set $c = 1$. Now consider the four cases for $a, b$.

(i) $a > 0, b > 0$. In this case $b^2 - 4ac < b$, so $m_{\pm}^2$ is always negative. Therefore the solutions $m_{\pm}$ are always imaginary. The only real solution is $m = 0$, which is a minimum having $F(0) = 0$.

(ii) $a < 0, b > 0$. In this regime, $b^2 + 4|a|c > b^2$, so $m_{\pm}^2 > 0$, so that $m_{\pm}$ is real. However $-b - (b^2 + 4|a|c)^{1/2}$ remains negative, so $m_{-}$ remains imaginary. The real solutions are thus a maximum at $m = 0$ and two symmetric minima at $m_{\pm}^2 = \frac{1}{2}([b^2 + 4|a|c]^{1/2} - b)$.

There is a phase transition between states (i) and (ii) that occurs at $a = 0$ where two new solutions emerge and the extremum at $m = 0$ changes from a maximum for $a < 0$ to a minimum for $a > 0$. The nature of the transition is found by making a small $|a|$ expansion of the solutions $m_{\pm}$, which leads to $m \approx |a|^{1/2}$. This is the Ising/Van der Waals universality class we have studied using mean field theory, where we found $|a| \approx |T - T_c|$.

(iii) $a < 0, b < 0$. In this regime, $b^2 + 4|a|c > b^2$, so $m_{+}$ is real but $m_{-}$ remains imaginary. Therefore, as in case (ii), there is a maximum at $m = 0$, and minima at $\pm m_{+}$.

(iv) $a > 0, b < 0$. In this regime there are several things going on. First, the discriminant $b^2 - 4a$ is negative for $b^2 < 2a$, so in this regime there is only one real solution, a minimum at $m = 0$. For $b^2 > 2a$, there are five real solutions because $|b| \pm (b^2 - 4a)^{1/2} > 0$. Moreover, we know that the solution at $m = 0$ is a minimum, so we know that $\pm m_{-}$ are maxima, while $\pm m_{+}$ are minima.

The final issue we have to resolve is the behavior of the minima $m_{+}$ as a function of $a, b$, in particular we need to know if $F(m_{+})$ is greater than or less than $F(0)$. If the lowest free energy state changes it corresponds to a phase
transition. We can solve this problem by evaluating $F(m_+)$, or we can find solutions where $F(m_0) = 0$ and then solve $m_0 = m_*$. The later leads to,

$$m_0^2 = \frac{3}{2} |b| \pm \left( \frac{b^2}{4} - \frac{4a}{3} \right)^{1/2}$$

and setting $m_0^2 = m_*^2$, we find,

$$3 |b| \pm \left( \frac{b^2}{4} - \frac{4a}{3} \right)^{1/2} = \frac{1}{2} |b| + (b^2 - 4a)^{1/2}$$

which has solution

$$|b|_* = 4 \left( \frac{a}{3} \right)^{1/2}; \quad \text{with} \quad m_*^2 = m_0^2 |b|_* \approx \frac{2(\alpha)}{3}^{1/2}$$

$m_*$ is the magnetization on the phase boundary defined by $|b|_*$. There is then a first order phase transition from magnetization $m_*$ for $|b| < |b|_*$, to magnetization $m = 0$ for $|b| > |b|_*$. The behavior of the magnetization on the phase boundary is $m_* \approx a^{1/4} \approx |T - T_c|^{1/4}$, which is the mean field result for the order parameter near a tricritical point where a line of second order phase transitions meets a line of first order phase transitions.

Assigned Problem 5. Consider a Landau theory with a cubic term,

$$F = a(T - T_c) m^2 + b m^3 + c m^4.$$  

Analyse the behavior of this model, particularly the nature of the different phases and phase transition(s) that occur.

Solutions

It is convenient to write this in the form,

$$F = \frac{\alpha}{2} m^2 - \frac{\beta}{3} m^3 + \frac{\gamma}{4} m^4,$$

We require that $\gamma > 0$ to ensure that the magnetization at the free energy minimum is bounded, and we can take $\gamma = 1$ without loss of generality. We also note that the transformation $\beta \to -\beta$, $m \to -m$ leaves $F$ invariant, so we only consider $\beta > 0$. First consider the case where $\beta = 0$. In that case we have the Landau theory that we studied before and we know that there is a continuous mean field phase transition at $\alpha = 0$ from a spontaneously ordered phase for $\alpha < 0 (T < T_c)$ to a disordered $m = 0$ phase for $\alpha > 0 (T > T_c)$. For $\beta > 0$, the positive magnetization state is further stabilized, so we look for a transition at $\alpha > 0$. To determine the behavior for $\beta > 0$, we find the extreme of $F$,

$$\frac{\partial F}{\partial m} = 0 = \alpha m - \beta m^2 + m^3,$$

where has solutions,

$$m = 0; m_\pm = \frac{1}{2} [\beta \pm \sqrt{\beta^2 - 4\alpha}]$$

when the discriminant is negative there is only one real solution ($m = 0$), while if the discriminant is positive, there are three real solutions. The critical condition is called the spinodal line and it is given by,

$$\beta_* = 2\sqrt{\alpha} \quad \alpha > 0$$

for $\beta < \beta_*$ there is no ordered phase, while for $\beta > \beta_*$ there are three extrema, but we don’t yet know if there is a stable ordered phase. To find out if a positive magnetization state is stable, we compare the free energies, $f(0)$ and $f(m_+)$ and find the critical condition by equating them,

$$f(0) = 0 = \frac{\alpha}{2} m_+^2 - \frac{\beta}{3} m_+^3 + \frac{1}{4} m_+^4$$
or,
\[
\frac{\alpha}{2} - \frac{\beta}{3} m_+ + \frac{1}{4} m_+^2 = 0
\]  (59)

We also have,
\[m_+^2 = \beta m_+ - \alpha \]  (60)

so that,
\[
\frac{\alpha}{2} - \frac{\beta}{3} m_+ + \frac{1}{4}(\beta m_+ - \alpha) = 0
\]  (61)

or
\[m_+ + \frac{3\alpha}{\beta} = 0. \]  (62)

Using the solution for \(m_+\), we find,
\[
\sqrt{\beta^2 - 4\alpha} = -\frac{6\alpha}{\beta} - \beta
\]  (63)

Solving yields,
\[
\beta_c = \frac{3}{\sqrt{2}} \sqrt{\alpha}.
\]  (64)

For \(\beta < \beta_c\), the model predicts an ordered phase with finite magnetization, and at \(\beta_c\) there is a first order transition into a phase with finite magnetization. In the regime \(\beta_s < \beta < \beta_c\) the system has zero magnetization but there is a metastable state with finite magnetization. For \(\beta < \beta_s\) the zero magnetization state is the only local minimum in the model.

---

**Assigned Problem 6.**

A spin half Ising model with four spin interactions on a square lattice has Hamiltonian,
\[
H = -\sum_{ijkl \; \text{in square}} JS_i S_j S_k S_l
\]  (65)

where the sum is over the smallest squares on an infinite square lattice, the interaction is ferromagnetic \(J > 0\) and \(S_i = \pm 1\). Each elementary square is counted only once in the sum.

Using a leading order expansion in the fluctuations (i.e. write \(S_i = m_i + (S_i - m_i)\) and expand to leading order in the fluctuations), find the mean field Hamiltonian for this problem (Here \(m_i = <S_i>\) is the magnetization at site \(i\)).

Using the mean field Hamiltonian and assuming a homogeneous state where \(m_i = m\), find an expression for the mean field Helmholtz free energy, and the mean field equation for this problem.

Taking \(J = 1\), sketch the behavior of the solutions to the mean field equation as a function of temperature. Does the non-trivial solution move continuously toward the \(m = 0\) solution as the temperature increases? Is the behavior of the order parameter at the critical temperature discontinuous or continuous? Do you expect the correlation length to diverge at the critical point in this problem?

**Solutions**

We start by writing a three spin term in terms of an expansion in the fluctuations,
\[
S_i S_j S_k S_l = [m_i + (S_i - m_i)][m_j + (S_j - m_j)][m_k + (S_k - m_k)][m_l + (S_l - m_l)]
\]  (66)

Expanding to leading order in the fluctuations, we then have,
\[
S_i S_j S_k S_l \approx m_i m_j m_k m_l + (S_i - m_i)m_j m_k m_l + m_i (S_j - m_j)m_k m_l + m_i m_j (S_k - m_k)m_l + m_i m_j m_k (S_l - m_l)
\]  (67)
Since the interaction is ferromagnetic we can make the uniform assumption \( m_i = m \), which yields,

\[
H_{MF} = - \sum_{ijkl \text{ in square}} [-3Jm^4 + m^3(S_i + S_j + S_k + S_l)] = 3JNm^4 - 4Jm^3 \sum_i S_i \tag{68}
\]

The mean field partition function is then,

\[
Z_{MF} = e^{-\beta J N m^4} [2 \cosh(4 \beta J m^3)]^N \tag{69}
\]

which leads to the free energy,

\[
F_{MF} = -k_B T \ln Z_{MF} = 3J N m^4 - k_B T N \ln [2 \cosh(4 \beta J m^3)] \tag{70}
\]

and the mean field equation is,

\[
m = \tanh(4 \beta J m^3) \tag{71}
\]

The mean field equation can be found in several ways, for example by doing the variation \( \delta F/\delta m = 0 \), or by finding the expectation \(< S_i >\) using the mean field Hamiltonian.

By plotting the graphs of \( m \) and \( \tanh(4 \beta J m^3) \), it is evident that at large values of \( K = \beta J \) (i.e. low temperature), there are two positive \( m \) solutions as well as the solution at \( m = 0 \). However as \( K \) decreases (i.e. \( T \) increases) there is a critical point at which the two non-trivial positive \( m \) solutions merge. This defines the critical point. At this point \( m \) is finite. For \( T > T_c \) the positive \( m \) solution disappears so there is a discontinuous jump in the magnetization from a finite value to zero at \( T_c \). The transition in this model is then first order, in contrast to the pair interaction case where the transition is continuous. The correlation length at the transition found here is then remains finite at the critical point.

**Assigned Problem 7.** The Dieterici equation of state for a gas is,

\[
P = \frac{k_B T}{v - b} e^{-a/(k_B T v)} \tag{72}
\]

where \( v = V/N \). Find the critical point and the values of the exponents \( \beta, \delta, \gamma \) for this model.

**Solution.** The critical point is found by solving,

\[
P_c = \frac{k_B T_c}{v_c - b} e^{-a/(k_B T_c v_c)}; \tag{73}
\]

\[
\frac{\partial P}{\partial v} = 0 = - \frac{k_B T_c}{(v_c - b)^2} e^{-a/(k_B T_c v_c)} + \frac{k_B T_c}{v_c - b} \frac{a}{k_B T_c v_c^2} e^{-a/(k_B T_c v_c)} \tag{74}
\]

Which simplify to,

\[
-\frac{1}{v_c - b} + \frac{a}{k_B T_c v_c^2} = 0; \quad \text{so} \quad \frac{a}{k_B T_c} = \frac{v_c^2}{v_c - b} \tag{75}
\]

The second derivative yields,

\[
\frac{\partial^2 P}{\partial v^2} = 0 = 2 \frac{k_B T_c}{(v_c - b)^3} e^{-a/(k_B T_c v_c)} - 2 \frac{k_B T_c}{v_c - b} \frac{a}{k_B T_c v_c^2} e^{-a/(k_B T_c v_c)}
\]

\[-2 \frac{k_B T_c}{v_c - b} k_B T_c v_c^3 e^{-a/(k_B T_c v_c)} + \frac{k_B T_c}{v_c - b} \frac{a}{k_B T_c v_c^2} e^{-a/(k_B T_c v_c)} \tag{76}
\]

so that,

\[
2 \frac{1}{(v_c - b)^2} - 2 \frac{1}{v_c - b} \frac{a}{k_B T_c v_c^2} - 2 \frac{a}{k_B T_c v_c^3} + \left( \frac{a}{k_B T_c v_c^2} \right)^2 = 0 \tag{77}
\]
and using Eq. (),
\[-2 \frac{1}{v_c} \frac{1}{v_c - b} + \left( \frac{1}{v_c - b} \right)^2 = 0; \quad \text{so} \quad v_c = 2b \tag{78}\]
so we find that,
\[v_c = 2b; \quad k_B T_c = \frac{a}{4b}; \quad P_c = \frac{a}{4e^2 b^2} \tag{79}\]
To find the critical exponents we write \(v = v_c + \delta v, T = T_c + \delta T, P = P_c + \delta P\), so that,
\[P_c + \delta P = \frac{k_B(T_c + \delta T)}{v_c + \delta v - b} e^{-a/[k_B(T_c + \delta T)(v_c + \delta v)]} = \frac{k_B T_c}{b} \left( 1 + \frac{\delta T}{T_c} \right)^{2} e^{-a/[k_B T_c v_c(1+\delta T/T_c)(1+\delta v/v_c)]} \tag{80}\]
This reduces to,
\[1 + p = e^2 \frac{1+t}{1+2x} E x p[-\frac{2}{(1+t)(1+x)}] \tag{81}\]
where \(p = \delta P/P_c, t = \delta T/T_c, x = \delta v/v_c\). To third order this expansion gives,
\[p = 3t + 2t^2 - \frac{2}{3} t^3 + (-2t - 4t^2)x + 2tx^2 - \frac{2}{3} x^3 \tag{82}\]
Taking a derivative with respect to \(v\) at setting \(x = 0\) leads to,
\[\kappa_T = (-V \frac{\partial P}{\partial V})^{-1} \approx |T - T_c|^{-1} \tag{83}\]
so \(\gamma = 1\). The exponent \(\delta\) is found by setting \(t\) to zero so that \(p \approx x^3\), so that \(\delta = 3\). To find \(\beta\) we assume that \(p_t = p_g, x_t = -x_g\), so that,
\[p_t = 3t + 2t^2 - \frac{2}{3} t^3 + (-2t - 4t^2)x_t + 2tx_t^2 - \frac{2}{3} x_t^3 \tag{84}\]
\[p - g = 3t + 2t^2 - \frac{2}{3} t^3 - (-2t - 4t^2)x_t + 2tx_t^2 + \frac{2}{3} x_t^3 \tag{85}\]
Setting these equations to be equal yields,
\[2(-2t - 4t^2)x_t = \frac{2}{3} x_t^3, \quad \text{so that} \quad x_t \approx |T - T_c|^{1/2} \tag{86}\]
where we dropped the \(t^2\) term as it is higher order. In the above analysis the signs of the \(t\) and \(x\) are consistent but have to be checked each time.

**Assigned Problem 8.** Consider a phase co-existence curve in a \(P - T\) phase diagram, separating two phases “A” and “B”. Consider two points on the phase coexistence curve at \(P, T\) and \(P + \Delta P, T + \Delta T\). Since the chemical potential of the phases \(A\) and \(B\) are the same at any given point on the co-existence curve, we have,
\[\Delta g_A = g_A(P + \Delta P, T + \Delta T) - g_A(P, T) = g_B(P + \Delta P, T + \Delta T) - g_B(P, T) = \Delta g_B \tag{87}\]
From this relation, prove the Clausius-Clapeyron relation,
\[\frac{\partial P}{\partial T} = \frac{L}{T(V_B - V_A)} \tag{88}\]
where \(L\) is the latent heat. Find the form of this relation for the van der Waals equation of state. What is the dependence of the latent heat as \(T \to T_c\). Is this exponent related to any of the other exponents in the problem?
**Solution**

The Gibb’s energies $G(B), G(A)$ are the same at temperature $T$ and at temperature $T + \Delta T$, so $dG_A = dG_B$, where $dG = G(T + dT) - G(T)$. We also have,

$$
  dG = -SdT + VdP; \quad \text{so} \quad \frac{dG}{dT} = -S + V \frac{dP}{dT}
$$

(89)

Using the latter expression for both phases we have,

$$
  -S_A + V_A \frac{dP}{dT} = -S_B + V_B \frac{dP}{dT}
$$

(90)

where we used the fact that the pressure is the same in the $A$ and $B$ phases. Now we use the Clausius relation $dS = dQ/T$, and the fact that $dQ = L$ to find,

$$
  \frac{dP}{dT} = \frac{S_B - S_A}{V_B - V_A} = \frac{L}{T(V_B - V_A)}
$$

(91)

**Assigned Problem 9.** Recent work on black hole thermodynamics has suggested that a black hole with charge $Q$ obeys the equation of state,

$$
  P = \frac{T}{v} - \frac{1}{2\pi v^2} + \frac{2Q^2}{\pi v^4}
$$

(92)

where the physical pressure and temperature are given by,

$$
  Press = \frac{hc}{l_P^2}; \quad Temp = \frac{hc}{k_B} T; \quad v = 2l_P r_+
$$

(93)

where $l_P = hG_N/c^3$ is the Planck length and $r_+$ is the black hole event horizon. Yes, the "Temp" temperature expression looks strange, but that is the expression in the paper I got this from and I have not had time to figure out if there is a typo in the paper. In any case you don’t need to use that equation. Find the critical point of this equation of state and find the critical exponents $\delta$ and $\beta$.

**Solution**

The conditions for the critical point are,

$$
  \frac{\partial P}{\partial v} = \frac{\partial^2 P}{\partial v^2} = 0
$$

(94)

which lead to the two equations,

$$
  -\frac{T}{v^2} + \frac{1}{\pi v^3} - \frac{8Q^2}{\pi v^5} = 0; \quad \frac{2T}{v^3} - \frac{3}{\pi v^4} + \frac{40Q^2}{\pi v^6} = 0
$$

(95)

which reduce to,

$$
  -Tv^3 + \frac{v^2}{\pi} - \frac{8Q^2}{\pi} = 0; \quad 2Tv^3 - \frac{3v^2}{\pi} + \frac{40Q^2}{\pi} = 0
$$

(96)

Multiplying the first equation by two and adding it to the second equation gives,

$$
  -\frac{v^2}{\pi} + \frac{24Q^2}{\pi} = 0; \quad \text{so} \quad v_c = \sqrt{24Q}
$$

(97)

and hence,

$$
  T_c = \frac{1}{3\sqrt{6\pi}Q}; \quad P_c = \frac{1}{96\pi Q^2}
$$

(98)

Defining $p = P/P_c$, $\nu = v/v_c$, $t = T/T_c$, we find,

$$
  8t = 3\nu(p + \frac{2}{\nu^2}) - \frac{1}{\nu^3}
$$

(99)
In these variables the critical point $p, t, v$ is at 1, 1, 1. To find the critical exponents we expand as in the van der Waals case, so we define, $t = 1 - \delta t, \nu = 1 + \delta \nu; p = 1 + \delta p$.

\[
\frac{8}{3} (1 - \delta t) = 1 + \delta p + \frac{2}{(1 + \delta \nu)^2} - \frac{1}{3(1 + \nu)^4}
\]  
(100)

Using the Taylor expansion,

\[
\frac{1}{(1 + x)^l} = 1 - lx + \frac{l(l + 1)x^2}{2} - \frac{l(l + 1)(l + 2)x^3}{3!} + ...
\]  
(101)

we find,

\[
\frac{8}{3} (1 - \delta t)(1 - \delta v + \delta v^2 - \delta v^3 + ...) = 1 + \delta p + 2(1 - 2\delta v + 3\delta v^2 - 4\delta v^3 + ...) - \frac{1}{3}(1 - 4\delta v + 10\delta v^2 - 20\delta v^3 + ...)
\]  
(102)

Expanding gives,

\[
\frac{8}{3}(1 - \delta v + \delta v^2 - \delta v^3 - \delta t + \delta t\delta v - \delta t\delta v^2 + ...) = \frac{8}{3} + \delta p - \frac{8}{3}\delta v + \frac{8}{3}\delta v^2 - \frac{4}{3}\delta v^3
\]  
(103)

which reduces to,

\[
\delta p = -\delta t + \delta t\delta v - \delta t\delta v^2 - \frac{4}{3}\delta v^3
\]  
(104)

Using the fact that $\delta v_y = -\delta v_t$ and subtracting equations for both the gas and liquid phases leads to,

\[
\delta v_y = \sqrt{0.75}\delta t^{1/2}.
\]  
(105)

Finally setting $\delta t = 0$, we find $\delta v_y \sim \delta p^{1/3}$. We thus find the exponents $\beta = 1/2$ and $\delta = 3$ as expected for mean field systems.

**Assigned Problem 10.** Consider a ferromagnetic nearest neighbor, spin 1/2, square lattice Ising model where the interactions along the x-axis, $J_x$, are different than those along the y-axis, $J_y$. Extend the low and high temperature expansions Eq. (150) and Eq. (152) to this case. Does duality still hold? From your expansions, find the internal energy and the specific heat.

**Solution**

\[
Z = \sum_{\{S_i = \pm 1\} <ij>} e^{K_i S_i S_j} = (Cosh(K_x))^N(Cosh(K_y))^N \sum_{\{S_i = \pm 1\} <ij>}(1 + t_{ij} S_i S_j).
\]  
(106)

$t_{ij} = t_x$ for horizontal bonds and $t_{ij} = t_y$ for vertical bonds, where $t_x = tanh(K_x), t_y = tanh(K_y)$. The diagrams used are similar, but now we have to treat subclasses with different numbers of horizontal and vertical bonds, so that,

\[
-\beta F = ln(Z) = \frac{zN}{2}ln(Cosh(K)) + Nln(2) + ln[1 + Nt^4 + 2Nt^6 + N(N + \frac{9}{2})t^8 + O(t^{10})]
\]  
(107)

becomes

\[
-\beta F = N[ln(2) + ln(Cosh(K_x)) + ln(Cosh(K_y))] + t_x^2 t_y^2 + t_x^2 t_y^2 (t_x^2 + t_y^2) + \frac{5}{2}(t_x^2 t_y^4) + t_x^2 t_y^4 + t_x^2 t_y^2 + ...]
\]  
(108)

Similarly, the extension of the low temperature expansion,

\[
Z = \sum_{\{S_i = \pm 1\} <ij>} e^{K S_i S_j} = e^{KzN[1 + Ns^4 + 2Ns^6 + N(N + \frac{9}{2})s^8 + O(s^{10})]}
\]  
(109)

to the anisotropic case leads to,

\[
-\beta F = N[K_x + K_y + s_x^2 s_y^2 + s_x^2 s_y (s_x^2 + s_y^2) + \frac{5}{2}s_x^4 s_y^4 + s_x^2 s_y^6 + s_x^2 s_y^2...]
\]  
(110)

where $s_x = e^{-2K_x}, s_y = e^{-2K_y}$. Duality holds for both x and y directions.
Assigned Problem 11. Find the second virial coefficient for four cases: (i) the classical hard sphere gas; (ii) non-interacting Fermions; (iii) non-interacting Bosons; (iv) the van der Waals gas.

Solution

\[ \frac{P v}{k_B T} = \sum_{l=1}^{\infty} a_l(T) \left( \frac{\lambda^3}{v} \right)^{l-1} \]  

(111)

where the first virial coefficient \( a_1(T) = 1 \), and the second virial coefficient is \( a_2(T) \). The virial expansion is most often carried out in the grand canonical ensemble, where we may write,

\[ \frac{P v}{k_B T} = \frac{1}{\lambda^3} \sum_{l=1}^{\infty} b_l z^l; \quad N / V = \frac{1}{\lambda^3} \sum_{l=1}^{\infty} l b_l z^l \]  

(112)

so that,

\[ \frac{P v}{k_B T} = \frac{\sum_{l=1}^{1} b_l z^l}{\sum_{l=1}^{\infty} l b_l z^l} = \sum_{l=1}^{\infty} a_l(T) \left( \frac{\lambda^3}{v} \right)^{l-1} \]  

(113)

which gives relations between the quantities \( a_l(T) \) and \( b_l(T) \). For the second virial coefficient the relationship is \( a_2(T) = -b_2(T) \). We have already calculated the coefficients \( b_l \) for the ideal Bose and Fermi gases, with the results,

\[ b_l = \frac{(-1)^{l+1}}{l^{5/2}}; \quad \text{(Ideal Fermi)} \]  

\[ b_l = \frac{1}{l^{5/2}}; \quad \text{(Ideal Bose)} \]  

(114)

so we have,

\[ \frac{P v}{k_B T} = 1 - \frac{1}{25/2} \frac{(\lambda^3 / v)^{5/2}}{} + \ldots; \quad \text{(Ideal Bose)} \]  

(115)

and

\[ \frac{P v}{k_B T} = 1 + \frac{1}{25/2} \frac{(\lambda^3 / v)^{5/2}}{} + \ldots; \quad \text{(Ideal Fermi)} \]  

(116)

The van der Waals equation of state may be expanded to find the second virial coefficient,

\[ P = \frac{k_B T}{v - b} - \frac{a^2}{v} \]  

so that

\[ \frac{P v}{k_B T} = \frac{1}{(1 - b / v)} - \frac{a}{k_B TV} \approx 1 + b - a / k_B T v + \ldots \]  

(117)

For the classical interacting gas, \( b_2 \) is given by,

\[ b_2 = \frac{1}{2V\lambda^3} \int d^3 r_1 \int d^3 r_2 \left[ e^{-\beta a (\vec{r}_1 - \vec{r}_2)} - 1 \right] = \frac{1}{2V^3} \int d^3 r \left[ e^{-\beta a (\vec{r})} - 1 \right] \]  

(118)

For the hard sphere problem, with a hard core radius of \( R \), we then find that \( b_2 = -2\pi R^3/(3\lambda^3) \), so the virial expansion for this case is

\[ \frac{P v}{k_B T} = 1 + \frac{2\pi R^3}{3v} + \ldots \]  

(119)

The behavior of the second virial coefficient as a function of temperature can be used to deduce the interaction potential, and the importance of quantum effects as they have different temperature dependences.

Assigned Problem 12. The BCS pairing Hamiltonian is a simplified model in which only pairs with zero center of mass momentum are included in the analysis. We also assume that the fermion pairing that leads to superconductivity occurs in the singlet channel. The BCS Hamiltonian is then,

\[ H_{pair} - \mu N = \sum_{k\sigma} (\epsilon_{k\sigma} - \mu) a_{k\sigma}^\dagger a_{k\sigma} + \sum_{k\ell} V_{k\ell} a_{k\uparrow}^\dagger a_{\ell\downarrow}^\dagger a_{-k\downarrow} a_{-\ell\uparrow}, \]  

(120)
where \( N = \sum_{k,\sigma} n_{k,\sigma} \) is the number of electrons in the Fermi sea. By making an expansion in the fluctuations and defining,

\[
b_k = \langle a_{-\vec{k},\downarrow} a_{\vec{k},\uparrow} \rangle, \quad \text{and} \quad b_k^* = \langle a_{\vec{k},\uparrow} a_{-\vec{k},\downarrow} \rangle.
\]  

(121)

where \( b_k^* \) is the average number of pairs in the system at wavevector \( \vec{k} \), show that the mean field BCS Hamiltonian is given by,

\[
H_{MF} - \mu N = \sum_{k,\sigma} (\epsilon_k - \mu) a_{k,\sigma}^\dagger a_{k,\sigma} + \sum_{\vec{k},\ell} V_{\vec{k}\ell} (a_{\vec{k},\uparrow}^\dagger a_{\vec{k},\downarrow}^\dagger b_{\ell} - b_{\ell}^* a_{-\vec{k},\downarrow} a_{\vec{k},\uparrow} - b_{\ell}^* b_{\ell}^*).
\]  

(122)

This is the Hamiltonian that we will solve to find the thermodynamic behavior of superconductors, using an atomistic model.

**Assigned Problem 13.** The BCS pairing Hamiltonian is a simplified model in which only pairs with zero center of mass momentum are included in the analysis. We also assume that the fermion pairing that leads to superconductivity occurs in the singlet channel. The BCS Hamiltonian is then,

\[
H_{pair} - \mu N = \sum_{k,\sigma} (\epsilon_k - \mu) a_{k,\sigma}^\dagger a_{k,\sigma} + \sum_{\vec{k},\ell} V_{\vec{k}\ell} (a_{\vec{k},\uparrow}^\dagger a_{\vec{k},\downarrow}^\dagger b_{\ell} - b_{\ell}^* a_{-\vec{k},\downarrow} a_{\vec{k},\uparrow} - b_{\ell}^* b_{\ell}^*),
\]  

(123)

where \( N = \sum_{k,\sigma} n_{k,\sigma} \) is the number of electrons in the Fermi sea. Defining,

\[
b_k = \langle a_{-\vec{k},\downarrow} a_{\vec{k},\uparrow} \rangle, \quad \text{and} \quad b_k^* = \langle a_{\vec{k},\uparrow} a_{-\vec{k},\downarrow} \rangle.
\]  

(124)

carry out a leading order expansion in fluctuations, leading to,

\[
H_{MF} - \mu N = \sum_{k,\sigma} (\epsilon_k - \mu) a_{k,\sigma}^\dagger a_{k,\sigma} + \sum_{\vec{k},\ell} V_{\vec{k}\ell} (a_{\vec{k},\uparrow}^\dagger a_{\vec{k},\downarrow}^\dagger b_{\ell} - b_{\ell}^* a_{-\vec{k},\downarrow} a_{\vec{k},\uparrow} - b_{\ell}^* b_{\ell}^*).
\]  

(125)

This is the Hamiltonian that we will solve to find the thermodynamic behavior of superconductors, using an atomistic model.

**Solution.** The mean-field Hamiltonian can be considered as a first order expansion in the fluctuations i.e.

\[
a_{-\vec{k},\downarrow} a_{\vec{k},\uparrow} = \langle a_{-\vec{k},\downarrow} a_{\vec{k},\uparrow} \rangle + [a_{-\vec{k},\downarrow} a_{\vec{k},\uparrow} - \langle a_{-\vec{k},\downarrow} a_{\vec{k},\uparrow} \rangle].
\]  

(126)

Substitution of this into the Hamiltonian, along with the definitions above lead to \( H_{MF} \).

**Assigned Problem 14.** Using the Bogoliubov-Valatin transformation (Eq. 163), show that the mean field BCS Hamiltonian (Eq. (162)) reduces to Eq. (166), provided Equations (167) and (168) are true.

**Solution.** With this transformation, the mean field Hamiltonian looks messy,

\[
H_{MF} - \mu N =
\]

\[
\sum_{k} (\epsilon_k - \mu) (a_{\vec{k},\uparrow}^\dagger a_{\vec{k},\downarrow}^\dagger + a_{\vec{k},\downarrow} a_{\vec{k},\uparrow}) - \sum_{\vec{k}} (\Delta_{\vec{k}} a_{\vec{k},\uparrow}^\dagger a_{-\vec{k},\downarrow}^\dagger + \Delta_{\vec{k}}^* a_{\vec{k},\uparrow} a_{-\vec{k},\downarrow} - b_{\vec{k}}^* \Delta_{\vec{k}}^*) = \sum_{\vec{k}}
\]

\[
(\epsilon_{\vec{k}} - \mu) ([u_{\vec{k}}^{\gamma\gamma} + v_{\vec{k}}^{\gamma\gamma}] + [u_{\vec{k}}^{\gamma\gamma} - v_{\vec{k}}^{\gamma\gamma}]) - \Delta_{\vec{k}} (u_{\vec{k}}^{\gamma\gamma} - v_{\vec{k}}^{\gamma\gamma}) + \Delta_{\vec{k}}^* (u_{\vec{k}}^{\gamma\gamma} + v_{\vec{k}}^{\gamma\gamma}) + b_{\vec{k}}^* \Delta_{\vec{k}}
\]

\[\sum_{\vec{k}} (\epsilon_{\vec{k}} - \mu) (u_{\vec{k}}^{\gamma\gamma} + v_{\vec{k}}^{\gamma\gamma} - u_{\vec{k}}^{\gamma\gamma} - v_{\vec{k}}^{\gamma\gamma}) - \Delta_{\vec{k}} (u_{\vec{k}}^{\gamma\gamma} - v_{\vec{k}}^{\gamma\gamma}) + \Delta_{\vec{k}}^* (u_{\vec{k}}^{\gamma\gamma} + v_{\vec{k}}^{\gamma\gamma}) + b_{\vec{k}}^* \Delta_{\vec{k}}
\]
Expanding this yields,

\[
\sum_{\vec{k}} (\epsilon_{\vec{k}} - \mu) [u_{\vec{k}}^* u_{\vec{k}}^\dagger \gamma_{\vec{k}\uparrow} \gamma_{\vec{k}\downarrow} + v_k^* u_{\vec{k}}^\dagger \gamma_{\vec{k}\downarrow} \gamma_{\vec{k}\uparrow} + v_k^* u_{\vec{k}}^\dagger \gamma_{\vec{k}\downarrow} \gamma_{\vec{k}\downarrow} + v_k^* u_{\vec{k}}^\dagger \gamma_{\vec{k}\downarrow} \gamma_{\vec{k}\uparrow} + v_k^* u_{\vec{k}}^\dagger \gamma_{\vec{k}\downarrow} \gamma_{\vec{k}\downarrow}]
\]

\[
+ (\epsilon_{\vec{k}} - \mu) [u_{\vec{k}}^* u_{\vec{k}}^\dagger \gamma_{\vec{k}\uparrow} \gamma_{\vec{k}\downarrow} - u_{\vec{k}}^* u_{\vec{k}}^\dagger \gamma_{\vec{k}\downarrow} \gamma_{\vec{k}\uparrow} - v_k^* u_{\vec{k}}^\dagger \gamma_{\vec{k}\uparrow} \gamma_{\vec{k}\downarrow} + v_k^* u_{\vec{k}}^\dagger \gamma_{\vec{k}\uparrow} \gamma_{\vec{k}\downarrow} + v_k^* u_{\vec{k}}^\dagger \gamma_{\vec{k}\uparrow} \gamma_{\vec{k}\downarrow}]
\]

\[
- \Delta_{\vec{k}} [u_{\vec{k}}^* u_{\vec{k}}^\dagger \gamma_{\vec{k}\uparrow} \gamma_{\vec{k}\downarrow} - u_{\vec{k}}^* u_{\vec{k}}^\dagger \gamma_{\vec{k}\downarrow} \gamma_{\vec{k}\uparrow} + v_k^* u_{\vec{k}}^\dagger \gamma_{\vec{k}\downarrow} \gamma_{\vec{k}\uparrow} - v_k^* u_{\vec{k}}^\dagger \gamma_{\vec{k}\downarrow} \gamma_{\vec{k}\downarrow}]
\]

\[
- \Delta_{\vec{k}} [u_{\vec{k}}^* u_{\vec{k}}^\dagger \gamma_{\vec{k}\uparrow} \gamma_{\vec{k}\downarrow} + u_{\vec{k}}^* v_k^\dagger \gamma_{\vec{k}\downarrow} \gamma_{\vec{k}\uparrow} - u_{\vec{k}}^* u_{\vec{k}}^\dagger \gamma_{\vec{k}\uparrow} \gamma_{\vec{k}\downarrow} - u_{\vec{k}}^* v_k^\dagger \gamma_{\vec{k}\uparrow} \gamma_{\vec{k}\downarrow}]
\]

We now collect the terms in this expression into three categories: Those which have no operators in them; those which can be reduced to diagonal form i.e. those which are of the form \(\gamma_{\vec{k}\uparrow} \gamma_{\vec{k}\downarrow}\); and those that are off diagonal (e.g. \(\gamma_{\vec{k}\uparrow} \gamma_{\vec{k}\downarrow}\)). The first stage is to collect together the terms which look to be in these three categories. First the constant term,

\[
H_{MF} - \mu N = \sum_{\vec{k}} b_{\vec{k}}^* \Delta_{\vec{k}}
\]

The following terms can be converted to diagonal form,

\[
+ (\epsilon_{\vec{k}} - \mu) [|u_{\vec{k}}|^2 \gamma_{\vec{k}\uparrow} \gamma_{\vec{k}\downarrow} + |v_{\vec{k}}|^2 \gamma_{\vec{k}\downarrow} \gamma_{\vec{k}\uparrow} + |u_{\vec{k}}|^2 \gamma_{\vec{k}\downarrow} \gamma_{\vec{k}\downarrow} + |v_{\vec{k}}|^2 \gamma_{\vec{k}\uparrow} \gamma_{\vec{k}\downarrow}]
\]

\[
- \Delta_{\vec{k}} [u_{\vec{k}}^* v_k^\dagger \gamma_{\vec{k}\uparrow} \gamma_{\vec{k}\downarrow} + v_k^* u_{\vec{k}}^\dagger \gamma_{\vec{k}\downarrow} \gamma_{\vec{k}\uparrow} - u_{\vec{k}}^* u_{\vec{k}}^\dagger \gamma_{\vec{k}\uparrow} \gamma_{\vec{k}\downarrow} - v_k^* v_k^\dagger \gamma_{\vec{k}\uparrow} \gamma_{\vec{k}\downarrow}]
\]

Finally the off-diagonal terms are,

\[
+ (\epsilon_{\vec{k}} - \mu) (u_{\vec{k}}^* u_{\vec{k}}^\dagger - u_{\vec{k}}^* u_{\vec{k}}^\dagger) - \Delta_{\vec{k}} [u_{\vec{k}}^* v_k^\dagger \gamma_{\vec{k}\uparrow} \gamma_{\vec{k}\downarrow} - u_{\vec{k}}^* u_{\vec{k}}^\dagger \gamma_{\vec{k}\uparrow} \gamma_{\vec{k}\downarrow}]
\]

\[
- \Delta_{\vec{k}} [u_{\vec{k}}^* v_k^\dagger \gamma_{\vec{k}\uparrow} \gamma_{\vec{k}\downarrow} - u_{\vec{k}}^* u_{\vec{k}}^\dagger \gamma_{\vec{k}\uparrow} \gamma_{\vec{k}\downarrow} - v_k^* v_k^\dagger \gamma_{\vec{k}\uparrow} \gamma_{\vec{k}\downarrow}]
\]

We have to rearrange the terms categorized as diagonal above, as we need them in the form \(\gamma \gamma^\dagger\). We do this using the commutation relation, i.e. \(\gamma \gamma^\dagger = 1 - \gamma^\dagger \gamma\). This yields,

\[
H_{MF} - \mu N = \sum_{\vec{k}} b_{\vec{k}}^* \Delta_{\vec{k}} + 2(\epsilon_{\vec{k}} - \mu) |v_{\vec{k}}|^2 - \Delta_{\vec{k}} u_{\vec{k}}^* v_{\vec{k}} - \Delta_{\vec{k}} u_{\vec{k}}^* u_{\vec{k}}^\dagger
\]

\[
+ (\epsilon_{\vec{k}} - \mu) [u_{\vec{k}}^* u_{\vec{k}}^\dagger \gamma_{\vec{k}\uparrow} \gamma_{\vec{k}\downarrow} - |v_{\vec{k}}|^2 \gamma_{\vec{k}\downarrow} \gamma_{\vec{k}\uparrow} + u_{\vec{k}}^* u_{\vec{k}}^\dagger \gamma_{\vec{k}\uparrow} \gamma_{\vec{k}\downarrow} - |v_{\vec{k}}|^2 \gamma_{\vec{k}\uparrow} \gamma_{\vec{k}\downarrow}]
\]

\[
+ \Delta_{\vec{k}} [u_{\vec{k}}^* v_k^\dagger \gamma_{\vec{k}\uparrow} \gamma_{\vec{k}\downarrow} + v_k^* u_{\vec{k}}^\dagger \gamma_{\vec{k}\downarrow} \gamma_{\vec{k}\uparrow} + \Delta_{\vec{k}} [u_{\vec{k}}^* v_k^\dagger \gamma_{\vec{k}\downarrow} \gamma_{\vec{k}\uparrow} + v_k^* u_{\vec{k}}^\dagger \gamma_{\vec{k}\uparrow} \gamma_{\vec{k}\downarrow}]
\]

Finally the off-diagonal terms are (as before),

\[
+ (\epsilon_{\vec{k}} - \mu) (u_{\vec{k}}^* v_k^\dagger \gamma_{\vec{k}\downarrow} \gamma_{\vec{k}\uparrow} - u_{\vec{k}}^* v_k^\dagger \gamma_{\vec{k}\uparrow} \gamma_{\vec{k}\downarrow} + v_k^* u_{\vec{k}}^\dagger \gamma_{\vec{k}\uparrow} \gamma_{\vec{k}\downarrow} - v_k^* u_{\vec{k}}^\dagger \gamma_{\vec{k}\uparrow} \gamma_{\vec{k}\downarrow})
\]

\[
- \Delta_{\vec{k}} [u_{\vec{k}}^* v_k^\dagger \gamma_{\vec{k}\uparrow} \gamma_{\vec{k}\downarrow} - u_{\vec{k}}^* v_k^\dagger \gamma_{\vec{k}\downarrow} \gamma_{\vec{k}\uparrow} + \Delta_{\vec{k}} [u_{\vec{k}}^* v_k^\dagger \gamma_{\vec{k}\downarrow} \gamma_{\vec{k}\uparrow} - (v_k^*)^2 \gamma_{\vec{k}\uparrow} \gamma_{\vec{k}\downarrow}]
\]

We note that \(n_{\vec{k}\uparrow} = n_{\vec{k}\downarrow}\), and that the expectation of other terms that transform into one another through the transformation \(\vec{k} \rightarrow -\vec{k}\), are equivalent. Collecting terms then leads to Eqs. (166)-(168) of the lecture notes.
Assigned Problem 15. We define
\[ v_k = \frac{g_k}{(1 + |g_k|^2)^{1/2}} \]  
show that Eq. (167) reduces to (173).

Solution Starting with,
\[ 2(\epsilon_k - \mu)(1 - |v_k|^2)^{1/2}v_k + \Delta_k v_k^2 - \Delta_k^*(1 - |v_k|^2) = 0, \]  
We have,
\[ |u_k|^2 = 1 - |v_k|^2; \quad u_k = \frac{1}{(1 + |g_k|^2)^{1/2}}. \]  
Substitution into Eq. (128) leads to,
\[ 2(\epsilon_k - \mu)g_k + \Delta_k g_k^2 - \Delta_k^* = 0. \]  

Assigned Problem 16. Show that \( E_k \) as defined in Eq. (174) is in agreement with Eq. (168).

Solution We need to show that the definitions,
\[ E_k = (\epsilon_k - \mu)(|u_k|^2 - |v_k|^2) + \Delta_k u_k^*v_k + \Delta_k^* u_k v_k, \]  
and
\[ E_k = [(\epsilon_k - \mu)^2 + |\Delta_k|^2]^{1/2}, \]  
are the same. To do this we use the results of Problem 9 in Eq. (53) to write,
\[ E_k = (\epsilon_k - \mu)[\frac{E_k + (\epsilon_k - \mu)^2}{4E_k^2} - \frac{E_k - (\epsilon_k - \mu)^2}{4E_k^2}] + \Delta_k \frac{\Delta_k^*}{2E_k} + \Delta_k^* \Delta_k \frac{1}{2E_k}, \]
which reduces to Eq. (54) as required.

Assigned Problem 17. Prove the relations Eq. (175-177).

Solution We have,
\[ g_k = \frac{E_k - (\epsilon_k - \mu)}{\Delta_k}; \quad E_k = [(\epsilon_k - \mu)^2 + |\Delta_k|^2]^{1/2}, \]
so that,
\[ |\Delta_k|^2 = E_k^2 - (\epsilon_k - \mu)^2; \]
so that,
\[ |g_k|^2 = \frac{E_k - (\epsilon_k - \mu)}{\Delta_k} = \frac{|E_k - (\epsilon_k - \mu)|^2}{E_k^2 - (\epsilon_k - \mu)^2} = \frac{E_k - (\epsilon_k - \mu)}{E_k + (\epsilon_k - \mu)} \]
We then find,
\[ |v_k|^2 = \frac{|g_k|^2}{1 + |g_k|^2} = \frac{E_k - (\epsilon_k - \mu)}{2E_k}; \quad |u_k|^2 = \frac{E_k + (\epsilon_k - \mu)}{2E_k} \]
and hence,
\[ u_k v_k^* = \frac{g_k}{1 + |g_k|^2} = \frac{\Delta_k^*}{2E_k} \]