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Michael Plischke
Simon Fraser University

Birger Bergersen
University of British Columbia
EQUILIBRIUM STATISTICAL PHYSICS, 2nd Edition
SOLUTIONS MANUAL

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Chapter 1

Review of
Thermodynamics

1.1.

We assume that the energy is a function of $N$ and $T$ and refer to Figure 1.1 in the text. Then

$$Q_1 = \int_{V_A}^{V_B} P \, dV = N k_B T_1 \ln \frac{V_B}{V_A}$$

$$Q_2 = N k_B T_2 \ln \frac{V_D}{V_C}.$$ 

Along an adiabat $TV^{\gamma-1} = \text{const.}$, with $\gamma = C_P/C_V$. It follows that

$$\ln V_A - \ln V_D = \ln V_B - \ln V_C$$

$$\ln \frac{V_D}{V_C} = - \ln \frac{V_B}{V_A}$$

and we get the desired result

$$\eta = \frac{Q_1 + Q_2}{Q_1} = 1 - \frac{T_2}{T_1}.$$
1.2

(a)

For a reversible process in a magnetic system we have \( dQ = TdS = dE - HdM \)
and \( A = E - TS \) with \( dA = -SdT + HdM \). Therefore
\[
\left( \frac{\partial S}{\partial M} \right)_T = - \left( \frac{\partial H}{\partial T} \right)_M = - \frac{H}{T}
\]
where the last step follows from the equation of state. Differentiation of \( E = A + TS \) with respect to \( M \) yields
\[
\left( \frac{\partial E}{\partial M} \right)_T = T \left( \frac{\partial S}{\partial M} \right)_T + H = 0.
\]

Therefore \( E(M, T) = E(T) \).

Consider an adiabatic reversible process:
\[
TdS = 0 = \left( \frac{\partial E}{\partial T} \right)_M dT - HdM
= C_M(T) dT - \frac{MT}{C} dM.
\]

Integrating, we find
\[
\frac{M^2}{2C} \bigg|^{f}_i = \int_{T_i}^{T_f} dT \left( \frac{C_M(T)}{T} \right).
\]

To make further progress, we may assume that the specific heat \( C_M \) is constant.

With this we have
\[
\frac{1}{T} \exp \frac{M^2}{2CC_M} = \text{const.}
\]
along an adiabat.

(b)

Assume that the four end-points of the Carnot cycle are given by \((H_1, T_1), (H_2, T_1), (H_3, T_2), (H_4, T_2)\). Along the isotherm at temperature \( T_1 \) we have
\[
\Delta Q_{1 \rightarrow 2} = - \int_1^2 HdM = -C \frac{H_2^2 - H_1^2}{2T_1}.
\]
Similarly,
\[ \Delta Q_{3 \rightarrow 4} = -C \frac{H_4^2 - H_3^2}{2T_2} \cdot \]

Therefore,
\[ \eta = 1 + \frac{T_1}{T_2} \frac{(H_4^2 - H_3^2)}{(H_2^2 - H_1^2)} \]

Along the adiabat connecting points 2 and 3, e.g. we have, since the energy is a function of \( T \) only
\[ \int_2^3 \frac{dE(T)}{T} = \phi(T_2, T_1) = \frac{1}{C} \int dMM = \frac{C}{2} \left( \frac{H_3^2}{T_2^2} - \frac{H_2^2}{T_1^2} \right) . \]

Similarly,
\[ \int_4^1 \frac{dE(T)}{T} = -\phi(T_2, T_1) = \frac{C}{2} \left( \frac{H_1^2}{T_1^2} - \frac{H_4^2}{T_2^2} \right) \]

where \( \phi \) is an unknown function. Adding, we obtain
\[ 0 = \frac{C}{2} \left[ \frac{H_3^2 - H_4^2}{T_2^2} + \frac{H_1^2 - H_2^2}{T_1^2} \right] . \]

Substituting into the expression for \( \eta \) we obtain
\[ \eta = 1 - \frac{T_2}{T_1} . \]

Notice that in this derivation we did not need to assume that \( C_M \) is independent of \( T \).

1.3.

Consider a system of fixed volume in contact with a reservoir at fixed temperature \( T_0 \) and chemical potential \( \mu_0 \). This system can exchange energy and particles with the reservoir. Fluctuations in \( S \) and \( N \) can only increase the grand potential
\[ \Omega(\mu, V, T) = E(S, V, N) - T_0 S - \mu_0 N . \]

Thus
\[ \delta \Omega = \delta S \left[ \left( \frac{\partial E}{\partial S} \right)_{V,N} - T_0 \right] + \delta N \left[ \left( \frac{\partial E}{\partial N} \right)_{V,S} - \mu_0 \right] \]
\[ + \frac{1}{2} \delta S^2 \frac{\partial^2 E}{\partial S^2} + \delta S \delta N \frac{\partial^2 E}{\partial S \partial N} + \frac{1}{2} \delta N^2 \frac{\partial^2 E}{\partial N^2} + \ldots \geq 0. \]

At equilibrium the first order terms are zero, requiring the second order terms to be positive semi-definite yields

\[ \frac{\partial^2 E}{\partial S^2} = \frac{\partial T}{\partial S} \geq 0 \quad \rightarrow \quad C_{V,N} \geq 0 \]
\[ \frac{\partial^2 E}{\partial N^2} = \frac{\partial \mu}{\partial N} \geq 0 \quad \rightarrow \quad \left( \frac{\partial N}{\partial \mu} \right)_{V,S} \geq 0 \]
\[ \frac{\partial^2 E}{\partial S^2} \frac{\partial^2 E}{\partial N^2} - \left( \frac{\partial^2 E}{\partial S \partial N} \right)^2 \geq 0 \quad \rightarrow \quad \frac{C_{V,N}}{T} \frac{\partial N}{\partial \mu} \leq \left( \frac{\partial S}{\partial \mu} \right)^2. \]

1.4.

The definitions

\[ C_M = T \left( \frac{\partial S}{\partial T} \right)_M \]
\[ C_H = T \left( \frac{\partial S}{\partial T} \right)_H \]
\[ \chi_T = T \left( \frac{\partial M}{\partial H} \right)_T \]
\[ \chi_S = T \left( \frac{\partial M}{\partial H} \right)_S \]

together with the Maxwell relation

\[ \left( \frac{\partial S}{\partial H} \right)_T = \left( \frac{\partial M}{\partial T} \right)_H \]

when substituted into the chain rule formula

\[ \left( \frac{\partial S}{\partial T} \right)_H = \left( \frac{\partial S}{\partial T} \right)_M + \left( \frac{\partial S}{\partial M} \right)_T \left( \frac{\partial M}{\partial T} \right)_H \]

gives the desired result

\[ C_H - C_M = \frac{T}{\chi_T} \left( \frac{\partial M}{\partial T} \right)_H^2. \quad (1.1) \]

To obtain the second formula we apply the chain rule expression

\[ \left( \frac{\partial M}{\partial H} \right)_T = \left( \frac{\partial M}{\partial H} \right)_S + \left( \frac{\partial M}{\partial S} \right)_H \left( \frac{\partial S}{\partial H} \right)_T \]

to obtain

\[ C_H(\chi_T - \chi_S) = T \left( \frac{\partial S}{\partial T} \right)_H \left( \frac{\partial M}{\partial S} \right)_H \left( \frac{\partial S}{\partial H} \right)_T = \]
\[ -T \left( \frac{\partial M}{\partial T} \right)_H \frac{\partial^2 G}{\partial H \partial T} = T \left( \frac{\partial M}{\partial T} \right)_H^2 \]

from which we find

\[ \chi_T - \chi_S = \frac{T}{C_H} \left( \frac{\partial M}{\partial T} \right)_H^2. \tag{1.2} \]

Finally, by combining (1.1) with (1.2) we find

\[ \chi_T (C_H - C_M) = C_H (\chi_T - \chi_H) \]

or

\[ \frac{\chi_T}{\chi_H} = \frac{C_H}{C_M}. \]

1.5.

(a)

Along part of the straight line segment the system will absorb heat, while the system will expel heat during the remaining part of the segment. The resolution of the apparent paradox is that while

\[
\text{work} = \text{absorbed heat} - | \text{expelled heat} | = Q_{12}
\]

\[ \eta = \frac{\text{work}}{\text{absorbed heat}} < 1. \]

(b)

We have \( C_V = \frac{3}{2} N k_B, \gamma = C_P/C_V = \frac{5}{3}. \) Along the straight line segment

\[ P = P_1 + (V - V_1) \frac{P_2 - P_1}{V_2 - V_1} \]

and

\[ dQ = PdV + C_VdT. \]

We define

\[
v = \frac{V}{V_1}; \quad r = \frac{V_2}{V_1}; \quad p = \frac{P}{P_1}; \quad t = \frac{T}{T_1}; \quad q = \frac{Q}{P_1 V_1}; \quad c = \frac{C_V}{N k_B}\]

and introduce

\[ z = \frac{\partial q}{\partial v} = (1 + c)p + cv \frac{dp}{dv}. \]
If \( z = 0 \) for \( u = x \) we find
\[
\eta = \frac{\int_1^r zdv}{\int_1^x zdv}.
\]
Numerically we find \( x = 1.537 \) and \( \eta = 0.259 \)

### 1.6.

The heat absorbed by the working substance in the step \( B \to C \) is \( Q_{B\to C} = C_P(T_C - T_B) \) and during \( D \to A \) it is \( Q_{D\to A} = C_P(T_A - T_D) \). The efficiency of the cycle is thus
\[
\eta = 1 + \frac{T_A - T_D}{T_C - T_B}.
\] (1.3)

Along an adiabat \( P^{1/\gamma} = \text{const.} \) where \( \gamma = C_P/C_V \). Therefore
\[
T_B = T_A \left( \frac{P_B}{P_A} \right)^{\frac{\gamma - 1}{\gamma}}
\]
\[
T_C = T_D \left( \frac{P_B}{P_A} \right)^{\frac{\gamma - 1}{\gamma}}.
\] (1.4)

If we substitute (1.4) into (1.3) we get the desired result.

### 1.7.

We have
\[
\alpha = \frac{1}{V} \left( \frac{\partial V}{\partial T} \right)_P = \frac{1}{V} \left( \frac{\partial}{\partial T} \frac{Nk_BT}{P} \right)_P = \frac{1}{T}
\] (1.5)
\[
\kappa_T = -\frac{1}{V} \left( \frac{\partial V}{\partial P} \right)_T = -\frac{1}{V} \left( \frac{\partial}{\partial P} \frac{Nk_BT}{P} \right)_T = \frac{1}{P}.
\] (1.6)

Combining (1.5) and (1.6) gives
\[
C_P - C_V = \frac{TV}{\kappa_T} \alpha^2 = Nk_B.
\]

### 1.8.

Since the added gas is inert, we can take take the Gibbs free energy in the gas phase to be equal to the sum of the Gibbs free energies of the two components,
evaluated at their respective partial pressures. At constant temperature small changes in the Gibbs free energy can be written \( \Delta g = v \Delta P \) where \( v \) is the volume per particle. For the system to remain in equilibrium, the change in chemical potential in the gas and liquid phases must remain the same. Thus

\[
\Delta \mu_L = v_L (P_i + \delta P) = \Delta \mu_g = v_g \delta P.
\]

Assuming that \( \delta P \ll P_i \ll P \) and \( v_g = k_B T / P \) we get the desired result

\[
\frac{\delta P}{P} = \frac{P_i v_L}{k_B T}.
\]

1.9.

Connect the two thermodynamic states by a reversible process, i.e. for gas \( A \) consider an isothermal expansion. Thus

\[
\Delta S_A = \int_{V_A}^{V_A + V_B} dV \frac{N_A k_B T}{V} = N_A k_B \ln \frac{V_A + V_B}{V_A}.
\]

A similar expression is obtained for gas \( B \) and we find for the entropy of mixing

\[
\Delta S = \frac{P}{T} \left( V_A \ln \frac{V}{V_A} + V_B \ln \frac{V}{V_B} \right).
\]

1.10

(a)

To show that in equilibrium the energy must be a minimum, consider the following argument. Suppose that we have an equilibrium state at volume \( V \) and entropy \( S \) in which the energy \( E \) is greater than \( E_{\text{min}} \), the minimum value of the energy compatible with the given values of the parameters. Extract \( E - E_{\text{min}} \) from the system by doing work on some other system. We can then return this energy in the form of heat. This will raise the entropy, implying that the initial state with \( E \) and \( V \) was not the state of maximum entropy and therefore not an equilibrium state.
Another way of at least partially demonstrating that \( E \) is a concave function is the following argument. The relation \( S(E + \Delta E) + S(E - \Delta E) - 2S(E, V) \leq 0 \) implies that any straight line connecting \( S(E_1) \) and \( S(E_2) \) lies below the curve \( S(E) \). By simply flipping the \( E \) and \( S \) axes one immediately sees that any straight line connecting \( E(S_1) \) and \( E(S_2) \) must lie above the curve \( E(S) \). The local convexity conditions on the energy are then

\[
\frac{\partial^2 E}{\partial S^2} \geq 0 \quad \frac{\partial^2 E}{\partial V^2} \geq 0 \quad \frac{\partial^2 E}{\partial S^2} \frac{\partial^2 E}{\partial V^2} - \left( \frac{\partial^2 E}{\partial S \partial V} \right)^2 \geq 0.
\]

(b)

We will prove that \( G \) is a concave function of \( P \) and \( T \) using the local conditions. We have \( A = E - TS \) and

\[
\frac{\partial^2 A}{\partial T^2} = -\left( \frac{\partial S}{\partial T} \right)_V = -\left( \frac{\partial^2 E}{\partial S^2} \right)_V \leq 0.
\]

Similarly, \( \partial^2 A / \partial V^2 \geq 0 \). A further Legendre transformation yields the Gibbs potential \( G = A + PV \) which has the properties

\[
\left( \frac{\partial^2 G}{\partial P^2} \right)_T = \left( \frac{\partial P}{\partial V} \right)^{-1} = -\left( \frac{\partial^2 A}{\partial V^2} \right)_T \leq 0
\]

and

\[
\left( \frac{\partial^2 G}{\partial T^2} \right)_P \leq 0
\]

which shows that \( G \) is a concave function of \( P \) and \( T \) separately. To show that the cross-derivatives satisfy the appropriate inequality we proceed somewhat indirectly. From part (a) we have

\[
\left( \frac{\partial^2 E}{\partial V^2} \right)_S = -\left( \frac{\partial P}{\partial V} \right)_S \geq 0.
\]

Let \( V = V(P, T) \). Then

\[
\left( \frac{\partial V}{\partial P} \right)_S = \left( \frac{\partial V}{\partial P} \right)_T + \left( \frac{\partial V}{\partial T} \right)_P \left( \frac{\partial T}{\partial P} \right)_S = \left( \frac{\partial^2 G}{\partial P^2} \right)_T + \left( \frac{\partial^2 G}{\partial P \partial T} \right)_P \left( \frac{\partial T}{\partial P} \right)_S.
\]
From the enthalpic Maxwell relations we have
\[
\left( \frac{\partial T}{\partial P} \right)_S = \left( \frac{\partial V}{\partial S} \right)_P
\]
and
\[
\left( \frac{\partial V}{\partial S} \right)_P = \left( \frac{\partial V}{\partial T} \right)_P \left( \frac{\partial S}{\partial T} \right)_P^{-1} = -\frac{\partial^2 G}{\partial T \partial P} \left( \frac{\partial^2 G}{\partial T^2} \right)^{-1}.
\]
Therefore
\[
-\left( \frac{\partial V}{\partial P} \right)_S = \frac{G_{PP}G_{TT} - G_{TP}^2}{G_{TT}} \geq 0
\]
where the subscripts indicate partial differentiation with respect to those variables. Since \( G_{TT} \leq 0 \) we obtain
\[
G_{PP}G_{TT} - G_{TP}^2 \leq 0
\]
which completes the proof that \( G \) is a concave function of \( P \) and \( T \).

1.11.

(a)

We combine
\[
T = \left( \frac{\partial E}{\partial S} \right)_{NV} = \frac{Ed}{Nk_B}
\]
and
\[
P = -\left( \frac{\partial E}{\partial V} \right)_{SN} = \frac{Ed}{V}
\]
to get \( PV = Nk_BT \).

(b)

Using (1.7) we find
\[
P(S, V, N) = \text{const } d \left( \frac{N}{V} \right)^{d+1} \exp \left[ \frac{dS}{Nk_B} \right]
\]
and find that \( \gamma = d + 1 \). Also, from \( E = Nk_BT/d \) we find \( C_V = Nk_B/d \) and \( C_P = \gamma C_V = Nk_B(d + 1)/d \).
Chapter 2

Statistical Ensembles

2.1

(a)

Let

\[ p = r \cos \phi; \quad q = r \sin \phi. \]

The constant energy surface \( \Gamma(E) \) in the \( q - p \) plane is the circle \( r = \text{const.} \). The equations of motion can be written

\[ \dot{r} = 0; \quad \dot{\phi} = 1 = \text{const}, \]

i.e., the phase space point moves with constant velocity and covers the whole "surface". It thus spends equal time in all regions of \( \Gamma(E) \).

(b)

The solutions to the equations of motion can be written

\[ q_1 = r_1 \sin \phi_1 + r_2 \sin \phi_2 \]
\[ q_2 = r_1 \sin \phi_1 - r_2 \sin \phi_2 \]
where \( r_1, r_2 \) are constants of the motion and

\[
\begin{align*}
\phi_1 &= \sqrt{\frac{3}{2} t} + \phi_1(0) \\
\phi_2 &= \sqrt{\frac{1}{2} t} + \phi_2(0).
\end{align*}
\]

The projection of the constant energy surface on the \( r_1, r_2 \) surface is the ellipse

\[
\frac{3}{4} r_1^2 + \frac{1}{4} r_2^2 = \text{const}.
\]

However, with given initial conditions only a single point on this ellipse is visited.

### 2.2.

(a)

Without the \( N! \) factor in the denominator the general expression for \( \Omega \) becomes

\[
\Omega(E,V,N) = \frac{V^N}{h^{3N}} \frac{(2m\pi E)^{3N/2}}{(\frac{3N}{2} - 1)!} \frac{\delta E}{E}.
\]

The general expression for the entropy is thus

\[
S(E,V,N) = Nk_B \ln V + \frac{3N}{2} k_B \ln \frac{4\pi m E}{3N\hbar^2} + \frac{3}{2} Nk_B. \quad (2.1)
\]

Before the partition is removed the entropy is

\[
S_A + S_B = 2S(E,V,N) = 2Nk_B \ln V + 3Nk_B \ln \frac{4\pi m E}{3N\hbar^2} + 3Nk_B. \quad (2.2)
\]

While after the partition is removed we have for the entropy

\[
S_{A+B} = S(2E,2V,2N) = 2Nk_B \ln 2V + 3Nk_B \ln \frac{4\pi m E}{3N\hbar^2} + 3Nk_B. \quad (2.3)
\]

Comparison of (2.3) and (2.2) gives

\[
S_{A+B} = S_A + S_B + 2Nk_B \ln 2
\]

which is the desired result.
(b)

With the N! factor in the expression for Ω we get the correct expression for entropy

\[ S(E, V, N) = Nk_B \ln \frac{V}{N} + \frac{3N}{2} k_B \ln \frac{4\pi mE}{3Nh^2} + \frac{5}{2} Nk_B . \]  

(2.4)

and

\[ S_{A+B} = S(2E, 2V, 2N) = S_A + S_B = 2S(E, V, N) . \]

(c)

The entropy of mixing is

\[ 2S(E, 2V, N) - 2S(E, V, N) = 2Nk_B \ln 2 = 2R \ln 2 \]

if \( N = N_{\text{Avogadro}}. \)

2.3

(a)

The partition function for a single oscillator is given by

\[ Z_c(T) = \frac{1}{\hbar} \int_{-\infty}^{\infty} dp \int_{-\infty}^{\infty} dq \exp \left\{ -\beta \left[ \frac{p^2}{2m} + \frac{Kq^2}{2} \right] \right\} = \sqrt{\frac{2m\pi k_B T}{\hbar^2}} \sqrt{\frac{2\pi k_B T}{K}} . \]

From

\[ \langle E \rangle = -\frac{\partial \ln Z_c}{\partial \beta} \]

we obtain

\[ \langle E \rangle = k_B T . \]

As well,

\[ -\frac{\partial \langle E \rangle}{\partial \beta} = \langle (E - \langle E \rangle)^2 \rangle = (k_B T)^2 . \]
The pressure $P(V/N, T)$ is given by the equation

$$\beta P(V/N, T) = -\frac{\partial}{\partial V} \ln \int d^{3N} r \exp\{-\beta U(r_1, r_2, \cdots, r_N)\}.$$  

(2.5)

Make the change of variables $r_j = \lambda r'_j$ in the integral on the right hand side. The factor $\lambda^{-3N}$ from the differential is irrelevant. The range of each integral is now reduced by a factor of $\lambda$. Using the scaling property of the potential energy we obtain

$$\beta P(V/N, T) = \lambda^{-3} P(V\lambda^{-3}/N, T\lambda^{-\gamma}).$$

Since $\lambda$ is arbitrary we may take it to be $T^{1/\gamma}$, which yields

$$P(V/N, T) = T^{1-3/\gamma} P(VT^{-3/\gamma}/N, 1) = T^{1-3/\gamma} f \left( \frac{V}{NT^{3/\gamma}} \right)$$

which is the desired result. The function $f$ can in principle be calculated from (2.5).

2.4

(a)

The first step is to rewrite the Hamiltonian in terms of canonical coordinates and momenta. Using $p_\theta = I \dot{\theta}$ and $p_\phi = I \sin^2 \theta \dot{\phi}$ we have, for the rotational part of $H$

$$H_{\text{rot}} = \frac{p_\theta^2}{2I} + \frac{p_\phi^2}{2I \sin^2 \theta} - \mu E \cos \theta.$$ 

The rotational partition function is given by

$$Z_{\text{rot}} = \frac{1}{\hbar^2} \int_0^{\pi} d\theta \int_0^{2\pi} d\phi \int_{-\infty}^{\infty} dp_\theta \int_{-\infty}^{\infty} dp_\phi e^{-\beta H_{\text{rot}}} = \frac{4\pi^2 I}{\beta \hbar^2} \int_0^{\pi} d\theta \sin \theta e^{\beta \mu E \cos \theta}$$

where the integrations over $\phi$ and the momentum variables have been carried out. With the change of variable $x = \cos \theta$ one easily performs the remaining integral to obtain the desired result.
(b) The polarization is given by

\[ P = \frac{N}{V} k_B T \frac{\partial}{\partial E} \ln Z_{\text{rot}} = \frac{N}{V} \left( \mu \coth(\beta \mu E) - \frac{k_B T}{E} \right). \]

(c) The low field, or high temperature, expression for the dielectric constant is simply obtained using the expansion \( \coth x \approx \frac{1}{x} + \frac{x}{3} + \cdots \) for small \( x \).

2.5

The grand partition function may be written as

\[ Z_G = \sum_N \int_{-\infty}^{\infty} \frac{dE}{\delta E} \exp\{\beta [TS(E, V, N) - E + \mu N]\}. \quad (2.6) \]

We assume that the contributions to the sum and integral come primarily from the region around \( N = \langle N \rangle \) and \( E = \langle E \rangle \) where the integrand attains its maximum value. Expanding around this point we obtain

\[ TS(E, V, N) - E + \mu N = TS(\langle E \rangle, V, \langle N \rangle) - \langle E \rangle + \mu \langle N \rangle \]

\[ + \frac{1}{2} (E - \langle E \rangle)^2 \frac{\partial^2 S}{\partial E^2} + \frac{1}{2} (N - \langle N \rangle)^2 \left( \frac{\partial^2 S}{\partial N^2} \right) + (E - \langle E \rangle)(N - \langle N \rangle) \left( \frac{\partial^2 S}{\partial N \partial E} \right) + \cdots \quad (2.7) \]

Substitution of (2.7) into (2.6) and approximating the sum over \( N \) by an integral yields

\[ Z_G = \exp(\beta [TS(\langle E \rangle, V, \langle N \rangle) - \langle E \rangle + \mu \langle N \rangle]) \times I \]

where

\[ I = \int_{-\infty}^{\infty} \frac{dE}{\delta E} \frac{dN}{\delta E} e^{-\frac{1}{k_B} [(E - \langle E \rangle)^2 \left( \frac{\partial^2 S}{\partial E^2} \right) + (N - \langle N \rangle)^2 \left( \frac{\partial^2 S}{\partial N^2} \right) + 2(E - \langle E \rangle)(N - \langle N \rangle) \left( \frac{\partial^2 S}{\partial N \partial E} \right) + \cdots]} \]

The Gaussian integrals can be evaluated and we are left with

\[ I = \frac{2\pi}{\delta E \sqrt{\left( \frac{\partial^2 S}{\partial N \partial E} \right)^2 - \left( \frac{\partial^2 S}{\partial E^2} \right) \left( \frac{\partial^2 S}{\partial N^2} \right)}}. \]
We thus find
\[
\frac{1}{\beta} \ln Z_G = -\langle A \rangle + \mu \langle N \rangle + \frac{1}{\beta} \ln 2\pi \delta E \sqrt{\left(\frac{\partial^2 S}{\partial N \partial E}\right)^2 - \left(\frac{\partial^2 S}{\partial E^2}\right)^2} (\frac{\partial^2 S}{\partial N^2})^2.
\]

The last term is a finite-size correction term. It will, for a large system, be small compared to the first two terms for all reasonable values of $\delta E$, and it can be made equal to zero by suitably choosing $\delta E$.

2.6

(a)

We have
\[
Z_1 = \frac{1}{h^3} \int_{V} d^3q \int_{-\infty}^{\infty} d^3p \exp \left( -\frac{\beta p^2}{2m} \right) = \frac{V}{h^3} \left( \frac{2\pi m}{\beta} \right)^{3/2} = \frac{V}{\lambda^3}.
\]

(b)

Using Stirling's formula, $\ln N! \approx N \ln N - N$, we find immediately
\[
A = -N k_B T \left( \ln \frac{V}{N\lambda^3} + 1 \right).
\]

(c)

The desired result follows immediately from
\[
Z_G = \sum_{N} e^{\beta N \mu} \frac{V^N}{N! \lambda^{3N}} = \exp \left[ e^{\beta \mu} \frac{V}{\lambda^3} \right].
\]

(d)

We have
\[
\Omega(N, V, T) = -\langle P \rangle V = -k_B T \ln Z_G.
\]

Giving
\[
\langle P \rangle = \frac{k_B T}{\lambda^3} \exp \frac{\mu}{k_B T}.
\]
\[ \langle N \rangle = \frac{V}{\lambda^3} \exp \left( \frac{\mu}{k_B T} \right) \]

\[ \langle S \rangle = \left( k_B - \frac{\mu}{T} - \frac{3k_B T}{\lambda} \frac{\partial \lambda}{\partial T} \right) \frac{V}{\lambda^3} \exp \left( \frac{\mu}{k_B T} \right). \]

Collecting terms we find

\[ E = TS - PV + \mu N = \left( k_B T - \mu + \frac{3k_B T}{\lambda} \frac{\partial \lambda}{\partial T} - k_B T + \mu \right) \frac{V}{\lambda^3} \exp \left( \frac{\mu}{k_B T} \right). \]

Using the definition of the thermal wavelength \( \lambda \) we finally obtain.

\[ E = \frac{3Nk_B T}{2}. \]

\[ \langle (\Delta E)^2 \rangle = k_B T^2 C_{V,N} = \frac{3Nk_B}{2} \]

and the formula for \( E \) we immediately find the desired result

\[ \frac{\sqrt{\langle (\Delta E)^2 \rangle}}{E} = \sqrt{\frac{2}{3N}}. \]

\[ (\Delta N)^2 = k_B T \frac{\partial \langle N \rangle}{\partial \mu}. \]

Differentiating (2.8) with respect to \( \mu \) then gives

\[ \langle (\Delta N)^2 \rangle = N. \]

2.7

(a) Photons are particles with zero chemical potential. Thus the grand partition function is given by

\[ Z_G = \prod_{k, \epsilon} \sum_{n_k = 0, \epsilon}^{\infty} \exp \{ -\beta \hbar \omega_k n_k \epsilon \} = \prod_{k, \epsilon} \frac{1}{1 - \exp (-\beta \hbar \omega_k)}. \]
Where the sum over $\epsilon$ is over the two transverse photon polarizations. Therefore the Helmholtz free energy is given by

$$A(V, T) = 2k_BT \sum_{k} \ln[1-\exp(-\beta\hbar\omega_k)] = \frac{Vk_BT}{\pi^2} \int_0^\infty k^2 dk \ln[1-\exp(-\beta\hbar ck)]$$

(2.9)

where, in the last step, we have converted the sum to an integral and used the fact that the frequency depends only on the magnitude of $k$. Substituting for $k$ in terms of $\omega$ yields the form of the answer in the text.

(b)

In (2.9) change the integration variable through $k = (k_BT/\hbar c)x$. This yields the following form

$$A(V, T) = \frac{V(k_BT)^4}{\pi^2\hbar^3 c^3} \int_0^\infty x^2 dx \ln(1 - e^{-x}) .$$

Since the volume and temperature dependence is now entirely in the prefactor, the result $PV = E/3$ follows directly by differentiation.

2.8

(a)

We write the mean energy as a sum of three terms $E = E_{\text{trans}} + E_{\text{vib}} + E_{\text{rot}}$ where, as usual $E_{\text{trans}} = \frac{3}{2}Nk_BT$. The contribution to the specific heat from the translational degree of freedom is thus $3Nk_B/2$.

The vibrational energy is given by

$$\langle E \rangle = \frac{N}{2}\hbar\omega_{\text{vib}} + \frac{N\hbar\omega_{\text{vib}}}{e^{\beta\hbar\omega_{\text{vib}}} - 1}$$

giving for the vibrational contribution to the specific heat

$$C_{\text{vib}} = \frac{\partial E_{\text{vib}}}{\partial T} = \frac{N(\hbar\omega_{\text{vib}})^2}{k_BT^2} \frac{e^{\beta\hbar\omega_{\text{vib}}}}{(e^{\beta\hbar\omega_{\text{vib}}} - 1)^2} .$$
We have
\[
C_{\text{vib}} \rightarrow \begin{cases} 
N k_B & ; T \gg \theta_{\text{vib}} \\
\frac{N (\hbar \omega_{\text{vib}})^2}{k_B T^2} e^{-\beta \hbar \omega_{\text{vib}}} & ; T \ll \theta_{\text{vib}} 
\end{cases}
\]

The rotational partition function must be evaluated separately in the high \((T \gg \theta_{\text{rot}})\) and low \((T \ll \theta_{\text{rot}})\) temperature limits. For low temperatures we sum the leading terms in the series for the partition function directly and find
\[
Z_{\text{rot}} \approx \left[ 1 + 3 \exp\{-2\theta_{\text{rot}}/T\} \right]^N
\]
\[
E_{\text{rot}} \approx \frac{6 N k_B \theta_{\text{rot}} \exp\{-2\theta_{\text{rot}}/T\}}{1 + 3 \exp\{-2\theta_{\text{rot}}/T\}} \approx 6 N k_B \theta_{\text{rot}} \exp\{-2\theta_{\text{rot}}/T\}
\]
and
\[
C_{\text{rot}} \approx 12 N k_B \left( \frac{\theta_{\text{rot}}}{T} \right)^2 \exp\{-2\theta_{\text{rot}}/T\}.
\]
Conversely, at high temperatures we use the Euler formula and obtain the expression
\[
Z_{\text{rot}} = \left( \sum_{j=0}^{\infty} (2j + 1) \exp\{j(j+1)\theta_{\text{rot}}/T\} \right)^N = \left( \frac{T}{\theta_{\text{rot}}} + \frac{\theta_{\text{rot}}}{15T} + \cdots \right)^N
\]
\[
E = N \frac{\partial}{\partial \beta} \ln \left( \frac{1}{\beta k_B \theta_{\text{rot}}} + \frac{1}{3} + \frac{\beta k_B \theta_{\text{rot}}}{15} + \cdots \right) = N k_B T \frac{1 - \frac{\theta_{\text{rot}}^2}{15T^2} + \cdots}{1 + \frac{\theta_{\text{rot}}}{3T} + \frac{\theta_{\text{rot}}^2}{15T^2} + \cdots}
\]
which has the series expansion
\[
E_{\text{rot}} = N k_B T \left( 1 - \frac{\theta_{\text{rot}}}{3T} - \frac{2\theta_{\text{rot}}^2}{45T^2} + \cdots \right).
\]
Finally we find
\[
C_{\text{rot}} = N k_B \left( 1 + \frac{2\theta_{\text{rot}}^2}{45T^2} + \cdots \right).
\]

(b) In region (i) the dominant contribution to the specific heat is \(3 k_B/2\) from the translational motion, with small exponential corrections from the other degrees of freedom. In region (ii) the rotational modes add a term \(N k_B\) giving \(C/N \approx 5 k_B/2\) while an additional contribution \(N k_B\) kicks in from the vibrational motion in region (iii) giving \(C/N \approx 7 k_B/2\).
2.9

We introduce Lagrange multipliers to ensure that the probability is normalized, that the energy and number of particles take on the correct mean values, and minimize

$$
\delta[-k_B \sum_i p_i \ln p_i + \lambda_1 \sum_i p_i + \lambda_E \sum_i p_i E_i + \lambda_N \sum_i p_i N_i] = 0 .
$$

This equation yields the following expression for $p_i$

$$
-k_B \ln p_i = 1 - \lambda_1 - \lambda_E E_i - \lambda_N N_i
$$

or

$$
S = 1 - \lambda_1 - \lambda_E \langle E \rangle - \lambda_N \langle N \rangle .
$$

The thermodynamic relation

$$
\frac{\partial S}{\partial \langle E \rangle} = \frac{1}{T}
$$

gives

$$
\lambda_E = -\frac{1}{T}
$$

while

$$
\frac{\partial S}{\partial \langle N \rangle} = -\frac{\mu}{T}
$$

yields

$$
\lambda_N = \frac{\mu}{T} .
$$

Combining these equations with the equation for $p_i$ above, we obtain

$$
p_i = \frac{\exp\{-\beta[E_i - \mu N_i]\}}{\exp\{[1 - \lambda_1]/k_B\}}
$$

and

$$
\exp\{[1 - \lambda_1]\} = \exp\{-\beta \Omega_G\}
$$

where $\Omega_G$ is the grand potential.
2.10

(a)

Assume that the \( n \) atoms originally occupying the vacancy sites in the in the lattice migrate to the surface, that the surface free energy is unaffected, and that the vacancy concentration is low enough that nearest neighbor vacancy pairs do not occur. With these assumptions we have \( qn \) oscillator modes which have the modified frequency \( \omega \) and \( 3N - qn \) modes that retain the original frequency \( \omega_0 \). Therefore the partition functions for the lattice vibrations is

\[
Z(n) = Z_0^{3N-qn} Z_1^{qn}.
\]

The single-mode partition functions are

\[
Z_0 = \frac{\exp\left\{-\beta \hbar \omega_0/2\right\}}{1 - \exp\{\beta \hbar \omega_0\}} = \frac{1}{2 \sinh\{\frac{1}{2} \beta \hbar \omega_0\}}
\]

\[
Z_1 = \frac{\exp\{-\beta \hbar \omega/2\}}{1 - \exp\{-\beta \hbar \omega\}} = \frac{1}{2 \sinh\{\frac{1}{2} \beta \hbar \omega\}}.
\]

The change in the Helmholtz free energy is therefore

\[
\Delta A = nq k_B T \ln \frac{\sinh(\beta \hbar \omega/2)}{\sinh(\beta \hbar \omega_0/2)}.
\]

(b)

For \( \beta \hbar \omega \ll 1 \) we approximate \( \sinh x \approx x \) and with \( q = 6 \), the result follows immediately. Similarly, at low temperatures, \( \beta \hbar \omega \gg 1 \) we use \( \sinh x \approx e^x/2 \), and obtain the other limiting result.

2.11

(a)

The Hamiltonian for the system consisting of \( N \) particles plus the friction-less piston of mass \( M \) is

\[
H = \sum_{i=1}^{N} \frac{p_i^2}{2m} + \frac{p_z^2}{2M} + Mgz.
\]
The partition function for a single gas molecule in a volume \( V = \mathcal{A}z \) is (see Problem 2.6(a))

\[
Z_1 = \frac{\mathcal{A}z}{\lambda^3}
\]

where

\[
\lambda = \sqrt[3]{\frac{\hbar^2}{2\pi m k_B T}}.
\]

The partition function for the complete system is then

\[
Z = \frac{\mathcal{A}^N}{N! \lambda^{3N}} \int_{-\infty}^{\infty} \frac{dp_z}{\hbar} \exp \left\{ -\frac{\beta p_z^2}{2M} \right\} \int_0^\infty dz z^N e^{-\beta Mg z}
\]

or

\[
Z = \frac{\mathcal{A}^N(\beta Mg z)^{N+1}}{\lambda^{3N}} \sqrt{\frac{2M \pi}{\beta \hbar^2}}.
\]

We find

\[
-k_B T \ln Z = -Nk_B T \ln \frac{\mathcal{A} k_B T}{\lambda^3 Mg}.
\]  

(2.10)

(b)

It was shown in the text that the chemical potential is given by

\[
\mu = k_B T \ln \left[ \frac{N \lambda^3}{V} \right] = \frac{G}{N}.
\]  

(2.11)

Identifying the pressure as \( Mg/A \) and using the ideal gas law \( PV = Nk_B T \)
we see that (2.10) and (2.11) are equivalent.

2.12

(a)

In the non-relativistic case we have

\[
E_{\text{kin}} = 2 \sum_{k < k_F} \frac{\hbar^2 k^2}{2m_e} = \frac{2V}{(2\pi)^3} 2m_e \frac{\hbar^2}{4\pi} \int_0^{k_F} k^4 dk = \frac{2R^3 \hbar^2 k_F^5}{15\pi m_e}.
\]  

(2.12)
\[ N = 2 \sum_{k<k_F} k_F^3 V \frac{3\pi^2}{3} \]

we have

\[ Rk_F = \left( \frac{9\pi N}{4} \right)^{1/3} \]  \hspace{1cm} (2.13)

Combining (2.12) and (2.13) we get the desired result

\[ E_{\text{kin}} = \frac{3\hbar^2}{10m_e} \left( \frac{9\pi}{4} \right)^{2/3} \frac{N^{5/3}}{R^2} \cdot \]

(b)

Let \( m_N \) be the nucleon mass. The mass density will then be approximately
\[ \rho = 2N m_N / V \] if there is an equal number of protons and neutrons. With \( G \) the gravitational constant we find for the potential energy

\[ E_{\text{pot}} = -\int_0^R dR 4\pi R^2 \frac{G\pi R^3}{3R} \rho^2 = -\frac{12}{5} m_N^2 G \frac{N^2}{R} \]  \hspace{1cm} (2.14)

(c)

Suppose \( N \) is fixed. The radius for which the kinetic plus potential energy is a minimum can then be found by differentiation. We find

\[ R_0 = \frac{1}{4} \left( \frac{9\pi}{4} \right)^{2/3} \frac{\hbar^2}{N^{1/3} m_e m_n^2 G} \]  \hspace{1cm} (2.15)

The gravitational constant is \( 6.67 \times 10^{-11} \text{Nm}^2/\text{kg}^2 \), the mass of a nucleon \( 1.67 \times 10^{-27} \text{kg} \), the mass of an electron is \( 9.11 \times 10^{-31} \text{kg} \). The solar mass is \( 1.99 \times 10^{30} \text{kg} \). The radius of the sun is \( 6.96 \times 10^8 \text{m} \). The radius for which the energy of a white dwarf with the same mass as the sun will be minimum will then be \( \approx 7.2 \times 10^6 \text{m} \) or \( \approx 1/100 \) that of the sun.
\[ e_{\text{tot}} = E_{\text{tot}} / (N m_e c^2) \]

Figure 2.1: Plot of \( e_{\text{tot}} \) vs. \( r \) for different values of \( n \) (see Problem 2-12.e).

(d)

Consider next an ultrarelativistic gas (\( \epsilon \approx c p \)) the electron kinetic energy will now be

\[
E_{\text{kin}} = 2 \sum_{k<k_F} \hbar k c = \frac{2V}{(2\pi)^3} 4\pi \hbar c \int_0^{k_F} k^3 dk = \frac{N^{4/3}}{R} \frac{\hbar c}{3\pi} \left( \frac{9\pi}{4} \right)^{4/3}
\]

while the potential energy is unchanged. Comparing (2.16) and (2.15) we find that for fixed \( N \) the potential and gravitational energies are both inversely proportional to \( R \). Since \( N^2 \gg N^{4/3} \) for large \( N \) we find that if the mass of the star is large enough the potential energy will dominate. This suggests that if a star is sufficiently heavy it will undergo a gravitational collapse. The critical value of \( N \) is

\[
N_{\text{crit}} = \left( \frac{5\hbar c}{36\pi m_n^2 G} \right)^{3/2} \left( \frac{9\pi}{4} \right)^2.
\]
Chapter 2. Statistical Ensembles

(e)

For the numerical calculation it is convenient to work with dimensionless quantities. Define

\[ e = \frac{E}{N m_e c^2} \]
\[ r = \frac{R}{R_0} \]

where our unit of length is

\[ R_0 = \left( \frac{9\pi}{4} \right)^{1/3} \frac{\hbar N^{1/3}}{mc} \]

corresponding to the radius of the star when the Fermi wavevector is an inverse Compton wavelength. The wave vector \( k \) is expressed in units of the inverse Compton wavelength

\[ x = \frac{\hbar k}{mc} \]

and we have at the Fermi surface

\[ x_F = \frac{1}{r} \]

We measure particle number in units of \( N_{\text{crit}} \)

\[ n = \frac{N}{N_{\text{crit}}} \]

where

\[ N_{\text{crit}} = \left( \frac{5\hbar c}{36\pi m_n^2 G} \right)^{3/2} \left( \frac{9\pi}{4} \right)^2 \]

Substitution gives

\[ e_{\text{tot}} = e_{\text{kin}} + e_{\text{pot}} = 3r^3 \int_0^{1/r} x^2 \sqrt{1 + x^2} dx - 1 - \frac{3n^{2/3}}{4r} \]

A plot of \( e_{\text{tot}} \) vs. \( r \) for different values of \( n \) is shown in Figure 2.1.
Chapter 3

Mean Field and Landau Theory

3.1

(a)

The Helmholtz free energy is given by

\[ A = \frac{qN}{2} \left[ e_{AA}c_A^2 + 2e_{AB}c_Ac_B + e_{BB}c_B^2 \right] + Nk_BT \left[ c_A \ln c_A + c_B \ln c_B \right]. \]

(b)

Let \( x = c_A - c_B \) so that

\[ c_A = \frac{1}{2}(1 + x); \quad c_B = \frac{1}{2}(1 - x) \]

and

\[ \frac{A}{qN} = \{\} + \frac{e_x^2}{4} + \frac{k_BT}{2q} [(1 + x) \ln(1 + x) + \ln(1 - x) \ln(1 - x)] \]

where

\[ \{\} = \frac{1}{4} \left\{ \frac{1}{2}(e_{AA} + 2e_{AB} + e_{BB}) + (e_{AA} - e_{BB})x \right\}. \]
The co-existence curve remains unchanged if we subtract constant terms, and terms linear in \( x \), from the free energy. We thus limit our attention to

\[
a = \frac{A}{qN} - \{ \} = \frac{\epsilon x^2}{4} + \frac{k_B T}{2q} \left[ (1 + x) \ln(1 + x) + (1 - x) \ln(1 - x) \right]
\]

(3.1)

where

\[
\epsilon = \frac{1}{2} e_{AA} + \frac{1}{2} e_{BB} - e_{AB}.
\]

By studying

\[
\frac{\partial^2 a}{\partial x^2} = \frac{\epsilon}{2} + \frac{k_B T}{2q} \left[ \frac{1}{1 + x} + \frac{1}{1 - x} \right]
\]

we see that for \( \epsilon < 0 \) the right hand side is negative for small \( x \) when \( k_B T < \frac{q|\epsilon|}{2} \).

The solution will thus phase separate for \( x \approx 0 \) for \( T < T_c = \frac{q|\epsilon|}{2k_B} \).

(c)

For \( T < T_c \) the reduced free energy (3.1) will look like Figure 3.1(a). If \( |x| \) is kept at a value larger than the \( x-\)value for which the free energy is a minimum, the system remains in a single phase and the critical temperature \( T_c(x) < T_c(0) \) is determined by the condition \( x_{\text{min}} = x \). The \( x \leftrightarrow -x \) symmetry simplifies the double tangent construction, the coexisting phases are those for which \( a \) has a minimum, or

\[
\frac{\partial a}{\partial x} = 0 = \frac{\epsilon x}{2} + \frac{k_B T}{2q} \ln \frac{1 + x}{1 - x}.
\]

In the notation of the text, the transition is discontinuous, since the concentrations in the two phases are different.

(d)

A plot of the coexistence curve is given in Figure 3.1(b).
Figure 3.1: (a). Plot of $a$ vs. $x$ for $T < T_c$. (b) Coexistence curve.

3.2

(a)

Writing $m = \langle \sigma \rangle$, the density matrices on the two sublattices can be written

$$\rho_{i1} = \begin{pmatrix} \frac{1+m}{2} & 0 \\ 0 & \frac{1-m}{2} \end{pmatrix}$$

$$\rho_{i2} = \begin{pmatrix} \frac{1-m}{2} & 0 \\ 0 & \frac{1+m}{2} \end{pmatrix}.$$ 

Therefore

$$\text{Tr} \rho H = \frac{qN}{2} \text{Tr} \sigma_{i1} \rho_{i1} \text{Tr} \sigma_{i2} \rho_{i2}$$

$$= -\frac{qNJ}{2} m^2.$$ 

Similarly, the entropy is

$$S = -\frac{Nk_B}{2} \text{Tr} \rho_{i1} \ln \rho_{i1} - \frac{Nk_B}{2} \text{Tr} \rho_{i2} \ln \rho_{i2}$$

$$= -\frac{Nk_B}{2} \left[ (1+m) \ln \frac{1+m}{2} + (1-m) \ln \frac{1-m}{2} \right].$$ 

Hence the minimization of the Helmholtz free energy $A = E - TS$ yields

$$\frac{\partial A}{\partial m} = 0 = -NqJm + \frac{Nk_BT}{2} \ln \frac{1+m}{1-m}$$

which is the desired result.
Figure 3.2: Plot of $m$ vs. $T$ for two values of $c_A$.

(b)

We can find the temperature dependence of the order parameter most easily if we first select a value of $m$ and use Equation (3.27) in the text to determine $T$. The resulting plot is shown in Figure 3.2 for the two cases $c_A = 0.5$ and $c_A = 0.45$. The insensitivity of the result to concentration represents an unrealistic aspect of the Bragg Williams approximation.

3.3

Let us define

$$x = e^{\beta h}; \quad y = e^{2\beta J}; \quad z = e^{2\beta h'}.$$

We have

$$Z_G = xyz + xy^{-1}z - 1 + 2x + x^{-1}y^{-1}z + x^{-1}yz^{-1} + 2x^{-1} \quad (3.2)$$

$$\langle \sigma_0 \rangle = \frac{1}{Z_C}[xyz + xy^{-1}z - 1 + 2x - x^{-1}y^{-1}z - x^{-1}yz^{-1} - 2x^{-1}] \quad (3.3)$$

$$\langle \sigma_1 \rangle = \frac{1}{Z_C}[xyz - xy^{-1}z^{-1} + x^{-1}y^{-1}z - x^{-1}yz^{-1}].$$

Putting $\sigma_0 = \sigma_1$ and solving for $z$ gives

$$z = \frac{1}{2} \left( y(x^2 - 1) + \sqrt{4x^2 + y^2 - 2x^2y^2 + x^4y^2} \right)$$

$$z^{-1} = \frac{1}{2x^2} \left( -y(x^2 - 1) + \sqrt{4x^2 + y^2 - 2x^2y^2 + x^4y^2} \right).$$
Substituting back into (3.2) and (3.3) gives after considerable algebra

$$\langle \sigma_0 \rangle = \frac{x^2 - 1}{\sqrt{x^4 - 2x^2 + 1 + 4x^2y^2}}. \quad (3.4)$$

This expression is equivalent to (3.57) in the text, i.e., the Bethe approximation gives the exact result for the magnetization. The algebra effort leading to (3.4) can ameliorated by employing a symbol-manipulating program such as "Mathematica".

### 3.4

(a)

We have $m = \tanh \{ \beta (qJm + h) \}$. Differentiating with respect to $h$ we find

$$\frac{\partial m}{\partial h} = \frac{\beta (qJ \frac{\partial m}{\partial h} + 1)}{\cosh^2 \beta qJm}.$$  

Solving for $\chi = \partial m / \partial h$ we obtain

$$\chi(h = 0, T) = \frac{\beta}{\cosh^2 \beta qJm - \beta qJ}.$$  

For $T > T_c$, $m = 0$ and we immediately have

$$\chi(0, T > T_c) = \frac{1}{k_B(T - T_c)}.$$  

For $T < T_c$, we use $\cosh^2 x \approx 1 + x^2 + \ldots$ for small $x$ and $m^2 \approx 3 \left( \frac{T}{T_c} \right)^3 \left( \frac{T}{T_c} - 1 \right)$ to obtain

$$\chi(0, T \to T_c^-) \approx \frac{1}{2k_B(T_c - T)}.$$  

(b)

This part as well as the next require us to determine how the effective field $h'$ approaches zero in the Bethe approximation. We change notation slightly from the text and write the equation that determines $h'$ in the form

$$\frac{1 + \tanh K \tanh h'}{1 - \tanh K \tanh h'} = \exp \frac{2h'}{q - 1}.$$  

where $h'$ here corresponds to $\beta h'$ in the text and $K = \beta J$. Near the critical point $\tanh K = 1/(q - 1) + t$ where $t$ is proportional to $T_c - T$. Now, assuming that $h' \ll 1$ we may expand the two sides of the constitutive equation. Gathering the first few terms we find

$$h'[2t] + h'^2\left[\frac{4t}{q - 1}\right] - h'^3\left[\frac{2}{3(q - 1)} - \frac{2}{(q - 1)^3} + \frac{4}{3(q - 1)^3} + O(t)\right] + \ldots$$

The term of order $h'^2 t$ is clearly of higher order than the term of order $h' t$ and can be neglected to lowest order. Therefore,

$$h'^2 \sim t \quad \text{as } t \to 0.$$ 

Without any further calculation we can now show that $C(h = 0, t)$ is discontinuous at $T_c$. Since $\langle \sigma_0 \sigma_1 \rangle = \langle \sigma_0 \sigma_1 \rangle|_{h' = 0} + a h'^2 + \ldots$ we obtain a discontinuity in $C$ from the derivative of the second term in this expression.

(c)

The analysis of part (b) shows that $m(h = 0) \sim b h' \sim t^{1/2}$.

(d)

The equation for the effective field at $T = T_c$ can be written in the form

$$\frac{1 + \frac{1}{q-1} \tanh\{h + h'\}}{1 - \frac{1}{q-1} \tanh\{h + h'\}} = \exp \frac{2h'}{q - 1}.$$

Proceeding to expand, as in part (b) we obtain the following equation for $h'$:

$$\frac{2}{q - 1} h + \frac{2}{(q - 1)^2} [2hh' + h'^2] - \left[\frac{2}{3(q - 1)} - \frac{2}{3(q - 1)^3}\right] h'^3 + O(h'h^2, h'^2h).$$

Clearly the solution is

$$h' \sim h^{1/3}$$

which implies, in turn, that $m(h, T_c) \sim h^{1/3}$, i.e., $\delta = 3$. 
3.5

The dimensionless Hamiltonian $\tilde{H} = -\beta H$ for the three spins on the central cluster in the molecular field approximation is

$$\tilde{H} = K (\sigma_1 \sigma_2 + \sigma_2 \sigma_3 + \sigma_3 \sigma_1) + 4mK (\sigma_1 + \sigma_2 + \sigma_3).$$

Therefore, the expectation value $m = \langle \sigma_j \rangle$ for any of the three spins on the triangle is given by

$$m = \frac{e^{3K} \sinh(12Km)}{e^{3K} \cosh(12Km) + 3e^{-K} \cosh(4Km)} = f(m).$$

The critical point is given by

$$\left. \frac{df}{dm} \right|_{m=0} = 1$$

which yields

$$K_c \frac{12e^{4K_c} + 4}{e^{4K_c} + 3} = 1.$$

Solving numerically, we find $K_c = J/k_B T_c \approx 0.177$ which is not much of an improvement over the simplest mean field theory. On the square lattice the dimensionless Hamiltonian is

$$\tilde{H} = K (\sigma_1 \sigma_2 + \sigma_2 \sigma_3 + \sigma_3 \sigma_4 + \sigma_4 \sigma_1) + 2mK (\sigma_1 + \sigma_2 + \sigma_3 + \sigma_4).$$

Proceeding as in the triangular case, we find the function $f(m)$ to be

$$f(m) = \frac{e^{4K} \sinh(8mK) + 2 \sinh(2mK)}{e^{4K} \cosh(8mK) + 4 \cosh(2mK) + 2 + e^{-4K}}.$$

Solving the equation $f'(0) = 1$ we find $K_c \approx 0.309$.

3.6

Imagine a one-dimensional random walk and represent a step to the right by $\sigma = 1$ and a step to the left by $\sigma = -1$. The position of the end-point of an $N$-step random walk is then given by $x_N - x_0 = \sum_{i=1}^{N} \sigma_i$. We can identify the
length $l$ of a polymer with the end-to-end distance of a random walk in the following way

$$l = \sqrt{\langle (x_N - x_0)^2 \rangle} = \sqrt{N + \sum_{i \neq j} \sigma_i \sigma_j}.$$

In the diagram we see that the length increases as function of temperature and we can therefore assume that at very low temperatures, neighboring spins prefer to point in opposite directions so as to shorten the walk. Therefore a possible model is the Ising antiferromagnet with

$$H = J \sum_{i=1}^{N-1} \sigma_i \sigma_{i+1}.$$

The correlation function for this model can be worked out in the same fashion as for the ferromagnet with the result

$$\langle \sigma_i \sigma_j \rangle = (-v)^{|i-j|}$$

where $v = \tanh K$ with $K = \beta J$. Therefore

$$l^2 = N + 2 \sum_{i=2}^{N} \sum_{j=1}^{i-1} (-v)^{i-j}.$$

Retaining only terms proportional to $N$ we arrive at the result

$$l = \sqrt{N \frac{1-v}{1+v}} = \sqrt{Ne^{-K}}$$

which shows the expected increase of the length of the chain as function of $T$.

### 3.7

The elements of the transfer matrix for the spin-1 Ising ferromagnet are given by

$$P_{\sigma, \sigma'} = \exp K \sigma \sigma'$$

where $K = \beta J$ and $\sigma = 0, \pm 1$. Therefore

$$P = \begin{bmatrix} e^K & 1 & e^{-K} \\ 1 & 1 & 1 \\ e^{-K} & 1 & e^K \end{bmatrix}.$$
The eigenvalues of this matrix can be obtained (e.g. using "Mathematica") as

$$\lambda_1 = \frac{x^2 - 1}{x}$$

$$\lambda_2 = \frac{1}{2x} \left( 1 + x + x^2 + \sqrt{1 - 2x + 11x^2 - 2x^3 + x^4} \right)$$

$$\lambda_3 = \frac{1}{2x} \left( 1 + x + x^2 - \sqrt{1 - 2x + 11x^2 - 2x^3 + x^4} \right)$$

where $x = e^K$. The largest eigenvalue is $\lambda_2$. The internal energy is thus

$$E = -NJx \frac{\partial \ln \lambda_2}{\partial x}$$

$$= NJ \left( 1 - \frac{x + 2x^2 + \frac{-2x + 2x - 6x^3 + 4x^4}{2\sqrt{1 - 2x + 11x^2 - 2x^3 + x^4}}}{1 + x + x^2 + \sqrt{1 - 2x + 11x^2 - 2x^3 + x^4}} \right) .$$

A plot of the internal energy vs the inverse temperature is shown in Figure 3.3.
3.8

Let the shift in position, \( x_n \), be \( \pm 1 \), depending on whether the move is to the left or to the right. The position after \( n \) steps is then

\[
x = \sum_{n=1}^{N} x_n
\]

and the mean square displacement after \( N \) steps is

\[
\langle x^2 \rangle = \sum_{n,k=1}^{N} \langle x_n x_k \rangle
\]

where \( \langle x_n x_k \rangle \) depends only on \(|n - k|\), and \( \langle x_n x_n \rangle = 1 \). Let \( a_i, b_i \) be the probabilities that \( x_{n+i}x_n = +1 \) or \(-1\), respectively. We have \( a_0 = 1, b_0 = 0 \), \( \langle x_{n+i}x_n \rangle = a_i - b_i \) and

\[
a_i = pa_{i-1} + (1 - p)b_{i-1}
\]

\[
b_i = (1 - p)a_{i-1} + pb_{i-1}
\]

giving

\[
\langle x_{n+i}x_n \rangle = (2p - 1)^{|i|}
\]

and we have

\[
\langle x^2 \rangle = \sum_{n=1}^{N} \sum_{i=1-n}^{N-n} (2p - 1)^{|i|} = N + 2 \sum_{n=1}^{N-1} \sum_{i=1}^{N-n} (2p - 1)^i.
\]

Carrying out the sums we find

\[
\langle x^2 \rangle = N + \frac{2p - 1}{1 - p} \sum_{n=1}^{N-1} (1 - (2p - 1)^{N-n})
\]

or

\[
\langle x^2 \rangle = N + \frac{2p - 1}{1 - p} \left( N - 1 - \frac{2p - 1}{2 - 2p} \left[ 1 - (2p - 1)^{N-1} \right] \right)
\]

which simplifies to

\[
\langle x^2 \rangle = \frac{Np}{1 - p} - \frac{2p - 1}{2(1 - p)^2} + \frac{(2p - 1)^{N+1}}{2(1 - p)^2}.
\]

As a check on the algebra, we note that if \( p = 0.5 \) we have \( \langle x^2 \rangle = N \), for large \( N \) the expression grows linearly with \( N \), while for \( N = 1 \) we have \( \langle x^2 \rangle = 1 \) independently of \( p \).
3.9

(a)

The probability that the chain has spins $j, j + 1 \ldots, j + n$ in the $\uparrow$ state and spin $j + n + 1$ in the $\downarrow$ configuration can be written in the form

$$P = \frac{1}{\lambda_1^N} \sum_{\sigma_{j-1} \sigma_{j+n+2} \ldots \sigma_{j-2}} P_{\sigma_{j-1}, \uparrow} [P_{\uparrow, \uparrow}]^n P_{\downarrow, \downarrow} P_{\downarrow, \sigma_{j-1}}^{N-n-2}$$

where $\lambda_1$ is the larger of the two eigenvalues of $P$. If we denote the eigenvector corresponding to $\lambda_1$ by $|\lambda_1\rangle$ and the original basis states by $|\uparrow\rangle$ and $|\downarrow\rangle$ then we clearly can write the above equation as follows:

$$P = \frac{\langle \uparrow | \lambda_1 \rangle \langle \lambda_1 | \downarrow \rangle [P_{\uparrow, \uparrow}]^n}{\lambda_1^{n+1}} P_{\downarrow, \downarrow}.$$

In arriving at this expression we have assumed $N - n - 1 \to \infty$ as $N \to \infty$.

(b)

If the configuration of spin $j + 1$ is arbitrary then the last equation in part (a) simply changes to

$$P = \frac{\langle \uparrow | \lambda_1 \rangle \langle \lambda_1 | \uparrow \rangle [P_{\uparrow, \uparrow}]^n}{\lambda_1^n}.$$

3.10

(a)

We have for the free energy

$$\frac{G}{N} = -k_B T \ln \left( 4\pi \int_0^1 d\mu \exp \left\{ \frac{\rho U}{k_B T} [(3\mu^2 - 1)Q - Q^2] \right\} \right).$$

(3.5)

We introduce the reduced variables

$$\beta = \frac{\rho U}{2k_B T}; \quad g = \frac{G}{N\rho U}.$$
for the inverse temperature and free energy respectively. We find
\[
g = -\frac{1}{\beta} \ln(4\pi) + Q^2 - \frac{1}{\beta} \ln \left( \int_0^1 d\mu \exp\{\beta Q(3\mu^2 - 1)\} \right).
\]

Taylor expanding the exponent yields
\[
g = -\frac{1}{\beta} \ln(4\pi) + Q^2 - \frac{1}{\beta} \ln \left[ \int_0^1 d\mu \left( 1 + \beta Q(3\mu^2 - 1) + \frac{1}{2} [\beta Q(3\mu^2 - 1)]^2 + \right.ight.
\[
\left. \left. \frac{1}{6} [\beta Q(3\mu^2 - 1)]^3 + \frac{1}{24} [\beta Q(3\mu^2 - 1)]^4 + \ldots \right) \right] \right]
\]

After integrating we find
\[
g = -\frac{1}{\beta} \ln(4\pi) + Q^2 - \frac{1}{\beta} \ln \left[ 1 + \frac{4}{10} (\beta Q)^2 + \frac{8}{105} (\beta Q)^3 + \frac{2}{35} (\beta Q)^4 + \ldots \right]
\]

Finally, after expanding the logarithm in a Taylor series we obtain the desired formula
\[
g = -\frac{1}{\beta} \ln(4\pi) + Q^2 (1 - \frac{2\beta}{5}) - \frac{8\beta^2 Q^3}{105} + \frac{4\beta^3 Q^4}{175} + \ldots
\]
\[\text{(3.6)}\]

(b)

If we rewrite (3.6) as
\[
g = a + \frac{bQ^2}{2} - \frac{cQ^3}{3} + \frac{dQ^4}{4} + \ldots
\]
we have \( b = 2 - 0.8\beta, \ c = \frac{8\beta^2}{35}, \ d = \frac{16\beta^3}{175} \). The transition occurs when
\[
b = \frac{2c^2}{9d}; \quad \beta_c = 2.16.
\]
The discontinuity of the order parameter is
\[
Q_0 = \frac{2c}{3d}; \quad Q_0 = 0.77.
\]

(c)

Define the dimensionless inverse temperature \( x = \rho U \beta \) and the reduced Gibbs energy per molecule
\[
g_r = \frac{g}{\rho U} = Q^2 - \frac{1}{x} \ln \left( 4\pi \int_0^1 \exp[xQ(3\mu^2 - 1)]d\mu \right).
\]
For a given value of \( y = Qx \) we can evaluate \( Q \) from the self-consistency equation

\[
Q = \frac{\int_0^1 \frac{1}{2}(3\mu^2 - 1) \exp[y(3\mu^2 - 1)]d\mu}{\int_0^1 \exp[y(3\mu^2 - 1)]d\mu}
\]

Once \( Q \) is found we determine \( x = y/Q \). We find numerically that \( g_r \) is the same for the isotropic (\( Q = 0 \)) and nematic phase when \( y = 0.974209 \), the value of the order parameter is then \( Q = 0.429029 \). By differentiating \( g_r \) with respect to the reduced temperature \( t = \frac{1}{k_B x} \) we find that the change of entropy in going from the isotropic to the nematic state is

\[
\Delta s = \ln \left( \int_0^1 \exp[y(3\mu^2 - 1)]d\mu \right) - \frac{y \int_0^1 \frac{1}{2}(3\mu^2 - 1) \exp[y(3\mu^2 - 1)]d\mu}{\int_0^1 \exp[y(3\mu^2 - 1)]d\mu}
\]

per particle. Evaluating this expression numerically we find \( \Delta s = -0.417964 k_B \).

### 3.11

\[
G(m, T) = a(T) + \frac{b}{2} m^2 + \frac{c}{4} m^4 + \frac{d}{6} m^6
\]

We let \( \cdot \) indicate partial differentiation with respect to \( T \). Then

\[
S = -G' = - \left( a' + \frac{1}{2} b' m^2 + \frac{1}{4} c' m^4 + \frac{1}{6} d' m^6 \right) - \frac{\partial G}{\partial m} m'.
\]

The last term vanishes, since at equilibrium \( \partial G/\partial m = 0 \). Above the transition \( m = 0 \), while below \( T_c \) \( m \neq 0 \). The discontinuity at the transition is

\[
m_0 = \sqrt{-\frac{3c}{4d}}.
\]

Substitution of this result gives the answer

\[
L = T_c[S(T_c^+ - S(T_c^-))] = T_c \left( -\frac{3b'c}{8d} + \frac{9c'c^2}{64d^2} - \frac{9d'c^3}{128d^3} \right).
\]  \( (3.7) \)

It is tempting to try to simplify 3.7 further by making use of

\[
b(T_c) = \frac{3c^2}{16d}.
\]

However, this equation only holds at \( T_c \). Differentiating both sides to eliminate \( b' \) is not allowed!
3.12

(a)

The leading terms in the expression for the free energy along the first order line are
\[
\frac{G}{N} = a(T, \Delta) + \frac{b(T, \Delta)}{2} m^2.
\]
The other terms are of higher order in \(T - T_t\) or \(\Delta - \Delta_t\) close to the tricritical point. Using \(x = -1/N \partial G/\partial \Delta\) we have
\[
x_+ = -a_\Delta - \frac{b_\Delta}{2} m^2 - \frac{b}{2} \frac{dm^2}{d\Delta}
\]
in the disordered and ordered phase respectively. Using \(m^2 = -\frac{3c}{4d}\) we find, to leading order,
\[
\delta x = x_+ - x_- = \frac{3}{8d} (b_\Delta c + c_\Delta b).
\]

(b)

Quite generally,
\[
\chi^{-1} = b + 3cm^2 + 5dm^4.
\]
In the tricritical region, \(b \sim (T - T_t), c \sim (T - T_t)\) and \(m^2 \sim \sqrt{-b/d}\). Therefore the terms \(b\) and \(dm^4\) both approach zero as \((T - T_t)^1\) and, hence, \(\gamma_t = 1\). The specific heat in the ordered phase contains the terms
\[
C = -T \left[ 2b_T \frac{dm^2}{dT} + b(T) \frac{d^2m^2}{dT^2} + \cdots \right].
\]
Asymptotically, \(b_T \rightarrow \text{const.}\) and \(m^2(T) \sim (T_t - T)^{1/2}\). Therefore, the two terms singled out above diverge as \((T_t - T)^{-1/2}\) which implies \(\alpha_t = \frac{1}{2}\).

(c)

In the critical region, \(b \sim c^2\) and \(m(T) \sim (T_t - T)^{1/2}\). With \(c \sim (T - T_t)\) we see that all terms in \(\chi^{-1}\) approach zero as \((T_t - T)^2\) and that higher order
terms will vanish still more rapidly. Therefore $\gamma_u = 2$. As far as the specific heat is concerned, $m^2 \sim T - T_t$ and the divergence that occurs in the tricritical region does not occur in the critical region. Indeed, since $b \sim c^2$ we must have $b_T \sim c c_T \sim |T - T_t|$. Therefore, the leading nontrivial terms in the specific heat

$$2b_T \frac{dm^2}{dT} + \frac{c_T}{4} \frac{dm^4}{dT} + \cdots$$

all approach zero linearly with the temperature deviation from $T_t$. This is different from the case of an ordinary critical point in that there is no discontinuity in $C$ and it therefore makes sense to speak of $\alpha_u = -1$ as the exponent which gives the leading analytical behavior near the tricritical point.

3.13

We write the order parameter in the form $\mathbf{m} = m(1,0,0)$ or $\mathbf{m} = \frac{m}{\sqrt{2}}(1,1,0)$ or $\mathbf{m} = \frac{m}{\sqrt{3}}(1,1,1)$ for the three possible types of order in a cubic lattice. To fourth order, only the two fourth order terms discriminate between the different phases and the fourth order contribution to the free energy becomes

$$G(100) = \frac{d}{4} m^4$$

$$G(110) = \frac{c + 2d}{16} m^4$$

$$G(111) = \frac{c + d}{12} m^4 .$$

Comparing, we find that if $c < 2d$ the (111) phase has the lowest free energy. If $c > 2d$ the (100) phase wins. The (110) phase is never selected at this level of the expansion. Clearly the transition will be first order if $d < 0$ in the (100) case and if $c + d < 0$ in the (111) case, assuming in either case that the coefficient $b$ remains positive to a lower temperature.
Figure 3.4: Equation for the order parameter in Problem (3.14). (a) $T > T_c$ (b) $T < T_c V$.

3.14

(a)

We require that the derivative of the free energy

$$A = M g R \cos(\phi) - N k_B T \left\{ \ln \left[ \frac{AR \left( \frac{\pi}{2} + \phi \right)}{N \lambda^3} \right] + \ln \left[ \frac{AR \left( \frac{\pi}{2} - \phi \right)}{N \lambda^3} \right] + 2 \right\}$$

with respect to the order parameter $\phi$ should be zero. This gives

$$0 = -M g R \sin \phi + N k_B T \left\{ \frac{1}{\frac{\pi}{2} - \phi} - \frac{1}{\frac{\pi}{2} + \phi} \right\}.$$ 

This expression simplifies to

$$M g R \sin \phi = \frac{8 N k_B T \phi}{\pi^2 - 4 \phi^2} \tag{3.9}$$

In Figure 3.4(a) the left and right side of Equation (3.9) is sketched for

$$T > T_c = \frac{M g R \pi^2}{8 N k_B}$$
Figure 3.5: Temperature dependence of the order parameter in Problem 3.14 for (a) $\delta = 0$, (b) $\delta = 0.05$.

while the two sides of the equation are sketched for $T < T_c$ in Figure 3.4(b). We note that for $T > T_c$ Equation (3.9) has only one solution, the symmetric solution, $\phi = 0$. For $T < T_c$ there are three solutions. It is easy to see, by looking at the sign of the second derivative of the free energy with respect to $\phi$, that the symmetric solution $\phi = 0$ is now unstable, corresponding to a local maximum in the free energy. Instead there are two equivalent stable solutions one with $\phi < 0$ and one with $\phi > 0$.

(b)

The temperature dependence of the equilibrium value of $\phi$ is sketched in Figure 3.5(a).

(c)

The equation for the order parameter is now

$$0 = -M g R \sin \phi + N k B T \left\{ \frac{1 + \delta}{\frac{\pi}{2} - \phi} - \frac{1 - \delta}{\frac{\pi}{2} + \phi} \right\}.$$ 

The temperature tempendence of $\phi$ is shown in Figure 3.5(b).
3.15

(a)

The matrix $PQ$ can be written

$$PQ = \begin{pmatrix} 2 \cosh(2\beta) & 2 \cosh(2\beta\epsilon) \\ 2 \cosh(2\beta\epsilon) & 2 \cosh(2\beta) \end{pmatrix}.$$ 

The eigenvalues of this matrix are

$$\lambda_1 = 2[\cosh(2\beta) + \cosh(2\beta\epsilon)]; \quad 2[\cosh(2\beta) - \cosh(2\beta\epsilon)]$$

with $\lambda_1$ being the largest.

(b)

The free energy is an analytic function of $\epsilon$ and we can use Landau theory. Expanding the free energy in powers of $\epsilon$ gives

$$g(\epsilon) = -\frac{1}{\beta} \ln[2 \cosh(2\beta) + 2] + \epsilon^2 \left( \omega - \frac{\beta}{\cosh(2\beta) + 1} \right) + \epsilon^4 \frac{\beta^3}{3} \frac{2 - \cosh(2\beta)}{(\cosh(2\beta) + 1)^2} + \ldots$$

For $\omega = 0.20$ we find numerically, that the second order term is negative between $\beta_1 = 0.516582$ and $\beta_2 = 1.08189$. At the highest temperature $\beta_1$ the fourth order term is found to be positive. This means that there will be a second order phase transition at $\beta = \beta_1$.

(c)

For $\omega = 0.24$ the second order term does not vanish for any value of $\beta$. However, the fourth order term is negative for $\beta > 0.658479$. To show that there is a first order transition, we plot in Figure 3.6 the free energy as a function of $\epsilon$ for some values of the temperature. It is seen that the transition temperature is near $\beta = 1.1$. 
Figure 3.6: Dependence of the free energy on $\varepsilon$ in Problem 3.15 for $\omega = 0.24$ and three values of $\beta$.

(d)

At the tricritical point both the second and fourth order terms vanish. We have already seen that the fourth order vanishes at $\beta = 0.658479$. Substituting this value into the second order term we find that $\omega = 0.219493$ at the tricritical point.
Chapter 4

Dense Gases and Liquids

4.1

(a)

Since the particles are unable to pass through each other they can be ordered and are therefore distinguishable. Therefore the factor $N!$ must be omitted from the partition function. Let the position of the left edge of particle $j$ be denoted by $x_j$. The partition function is then given by

$$Z = \int_0^{L-(N-1)a} dx_1 \int_{x_1+a}^{L-(N-2)a} dx_2 \ldots \int_{x_{N-2}+a}^{L-a} dx_{N-1} \int_{x_{N-1}+a}^{L} dx_N.$$ 

These integrals can be carried out in sequence to yield

$$Z = \frac{1}{N!} [L - (N - 1)a]^N$$

and the one-dimensional pressure is given by

$$p = -\frac{\partial A}{\partial L} = \frac{\partial}{\partial L} Nk_B T \ln [L - (N - 1)a] = \frac{Nk_B T}{L - (N - 1)a}.$$ 

The expression $(N - 1)a$ is just the ‘excluded length’ seen by each particle. Ignoring the difference between $N$ and $N - 1$, we may obtain a virial expansion of the pressure:

$$\beta p = n [1 + na + n^2 a^2 + \ldots]$$
(b) In the Mayer theory the first two virial coefficients are given by

\[
B_2(T) = -\frac{1}{2} \int dx f(x)
\]

\[
B_3(T) = -\frac{1}{3} \int dx dy f(x) f(y) |x - y|.
\]

The Mayer function for the Tonks gas has the property \( f(x) = -1 \) for \(-a < x < a\) and \( f(x) = 0 \) otherwise. Therefore, we trivially obtain \( B_2(T) = a \) in agreement with the result of part (a). The integral for \( B_3 \) can be put into the form

\[
\int dx dy f(x) f(y) |x - y| = -\int_{-a}^{a} dx \int_{\max(-a, x-a)}^{\min(a, x+a)} dy = 3a^2
\]

which yields \( B_3(T) = a^2 \) as expected.

4.2

Label the vertices of graph \( g \) with numbers \( 1, 2, \ldots, (n_1, n_1), n_1+1 \ldots n_1+n_2-1 \) where the double entry of vertex \( n_1 \) indicates that it belongs to both subgraph \( g_1 \) and \( g_2 \). The integral

\[
I(g) = \frac{1}{V} \int d^3r_1 \ldots d^3r_{n_1+n_2-1} \prod_{i,j} f_{ij}
\]

can now be carried out in two steps. Define \( x_j = r_j - r_{n_1} \) for all \( j \neq n_1 \). With this transformation, the variable \( r_{n_1} \) is eliminated from the integrand and the integration factors into the corresponding integrals for each of the subgraphs \( g_1 \) and \( g_2 \), i.e.,

\[
I(g) = I(g_1)I(g_2).
\]

The number of distinct assignment of particle numbers to the vertices of \( g \) cannot be written down in complete generality as it depends on partial symmetries of the subgraphs. Let \( \mathcal{N}(g) \) be this number and let \( \mathcal{N}'(g_1), \mathcal{N}'(g_2) \) be the number of distinct labelings of the \( n_1 - 1 \) and \( n_2 - 1 \) vertices of \( g_1 \) and
\( g_2 \) given that a particular label has been assigned to the vertex at which they are joined to form \( g \). Finally define \( S(g_1, g_2) = 2 \) if graph \( g \) has a reflection symmetry about the vertex \( n_1 \) (e.g. two triangles joined at one of the vertices or two single lines joined). If there is no reflection symmetry, \( S(g_1, g_2) = 1 \). Then

\[
N(g) = (n_1 + n_2 - 1) \left[ \frac{(n_1 + n_2 - 2)!}{(n_1 - 1)!(n_2 - 1)!} \right] \frac{N'(g_1)N'(g_2)}{S(g_1, g_2)}.
\]

In this expression, the first factor represents the number of ways of choosing a label for the common vertex, the second factor the number of ways of assigning the remaining labels to the two sets of vertices \( n_1 - 1, n_2 - 1 \) and the final factor accounts for the number of inequivalent permutations of labels. As an example, consider the case of two triangles joined at a vertex. Direct enumeration shows that \( N'(g) = 15 \). In this case, \( N'(g_1) = N'(g_2) = 1 \) and \( S(g_1, g_2) = 2 \) and we get the same result from the above expression. Therefore,

\[
b(g) = \frac{n_1n_2}{S(g_1, g_2)} \frac{N'(g_1)N'(g_2)}{N(g_1)N(g_2)} b(g_1)b(g_2).
\]

4.3

We begin with the two-particle correlation function \( n_2 = \sum_{i \neq j} \langle \delta(x_1 - r_i)\delta(x_2 - r_j) \rangle \). In the grand canonical formalism this function is given by

\[
e^{\beta U(x_1 - x_2)}n_2(x_1, x_2) = \sum_{N=2}^{\infty} \frac{x^N}{(N-2)!} \int d^{N-2}r \left[ \prod_{m \neq 2}(1 + f_{1m}) \prod_{m \neq 1}(1 + f_{2m}) \prod_{i,j \neq 1,2}(1 + f_{ij}) \right] \]

\[
\sum_{N=0}^{\infty} \frac{x^N}{N!} \int d^N r \prod_{ij}(1 + f_{ij})
\]

where \( x = e^{\beta \mu} / \lambda^3 \) and where we have arbitrarily chosen particles 1 and 2 to be at \( x_1 \) and \( x_2 \) respectively. In the numerator, coordinates 1 and 2 are therefore not integrated over and will need to be specially labeled in a graphical expansion. If we expand the products in the numerator, we see that exactly the same graphs appear as in the partition function. However, because of vertices 1 and 2 we must take these graphs and attach 0, 1 or 2 of the special labels, e.g. an open circle in all possible ways to each of the graphs. Physically it is clear that since \( n_2 \) is a function only of \( |x_1 - x_2| \) the final result must contain
only contributions from graphs in which two open circles are joined by any
number of lines. Everything else must cancel and this serves as a useful check
on the algebra.

Consider first the terms of order \( (f)^0 \) and order \( f \). Clearly, in the numer-
ator the terms of order \( (f)^0 \) produce merely \( x^2 \exp \{ xV \} \) and \( \exp \{ xV \} \) in the
denominator. Let \( I_2 \equiv \int d^3 r f(r) \) and \( M = N - 2 \) in the numerator. Then the
terms of order \( f \) in the numerator give the following contributions:

\[
\sum_{M=1}^{\infty} \frac{2MV^{M-1}I_2x^{M+2}}{M!} = 2x^3I_2 e^{xV}
\]

where this comes from the one-line graphs with an open circle at one end. Note
that since we have taken the term \( (1 + f_{12}) \) to the left hand side, two open
circles cannot be joined by a single line. The other contribution comes from
the graph with no open circles:

\[
\sum_{M=2}^{\infty} \frac{M(M-1)V^{M-1}x^{M+2}I_2}{2M!} = \frac{1}{2}x^2V I_2 e^{xV}.
\]

The corresponding term in the denominator gives \( \frac{1}{2}x^2V \exp \{ xV \} I_2 \).

In the next order in \( f \), there are 7 different graphs as a result of decorating
the two plain graphs with open circles. All except the two-line graph with
open circles at each end give a contribution proportional to \( I_2 \). The unique
graph is proportional to the integral

\[
I_3 = \int d^3 r f(x_1 - r) f(r - x_2)
\]

and, according to the argument given above should represent the only surviving
contribution after all rearrangements have been carried out. Carrying out the
combinatorics for both numerator and denominator we find, to order \( f^2 \):

\[
e^{\beta U(x_1 - x_2)} n_2(x_1, x_2) =
\]

\[
x^2 \frac{1 + I_2(2x + \frac{1}{2}x^2V) + xI_3 + I_2^2(4x^2 + \frac{3}{2}x^3V + \frac{1}{8}x^4V^2)}{1 + \frac{1}{2}x^2V I_2 + I_2^2(\frac{1}{2}x^3V + \frac{1}{8}x^4V^2)}.
\]

Expanding the denominator and retaining terms to order \( I_2^2 \) we find

\[
e^{\beta U(x_1 - x_2)} n_2(x_1, x_2) = x^2 \left[ 1 + 2xI_2 + xI_3 + 4x^2I_2^2 + \ldots \right].
\]
Note that the volume \( V \) has disappeared from this expression as is required. The final step is to substitute for the chemical potential in terms of the density. This is easily done by inverting the expression

\[
n = x \frac{\partial}{\partial x} \ln Z_G = x \frac{\partial}{\partial x} \ln \{e^x V [1 + \frac{1}{2} x^2 I_2 + \frac{1}{2} x^3 V + \frac{1}{8} x^4 V^2]\}
\]

which yields

\[
x = n - I_2 n^2 + \frac{1}{2} I_2^2 n^3.
\]

Substituting, we finally obtain

\[
e^{\beta U(x_1 - x_2)} n_2(x_1, x_2) \equiv e^{\beta U} n^2 y_1(x_12) = n^2 [1 + n I_3(x_12) + \ldots].
\]

4.4

Assume that \( T = T(S, P) \). Then

\[
\left( \frac{\partial T}{\partial P} \right)_H = \left( \frac{\partial T}{\partial S} \right)_P \left( \frac{\partial S}{\partial P} \right)_H + \left( \frac{\partial T}{\partial P} \right)_S.
\]

Using

\[
\left( \frac{\partial S}{\partial P} \right)_H = -\frac{V}{T},
\]

\[
\left( \frac{\partial T}{\partial P} \right)_S = -\left( \frac{\partial S}{\partial P} \right)_T / \left( \frac{\partial S}{\partial T} \right)_P
\]

and the Maxwell relation

\[
\left( \frac{\partial S}{\partial P} \right)_T = -\left( \frac{\partial V}{\partial T} \right)_P
\]

we obtain

\[
\left( \frac{\partial T}{\partial P} \right)_H = \frac{1}{C_P} \left[ T \left( \frac{\partial V}{\partial T} \right)_P - V \right].
\]

Since the specific heat \( C_P \) is always positive, the locus of the inversion temperature is given by the expression

\[
T \left( \frac{\partial V}{\partial T} \right)_P - V = 0.
\]
Setting $dP = 0$ in the virial equation of state we find

$$\left( \frac{\partial V}{\partial T} \right)_p = \frac{V}{T} \frac{1 + n(TB_2)' + n^2(TB_3)'}{1 + 2B_2n + 3B_3n^2}$$

where $n = N/V$ and where the prime indicates differentiation with respect to $T$. Substituting into the equation for the inversion temperature we have

$$0 = T \frac{dB_2}{dT} - B_2 + n \left[ T \frac{dB_3}{dT} - 2B_3 \right]$$

to convert this expression into an equation for the inversion curve in the $P-T$ plane we may invert the virial expansion and write $n = \beta P + a(\beta P)^2 + b(\beta P)^3 + \ldots$ and solve for the coefficients $a$ and $b$. To lowest order in $\beta P$ we obtain

$$\beta P = \frac{B_2(T) - TdB_2/dT}{TdB_3/dT - 2B_3(T)}.$$
Chapter 5

Critical Phenomena,
Part 1

5.1

The calculation proceeds in exactly the same way as the diagonalization of the exact transfer matrix. After the Jordan–Wigner transformation we have

\[ V = (2 \sinh 2K)^{M/2} e^\mathcal{H} \]

with

\[ \mathcal{H} = K \sum_{j=1}^{M} (c_j^\dagger - c_j)(c_j^\dagger + c_{j+1}) + 2K^* \sum_{j=1}^{M} (c_j^\dagger c_j - \frac{1}{2}) \]

and antiperiodic boundary conditions in the subspace with an even number of fermions, periodic boundary conditions in the odd subspace. We now carry out the canonical transformation

\[ c_j = \frac{1}{\sqrt{M}} e^{-i\pi/4} \sum_q a_q e^{iqj} \]

\[ c_j^\dagger = \frac{1}{\sqrt{M}} e^{i\pi/4} \sum_q a_q^\dagger e^{-iqj} \]
and substituting, obtain
\[ \mathcal{H} = \sum_{q \geq 0} \mathcal{H}_q \]
with
\[ \mathcal{H}_q = (2K^* + 2K \cos q) \left( a_q^\dagger a_q + a_{-q}^\dagger a_{-q} \right) + 2K \sin q \left( a_q^\dagger a_{-q}^\dagger + a_{-q} a_q \right) - 2K^* . \]
The allowed values of \( q \) are precisely the same as in the case of the exact transfer matrix. The diagonalization of this operator is straightforward. The single-particle states \( a_q^\dagger |0\rangle \) and \( a_{-q}^\dagger |0\rangle \) are eigenstates of \( \mathcal{H}_q \) with eigenvalues \( 2K \cos q \). In the subspace spanned by the states \( |0\rangle \) and \( |2\rangle \) we obtain a \( 2 \times 2 \) matrix with eigenvalues
\[ \lambda_{\pm}(q) = 2K \cos q \pm 2\sqrt{K^{*2} + K^2 + 2K^*K \cos q} . \]
Clearly the largest eigenvalue is given by \( \lambda_+ \) in the above expression. As in the exact case, the two largest eigenvalues in the even and odd subspaces become degenerate at \( K = K^* \) so that the critical temperature is given exactly. The free energy per site of an \( M \times M \) lattice is then
\[ \frac{\beta G(0,T)}{M^2} = -\frac{1}{2} \ln [2 \sinh 2K] - \frac{1}{M} \sum_{q \geq 0} \lambda_+(q) . \]
The singularities in the thermodynamic functions result from the second term and we define the singular piece of the dimensionless free energy as
\[ g_s = -\frac{1}{M} \sum_{q \geq 0} \lambda_+(q) = -\frac{1}{\pi} \int_0^{\pi} dq \sqrt{K^{*2} + K^2 + 2K^*K \cos q} . \]
Substituting \( \cos q = 1 - 2\sin^2 q/2 \) we have
\[ g_s = -\frac{2}{\pi} (K^* + K) \int_0^{\pi/2} d\phi \sqrt{1 - q^2(K) \sin^2 \phi} \]
where \( q^2(K) = 4K^*K/(K^* + K)^2 \). The following simple argument shows that the internal energy remains finite at \( T = T_c \) or, equivalently, at \( q = 1 \). The singular piece of the internal energy is given by
\[ u_s = \frac{dg_s}{d\beta} \approx -\frac{2}{\pi} (K^* + K) \int_0^{\pi/2} \frac{q dq}{\sqrt{1 - q^2 \sin^2 \phi}} . \]
Since \( dq/d\beta = 0 \) at \( q = 1 \) and vanishes more rapidly as function of temperature than the weak singularity of the elliptic integral diverges, we have that \( u \) does not diverge. Either the more complete derivation of the next problem or the simple argument that \( d^2 q/d\beta^2 \) remains finite at \( q = 1 \) then shows that the approximate specific heat has the same logarithmic singularity as that found from the exact transfer matrix.

5.2

(a)

The simplest way to verify the identity

\[
\frac{\partial F(\phi, q)}{\partial q} = \frac{1}{1 - q^2} \left[ \frac{E(\phi, q) - (1 - q^2)F(\phi, q)}{q} - \frac{q \sin \phi \cos \phi}{\sqrt{1 - q^2 \sin^2 \phi}} \right]
\]

is to let \( A(\phi, q) = q \partial F(\phi, q)/\partial q \) and \( B(\phi, q) \) be the right hand side of the above expression multiplied by \( q \). It is then straightforward to show that

\[
\frac{\partial A(\phi, q)}{\partial \phi} = \frac{\partial B(\phi, q)}{\partial \phi}
\]

and therefore that \( A(\phi, q) = B(\phi, q) + C \) where \( C \) is an integration constant. Since \( A(0, q) = B(0, q) = 0 \) we have \( C = 0 \) and the desired result. The equation

\[
\frac{dK_1(q)}{dq} = \frac{E_1(q)}{q(1 - q^2)} - \frac{K_1(q)}{q}
\]

then follows simply by substituting \( \phi = \pi/2 \). The derivation of the expression (1.53) is then a simple matter of differentiation and substituting for \( dK_1/dq \).

(b)

To demonstrate the logarithmic singularity in the specific heat, we must analyze the behavior of the elliptic integral \( K_1 \) as \( q \to 1 \). The elliptic integral \( E_1 \) is clearly finite and since the factor \( (2 \tanh^2 2K - 1) \to 0 \) as \( K \to K_c \), the singularity in \( C(T) \) is entirely due to the term \( 4/\pi(K \coth 2K)^2 K_1(q) \). Let
\[ q^2 = 1 - \delta^2 \] where \( \delta \propto |T - T_c| \). Then we may write \( K_1 \) in the form

\[
K_1 = \int_0^{\pi/2} d\phi \frac{1}{\sqrt{\cos^2 \phi + \delta^2 \sin^2 \phi}} = \int_0^{\pi/2} d\phi \frac{1}{\sqrt{\sin^2 \phi + \delta^2 \cos^2 \phi}}.
\]

If \( \delta = 0 \) this integral diverges because of the singularity at \( \phi = 0 \). For small but finite \( \delta \) we write

\[
K_1(q) = \int_0^{\pi/2} d\phi \frac{1}{\sqrt{\phi^2 + \delta^2}} + \int_0^{\pi/2} d\phi \left[ \frac{1}{\sqrt{\sin^2 \phi + \delta^2 \cos^2 \phi}} - \frac{1}{\sqrt{\phi^2 + \delta^2}} \right].
\]

As \( \delta \to 0 \), the second integral remains finite and the first integral is a standard integral, the value of which is \( \ln \pi/\delta = -\ln |1 - T/T_c| + \text{const} \). Ignoring the constant, we therefore obtain

\[
\frac{C}{k_B} \approx -\frac{8k_B^2}{\pi} \ln \left| 1 - \frac{T}{T_c} \right|
\]

for \( T \to T_c \).

5.3

(a)

It is convenient to work with the reduced temperature variable \( \beta \equiv J h^2 / 4k_B T \). With this definition we have

\[
\chi = \beta + \frac{\beta \text{Tr} \sum_{j \neq i} \sigma_i \sigma_j \exp \{ \beta \sum_{nm} \vec{\sigma}_n \cdot \vec{\sigma}_m \}}{\text{Tr} \exp \{ \beta \sum_{nm} \vec{\sigma}_n \cdot \vec{\sigma}_m \}}
\]

where \( \vec{\sigma} = \{\sigma_x, \sigma_y, \sigma_z\} \) are the Pauli spin matrices. The lowest order nonzero term when the numerator is expanded in powers of \( \beta \) is of order \( \beta^2 \). Since we only require the expansion to order \( \beta^3 \) we can simply replace the denominator by \( \text{Tr}1 \). We therefore obtain

\[
\chi = \beta + \frac{\beta^2 \text{Tr} \sum_{j \neq i, (nm)} \sigma_i \sigma_j \vec{\sigma}_n \cdot \vec{\sigma}_m + \frac{\beta^3}{2} \text{Tr} \sum_{j \neq i, (nm), (kl)} \sigma_i \sigma_j \vec{\sigma}_n \cdot \vec{\sigma}_m \vec{\sigma}_k \cdot \vec{\sigma}_l}{\text{Tr}1}.
\]
In the first term of the numerator, the only nonzero contribution comes from the case when the set \((n, m)\) is the same as the set \((i, j)\) and from the term \(\sigma_{nx}\sigma_{mx}\) in the dot product. There are therefore six choices for the site \(j\). For the second term, we obtain a contribution when \(i = n, m = k \neq i\) and \(k \neq j, l = j\). There are \(q = 6\) possible choices for the site \(m\) and for each such choice, \(q - 1 = 5\) choices for \(j\). Another contribution comes from \(i = n = k, j = m = l\). In this case the \(x\) component of one scalar product and the \(y\) component of the other must be selected and there are \(q = 6\) choices for site \(j\). The result to order \(\beta^3\) is

\[
\chi = \beta + 6\beta^2 + 24\beta^3.
\]

(b) The lowest Padé approximant to this series is

\[
\chi = \frac{\beta + 2\beta^2}{1 - 4\beta}.
\]

(c) The transition occurs at \(\chi = \infty\) or \(\beta = \frac{1}{4}\). In the original units this corresponds to \(k_B T_c / J \hbar^2 = 1.0\) which is not a terrible result.

5.4

The coefficients \(a_n\) in the series \(k_B T \chi(0, T) = \sum_n a_n v^n\) for the Ising model on the triangular and the sequence of estimates \(r_n\) for \(v_c^{-1}\) and \(S_n\) for \(\gamma\) are given in the table below. Both the ratios \(a_n / a_{n-1}\) and the sequence \(r_n\) plotted as function of \(1/n\) fall essentially on straight lines that yield the estimate \(k_B T_c / J \approx 3.636\) in very good agreement with the exact result \(k_B T_c / J = 3.64098\ldots\). The extrapolated value of the exponent \(\gamma\) from the biased estimate \(S_n\) is 1.764, in quite good agreement with the exact value of 1.75.
\begin{tabular}{|c|c|c|c|}
\hline
\(n\) & \(a_n\) & \(r_n\) & \(S_n\) \\
\hline
1 & 6 & & \\
2 & 30 & 4 & 1.684 \\
3 & 138 & 3.8 & 1.703 \\
4 & 606 & 3.765 & 1.714 \\
5 & 2586 & 3.7713 & 1.726 \\
6 & 10818 & 3.7633 & 1.736 \\
7 & 44574 & 3.7430 & 1.740 \\
8 & 181542 & 3.7396 & 1.744 \\
9 & 732678 & 3.7407 & 1.748 \\
10 & 2935218 & 3.7384 & 1.751 \\
\hline
\end{tabular}

5.5

(a)

On the critical isotherm, the Landau–Ginzburg equation becomes

\[
h(r) = c(T_c)m^3(r) + d(T_c)m^5(r) \ldots - f \nabla^2 m(r) .
\]

Letting \(h(r) = h_0 + h_1 \delta(r)\) and \(m(r) = m_0(T_c, h) + \phi(r)\) and retaining only the leading powers of \(m_0\) and terms linear in \(\phi\) we obtain the equation

\[
\nabla^2 \phi - \left( \frac{3m_0^2}{f} \right) \phi(r) = -\frac{h_1}{f} \delta(r) .
\]

This has the solution

\[
\phi = \frac{h_1}{4\pi f} \frac{e^{-r/\xi}}{r}
\]

where

\[
\xi = \frac{f}{3cm_0^2} = \frac{f}{3c} |h_0|^{-2/3} .
\]

Therefore, \(\nu_H = 2/3\) and \(\eta_H = 0\) in the Landau–Ginzburg approximation.
(b)

Very generally,

\[ k_B T \chi = \int d^d r g(r, h, T) \sim \int d r r^{1-\eta_H} e^{-r/\xi} \sim \xi^{2-\eta_H}. \]

Therefore, \( \chi \sim |h|^{-\nu_H(2-\eta_H)} \) and \( \gamma_H = \nu_H(2-\eta_H) \).

(c)

From the scaling form of the free energy \( G(t, h) = \lambda G(\lambda^s t, \lambda^r h) \) we obtain \( \beta = -(r+1)/s, \gamma = (2r+1)/s, \delta = -r/(r+1) \) and \( \gamma_H = (2r+1)/r \). Therefore \( \gamma_H \delta = \gamma/\beta \).

5.6

(a)

The expression

\[ \phi(r) - \phi(0) = \frac{1}{\sqrt{N}} \sum_k \left( e^{i k \cdot r} - 1 \right) \phi_k \]

can be rewritten in the form

\[ \phi(r) - \phi(0) = \sum_k (\alpha_k + i \gamma_k) \tilde{\psi}_k = \sum_k \left[ \alpha_k (\tilde{\psi}_k + \tilde{\psi}_{-k}) + i \gamma_k (\tilde{\psi}_k - \tilde{\psi}_{-k}) \right] \]

where

\[ \tilde{\psi}_k = e^{i k \cdot r} - 1. \]

Therefore,

\[ g(r) = \prod_k \frac{\int_{-\infty}^{\infty} d \alpha_k d \gamma_k \exp \{ B \}}{\int_{-\infty}^{\infty} d \alpha_k d \gamma_k \exp \{ -\beta J S^2 a^2 k^2 (\alpha_k^2 + \gamma_k^2) \}} \]

where

\[ B = -\beta J S^2 a^2 k^2 (\alpha_k^2 + \gamma_k^2) + i \alpha_k (\tilde{\psi}_k + \tilde{\psi}_{-k}) + i \gamma_k (\tilde{\psi}_k - \tilde{\psi}_{-k}). \]
In the numerator we simply complete the squares in the exponential and integrate. This yields

\[ \ln g(r) = -\frac{k_B T}{4 JS^2 a^2} \sum_k \frac{1}{k^2} \left[ (\Psi_k + \Psi_{-k})^2 - (\Psi_k - \Psi_{-k})^2 \right]. \]

Substituting

\[ \Psi_k + \Psi_{-k} = \frac{1}{\sqrt{N}} (2 \cos k \cdot r - 2) \]
\[ \Psi_k - \Psi_{-k} = \frac{2i}{\sqrt{N}} \sin k \cdot r \]

and converting the sum to a sum over the entire Brillouin zone, we obtain

\[ g(r) = \exp \left\{ -\frac{k_B T}{JS^2 a^2 N} \sum_k \frac{1 - \cos k \cdot r}{k^2} \right\} \]

which is the desired result.

(b)

In three dimensions we have

\[ \ln g(r) = -\frac{ak_B T}{(2\pi)^3 JS^2} \int_0^{\pi/a} dk k^2 \int_{-1}^1 d(cos \theta) \int_0^{2\pi} d\phi \frac{1 - \cos \{kr \cos \theta\}}{k^2} \]

where we have replace the sum over \( k \) by an integral over a ‘spherical Brillouin zone’. Carrying out the angular integrals, we obtain

\[ \ln g(r) = -\frac{ak_B T}{2\pi^2 JS^2} \int_0^{\pi/a} dk \left( 1 - \frac{\sin kr}{kr} \right). \]

Substituting \( k = x/r \) we have

\[ \ln g(r) = -\frac{ak_B T}{2\pi^2 JS^2} \frac{1}{r} \int_0^{\pi r/a} \left( 1 - \frac{\sin x}{x} \right). \]

Since the integral of \((\sin x)/x\) is finite in the limit \( r \to \infty \), the integral is clearly proportional to \( r \) at large distances and this shows that \( g(r) \) approaches a finite limit as \( r \to \infty \).
Chapter 6

Critical Phenomena II:
The Renormalization Group

6.1

This problem is a simple matter of plugging numbers into the recursion relations for $K$ and for the free energy. The results are $K^{(0)} = 1.0$, $K^{(1)} = 0.6625$, $K^{(2)} = 0.3501$, $K^{(3)} = 0.1137$ and $K^{(4)} = 0.0128$. The free energy to this order is $f = 1.1269$.

6.2

(a)

We use the simple majority rule to define the projection operator which connects the site and block spins. For the five-spin cluster on the square lattice we have 16 states for each value of the block-spin. Consider the case of $\mu_I = +1$. The states and corresponding energies are, with $\sigma_0$ the central
spin: (1) $\sigma_0 = 1$, all other spins up, $-\beta E = 4K$; (2) $\sigma_0 = 1$, one perimeter spin down, $-\beta E = 2K$, 4 different states; (3) $\sigma_0 = 1$, two perimeter spins down, $-\beta E = 0$, six different states; (4) $\sigma_0 = -1$, one perimeter spin down, $-\beta E = -2K$, 4 different states; and (5) $\sigma_0 = -1$; all perimeter spins up, $-\beta E = -4K$. Therefore the restricted partition function for the block is

$$Z_0(+) = e^{4K} + e^{-4K} + 4 (e^{2K} + e^{-2K}) + 6$$

and the expectation value of $\langle \sigma_i \rangle$ for each of the perimeter spins is given by:

$$\langle \sigma_i \rangle = \frac{e^{4K} + e^{-4K} + 2 (e^{2K} + e^{-2K})}{Z_0(+)}. $$

The partition function $Z_0(-)$ is identical to $Z_0(+)$ and the magnetization simply changes sign. Therefore, in the cumulant approximation we have

$$K' = 3K \langle \sigma_{I,i} \rangle \langle \sigma_{J,j} \rangle = 3KB(K)^2$$

where

$$B(K) = \frac{\cosh 4K + 2 \cosh 2K}{\cosh 4K + 4 \cosh 2K + 3}.$$

Using $\cosh 4K = 2 \cosh^2 2K - 1$ one can obtain a quadratic equation for $\cosh 2K$. Solving we find $K^* = K_c = 0.5931$. The thermal critical exponent is given by

$$\left( \sqrt{5} \right)^{y_1} = \left. \frac{\partial K'}{\partial K} \right|_{K^*}.$$

Differentiating and substituting, we find $y_1 = 0.901$ or $\alpha = -0.22$.

(b)

The recursion relation on the triangular lattice is given by

$$K' = 3K \langle \sigma_I \rangle \langle \sigma_J \rangle$$

where $\sigma_I$ represents any of the six spins on the outer ring of hexagon $I$ and $\sigma_J$ an appropriate spin on neighboring hexagon $J$. Again, using the majority rule we have 64 states in each subspace. The complicating feature in this case is that the energy depends on the relative location of aligned spins on the
perimeter. In the $\mu_I = +1$ subspace, consider the case of the central spin up. For six or five perimeter spins up there is no problem and the energies are $12K$ and $6K$ respectively. If there are two down spins on the perimeter, the six states in which the down spins are adjacent have energy $4K$, the remaining 9 states all have energy 0. Similarly, if there are three spins down on the perimeter, we have three separate cases: (1) adjacent, $-\beta E = 2K$, 6 states; (2) two down spins together, the third separated, $-\beta E = -2K$; (3) alternating $+/-$, $-\beta E = -6K$. Similar considerations yield the energies for the case when the central spin is down. The partition function is therefore

$$Z_0(+) = e^{12K} + 6e^{6K} + 6e^{4K} + 6e^{2K} + 16 + 18e^{-2K} + 9e^{-4K} + 2e^{-6K}.$$  

Similarly, we obtain

$$Z_0(+) \langle \sigma_i \rangle = e^{12K} + 4e^{6K} + 2e^{4K} + 6 + 4e^{-2K} + 3e^{-4K}$$

and from above, the recursion relation. The solution of this equation requires a small computer program or a software package such as Mathematica. The results for the critical coupling constants and exponents are: $K^* \approx 0.30033$, $y_1 \approx 0.919$ or $\alpha \approx -0.18$.

(c) The blocks on the honeycomb lattice have an even number of spins and we therefore have to modify the majority rule. We could take the six states with $\sum_i \sigma_i = 0$ and give them all a weight of $\frac{1}{2}$ but count them for both the up-spin and down-spin subspace. We have chosen to count the three that have two of the exterior spins up as part of the up-spin subspace, the other three as part of the down-spin subspace. With this choice, the calculation is trivial and

$$Z_0(+) = 2 \cosh 3K + 6 \cosh K$$

and

$$\langle \sigma_i \rangle = \frac{\cosh 3K + \cosh K}{\cosh 3K + 3 \cosh K}.$$  

By reexpressing $\cosh 3K$ in terms of $\cosh K$ one can reduce the equation determining the fixed point to a linear equation in $\cosh^2 K$. This produces $K^* = K_c = 0.764$ and $y_1 = 0.86$ or $\alpha = -0.326$. 
6.3

Refer to Figure 6.3 for the labeling of the blocks. Blocks \( I \) and \( L \) are second neighbors and block \( L \) can be reached from \( I \) via either \( J \) or \( K \). There are four terms of order \( K_1^2 \) from each of these paths with one special term:

\[
K_1^2 \langle \sigma_1 \sigma_3 J \sigma_3 J \sigma_2 \rangle = K_1^2 D^2 (K_1) \mu_I \mu_L.
\]

The other 7 terms are all of the same form as

\[
K_1^2 \langle \sigma_1 \sigma_2 J \sigma_3 J \sigma_2 \rangle = K_1^2 D^2 (K_1) E(K_1) \mu_I \mu_L.
\]

Therefore, the contribution from \( \frac{1}{2} [(V^2) - \langle V \rangle^2] \) to the coupling between blocks \( I \) and \( L \) is \( K_1^2 [D^2 + 7D^2 E - 8D^4] \). As well, there is a contribution of order \( K_3 \) from the direct third-neighbor interaction \( K_3 \sigma_1 \sigma_2 \). Therefore,

\[
K_2' = K_1^2 [7D^2 E + D^2 - 8D^4] + K_3 D^2
\]

The terms of second order that contribute to \( K_1' \) involve either the block \( K \) or the symmetrically placed unlabeled block to the left of the pair \( IJ \). The contributions from these two paths are the same. The total is

\[
\langle V^2 \rangle_{IJ} = 4K_1^2 \langle \sigma_1 \sigma_2 K \sigma_2 K \sigma_3 J \rangle + 4 \langle \sigma_1 \sigma_2 K \sigma_1 K \sigma_3 J \rangle
\]

\[
= 4 [D^2(K_1) + D^2(K_1) E(K_1)] \mu_I \mu_J.
\]

There are also three direct second neighbor couplings between blocks \( I \) and \( J \) as well as two third neighbor couplings. Therefore, the final result is

\[
K_1' = 2K_1 D^2(K_1) + 4K_1^2 \left[ D^2(K_1) + D^2(K_1) E(K_1) - 2D^4(K_1) \right] + 3K_2 D^2(K_1) + 2K_3 D^2(K_1).
\]

The calculation of \( K_3' \) is given in the text.

6.4

The trace over the spins connecting alternate rows is of the form

\[
\text{Tr}_{\sigma_0} \exp\{K \sigma_0 (\sigma_1 + \sigma_2)\} = 2 \cosh K (\sigma_1 + \sigma_2) = \exp\{a(K) + \gamma(K) \sigma_1 \sigma_2\}.
\]
Therefore, \( \gamma(K) = \frac{1}{2} \ln \cosh 2K \). By the same reasoning \( \gamma'(K) = \frac{1}{2} \ln \cosh 4K \).

Thus the recursion relation is

\[
K' = \frac{1}{2} \left[ \ln \cosh 2K + \ln \cosh 4K \right].
\]

Numerically solving for the fixed point we obtain \( K^* \approx 0.544 \) and from

\[
2^{y_1} = \tanh 2K^* + 2 \tanh 4K^*
\]

\( y_1 \approx 1.46 \) which is not in spectacular agreement with the exact value \( y_1 = 1 \).

### 6.5

**Note to the instructor:** The calculation of part (a) is rather lengthy. Parts (b)–(e), taking the recursion relations as given, form a useful exercise on their own.

(a)

We write the dimensionless Hamiltonian \( H \) in the form

\[
H = H_{s,0} + H_{n,0} + \tilde{V}_1 + \tilde{V}_2 + \tilde{V}_3
\]

where \( H_{s,0} \) and \( H_{n,0} \) are the Gaussian terms for the first \( m \) components and for the \( n \)-th component respectively. The terms \( \tilde{V}_j \) refer to the three different four-spin terms. Through second order in perturbation theory the new Hamiltonian—before rescaling—will be of the form

\[
e^{H'} = \exp \left\{ H_{s,0} + H_{n,0} + \left[ \tilde{V}_1 + \tilde{V}_2 + \tilde{V}_3 \right] + \sum_{i,j=1}^{3} \frac{1}{2} \left[ \left( \tilde{V}_i \tilde{V}_j \right) - \left( \tilde{V}_i \right) \left( \tilde{V}_j \right) \right] \right\}
\]

where only spins with wavevector \( |q| < \pi/l \) remain. We briefly describe the calculation of the various terms.

(i) \( \langle \tilde{V}_1 \rangle \) and \( \langle \tilde{V}_3 \rangle \)

These two cases are exactly the same as the calculation in the book except that \( n \) is replaced by \( m \) and by 1 and \( r \) is replaced by \( r_s \) and \( r_n \) respectively.
(ii) \( \langle \tilde{V}_2 \rangle \)
Here we must take either the pair \( q_1, q_2 \) or the pair \( q_3, q_4 \) in the region \( |q| > \pi/l \). Other terms vanish by symmetry. The result is

\[
\langle \tilde{V}_2 \rangle = 2V_2 \sum_{|q|<\pi/l} \sum_{\alpha=1}^{m} S_\alpha^q S_\alpha^{-q} \left[ \frac{1}{N} \sum_{|q|>\pi/l} \frac{1}{r_n + q^2} \right] \\
+ 2mV_2 \sum_{|q|<\pi/l} S_\alpha^q S_\alpha^{-q} \left[ \frac{1}{N} \sum_{|q|>\pi/l} \frac{1}{r_s + q^2} \right].
\]

(iii) \( \frac{1}{2} \left[ \langle \tilde{V}_i^2 \rangle - \langle \tilde{V}_i \rangle^2 \right] \) for \( i = 1, 3 \).
As in case (i), the results may be directly transcribed from the \( n \)-vector model.

(iv) \( \frac{1}{2} \left[ \langle \tilde{V}_2^2 \rangle - \langle \tilde{V}_2 \rangle^2 \right] \)
The starting point is the expectation value of terms of the form

\[
S_{\alpha_1}^q S_{\alpha_2}^q S_{\alpha_3}^n S_{\alpha_4}^n S_{\alpha_5}^\beta S_{\alpha_6}^\beta S_{\alpha_7}^n S_{\alpha_8}^n \Delta(q_1 + q_2 + q_3 + q_4) \Delta(q_5 + q_6 + q_7 + q_8).
\]

The nonzero contributions come from three different cases. The first two are when either the four wavevectors \( q_1, q_2, q_5, q_6 \) are in the outer shell or, conversely when the other set of four \( q \)'s are in this region. In the first case, we can pair the wavevectors in two different ways. This also requires \( \alpha = \beta \) and the resulting expression is

\[
4mV_2^2 \sum_{q_1, q_2, q_3, q_4} S_{\alpha_1}^n S_{\alpha_2}^n S_{\alpha_3}^n S_{\alpha_4}^n \\
\times \sum_{q, q' > \pi/l} \Gamma_s(q) \Gamma_s(q') \Delta(q_1 + q_2 + q_3 + q_4) \Delta(q_3 + q_4 - q - q')
\]

where \( \Gamma_s(q) = [r_s + q^2]^{-1} \) and \( \Gamma_n = [r_n + q^2]^{-1} \) The second case contributes to the renormalization of the coupling \( V_1 \). The resulting expression is entirely analogous except that \( m \) is replaced by 1 and \( \Gamma_s \) by \( \Gamma_n \). Finally, there are 16 different ways of selecting pairs of wavevectors of the type \( q_1, q_5, q_3, q_7 \). This choice imposes \( \alpha = \beta \) and we obtain a contribution to the renormalization of the coupling constant \( V_2 \). The result of averaging is

\[
32V_2^2 \sum_{q_1, q_2, q_3, q_4} S_{\alpha_1}^\alpha S_{\alpha_2}^\alpha S_{\alpha_3}^\alpha S_{\alpha_4}^\alpha
\]
\begin{align*}
&\times \sum_{q,q' \gg \pi/l} \Gamma_s(q) \Gamma_n(q') \Delta(q_1 + q_2 + q_3 + q_4) \Delta(q_3 + q_4 - q - q').
\end{align*}

\textbf{(v) } \langle \tilde{V}_1 \tilde{V}_2 \rangle - \langle \tilde{V}_1 \rangle \langle \tilde{V}_2 \rangle.

We first note that the factor of $\frac{1}{2}$ disappears because this term can be generated in two different ways. To obtain a contribution to the renormalized four-spin terms, we must choose four of the $q$-vectors in the expression

$$S_1^\alpha, S_2^\alpha, S_3^\beta, S_4^\beta, S_5^\delta, S_6^\delta, S_7^m, S_8^m \Delta(q_1 + q_2 + q_3 + q_4) \Delta(q_5 + q_6 + q_7 + q_8)$$

to lie in the outer shell. Two of these must come from the first four $q$'s and, of course, the pair $q_7, q_8$ must be either in the inner shell or the outer shell. If $q_7, q_8$ are in the outer shell, then there is no way to match them with a pair of wave-vectors from the first four and all contributions are canceled by the same terms in $\langle \tilde{V}_1 \rangle \langle \tilde{V}_2 \rangle$. Therefore, we must choose $q_5, q_6$ and two wavevectors from $q_1 \ldots q_4$. If we choose either the pair $q_1, q_2$ or the pair $q_3, q_4$ we get $2m$ identical contributions. If we choose one from each of these pairs, we lose a sum over $\alpha$ and there are only 8 further terms. The resulting expression is

$$(2V_2V_1)(4m + 8) \sum_{q_1, q_2, q_3, q_4} S_1^\alpha S_2^\alpha S_3^m S_4^m$$

$$\times \sum_{q, q' \gg \pi/l} \Gamma_s(q) \Gamma_n(q') \Delta(q_1 + q_2 + q_3 + q_4) \Delta(q_3 + q_4 - q - q'),$$

where the index $\alpha$ is understood to be summed from 1 to $m$.

\textbf{(vi) } \langle \tilde{V}_1 \tilde{V}_3 \rangle - \langle \tilde{V}_1 \rangle \langle \tilde{V}_3 \rangle.

This term does not contribute because there are no nonzero averages when spins from the two terms are paired.

\textbf{(vii) } \langle \tilde{V}_2 \tilde{V}_3 \rangle - \langle \tilde{V}_2 \rangle \langle \tilde{V}_3 \rangle.

This case is very similar to case (v). In fact the resulting expression can be directly transcribed by replacing $m$ by 1, $V_1$ by $V_3$ and $\Gamma_s$ by $\Gamma_n$.

The next step is to combine all this information. As in formulas (6.144)-(6.148) we approximate the sums of $\Gamma_{s,n}(q)$ by $c\delta/(1 + r_{s,n})$ and the sum over a product of these functions by the analogue of (6.148). We also carry out the spin and spatial rescaling to obtain the recursion relations given in the book.
Since \( l = 1 + \delta \) we write, as in the text, \( K'_j - K_j = \delta \partial K_j / \partial l \) where \( K_1 \) is any of the five coupling constants, and keep only linear order in \( \delta \). Noting that \( K'_j \sim O(\varepsilon) \) we disregard the factors \([1+r_{s,n}]^{-1}\) in the expressions for \( V'_j \). After dividing by \( \delta \) the recursion relations are

\[
\begin{align*}
\frac{\partial r_s}{\partial l} &= 2r_s - \frac{4(n + 1)}{1 + r_s} c V_1 - \frac{4c}{1 + r_n} V_2 \\
\frac{\partial r_n}{\partial l} &= 2r_n - \frac{4(n - 1)c}{1 + r_s} V_2 - \frac{12c}{1 + r_n} V_3 \\
\frac{\partial V_1}{\partial l} &= \varepsilon V_1 + 4(n + 7c V_1^2 + 4c V_2^2) \\
\frac{\partial V_2}{\partial l} &= \varepsilon V_2 + 16c V_3^2 + 4(n + 1)c V_1 V_2 + 12c V_2 V_3 \\
\frac{\partial V_3}{\partial l} &= \varepsilon V_3 + 4(n - 1)c V_2^2 + 36c V_3^2.
\end{align*}
\]

Setting these equations equal to zero yields the fixed points. It is easy to verify that the Ising, Heisenberg and \( XY \) fixed points are solutions of this equation and that they correspond to the solutions found in the text:

**Ising**

Set \( r_s^* = \infty \) and \( V_2 = V_3 = 0 \). Then \( V_3^* = -\varepsilon / 36c \) and \( r_n^* = -\varepsilon / 6 \).

**Heisenberg**

For \( r_s = r_n = r \) and \( V_1 = V_2 = V_3 = V \) the first two and last three equations become identical and yield the solution \( r^* = -\varepsilon (n+2) / 2(n+8) \), \( V^* = -\varepsilon / 4(n+8)c \).

**XY**

Setting \( r_n = \infty \) and \( V_2 = V_3 = 0 \) produces the same solution as for the Heisenberg model with \( n \) replaced by \( n - 1 \). Thus we have the fixed point of an \( n - 1 \) component isotropic Heisenberg model or, in the case of \( n = 3 \), an \( XY \) model.

Since the recursion relations are exactly of the form (6.150)–(6.151) it is clear that the linearized versions and the critical exponents will correspond to special cases of the \( n \)-vector model.
(c)

Following exactly the same procedure as in (6.154)–(6.157) we can calculate the elements of the $5 \times 5$ matrix $M$, the eigenvalues of which determine the critical exponents and the stability of the various fixed points. Clearly, we have $\partial V'_j/\partial r_{n,s} = O(c^2)$ at the fixed points since these derivatives involve products of the fixed point values of the various $V$'s. Therefore, the matrix $M$ has $M_{j1} = M_{j2} = 0$ for $j = 3, 4, 5$. To determine the scaling fields we would have to find the left eigenvectors. However, the right eigenvectors have the same set of eigenvalues and we can therefore use them if we only want the eigenvalues. Clearly, the vector

$$\Psi = \begin{bmatrix} a \\ b \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

satisfies the equation

$$M\Psi = \lambda\Psi .$$

The secular determinant is simply a $2 \times 2$ determinant and the eigenvalues are given by

$$\lambda_{\pm} = \frac{M_{11} + M_{22}}{2} \pm \frac{1}{2} \sqrt{(M_{11} - M_{22})^2 + 4M_{12}M_{21}} .$$

Evaluating derivatives of the recursion relations, we have quite generally

$$M_{11} = 1 + 2\delta + 4(n + 1)c\delta V_1^* ,$$

$$M_{12} = 4c\delta V_2^* ,$$

$$M_{21} = 4(n - 1)c\delta V_2^* ,$$

$$M_{22} = 1 + 2\delta + 12c\delta V_3^* .$$

Substituting, we obtain $\lambda_{\pm} = 1 + 2\delta - 2\epsilon/(n + 8) \approx (1 + \delta)y_2$ or $y_2 = 2 - 2\epsilon/(n + 8)$ and $\lambda_{\pm} = 1 + 2\delta - \epsilon(n + 2)/(n + 8) \approx (1 + \delta)y_1$ or $y_1 = 2 - (n + 2)\epsilon/(n + 8)$.
A reasonable estimate for the onset of Ising-like critical behavior is $|t|^\phi \approx a = 10^{-3}$. In three dimensions with $\phi = 22/25$ we get $|t| < .0023$.

At the Ising fixed point, we have $r_s = \infty$. Instead of $r_s$ and $r_n$ as coupling constants, it is more appropriate to take $r_n$ and $r_s^{-1}$. The recursion relation for $r_s^{-1}$ then becomes

$$r_s^{-1} = l^{-2}(r_s^{-1} + O(\epsilon)).$$

Clearly, the terms of order $\epsilon$ cannot compensate for the $l^{-2}$ and the Ising fixed point therefore has only one positive exponent and is stable. Similar considerations lead to the conclusion that the $XY$ fixed point is stable.
Chapter 7

Simulations

The problems in this chapter are, with the exception of Problem 7.3 computer projects. Since nobody wants to copy by hand long computer listings (and simulation source code tends to be rather long) we do not include any listings in this solution manual. However, source code in "c" is available by electronic mail upon request to birger@physics.ubc.ca. These programs are rather primitive, and there has not been a great deal of effort put into casting the programs into the currently recommended object-oriented programming style.

7.3

We have $P_{\alpha\leftarrow\alpha} = 1/2$, $P_{\alpha\leftarrow\beta} = 1$, $P_{\beta\leftarrow\alpha} = 1/2$, $P_{\beta\leftarrow\alpha} = 0$. The normalized solutions to

$$\begin{pmatrix} P_\alpha \\ P_\beta \end{pmatrix} = \begin{pmatrix} \frac{1}{2} & 1 \\ \frac{1}{2} & 0 \end{pmatrix} \begin{pmatrix} P_\alpha \\ P_\beta \end{pmatrix}.$$ 

Giving for the normalized probabilities $P_\beta = \frac{1}{3}$, $P_\alpha = \frac{2}{3}$.
Chapter 8

Polymers and Membranes

8.1

(a)

The vector \( \mathbf{w}_i \) is perpendicular to \( \mathbf{r}_{i-1} \) and is uncorrelated with \( \mathbf{r}_i \). Therefore

\[
\langle \mathbf{r}_i \cdot \mathbf{r}_{i-n} \rangle = \langle \mathbf{r}_{i-1} \cdot \mathbf{r}_{i-n} \rangle \cos \theta + \langle \mathbf{w}_i \cdot \mathbf{r}_{i-n} \rangle = \langle \mathbf{r}_{i-1} \cdot \mathbf{r}_{i-n} \rangle \cos \theta.
\]

Clearly this procedure can be continued:

\[
\langle \mathbf{r}_i \cdot \mathbf{r}_{i-n} \rangle = \langle \mathbf{r}_{i-2} \cdot \mathbf{r}_{i-n} \rangle \cos^2 \theta = \ldots = \langle \mathbf{r}_{i-n} \cdot \mathbf{r}_{i-n} \rangle \cos^n \theta = a^2 \cos^n \theta.
\]

(b)

Let \( v = \cos \theta \) and write

\[
S_N^2 = N a^2 + \sum_{n \neq m} \langle \mathbf{r}_n \cdot \mathbf{r}_m \rangle
\]

\[
= N a^2 + 2 \sum_{n > m} \langle \mathbf{r}_n \cdot \mathbf{r}_m \rangle
\]

\[
= N a^2 + 2a^2 \sum_{n=2}^{N} \sum_{m=1}^{n-1} v^{n-m}.
\]
Carrying out the sum over \( m \) we obtain, at fixed \( n \),

\[
\sum_{m=1}^{n-1} v^{n-m} = \frac{v}{1-v} - \frac{v^n}{1-v}.
\]

The sum over \( n \) is also carried out quite easily with the result:

\[
S_N^2 = Na^2 + (N-1) \frac{2a^2v}{1-v} - \frac{2a^2v^2}{1-v} \frac{1 - v^{N-1}}{1-v}.
\]

Combining the terms proportional to \( N \) and the remainder we find

\[
S_N^2 = Na^2 \frac{1+v}{1-v} - 2a^2v \frac{1 - v^N}{(1-v)^2}
\]

which is the required result.

8.2

(a)

The Hamiltonian of the Gaussian chain is

\[
H = \frac{3k_B T}{2a^2} \int_0^N dn \left( \frac{\partial R}{\partial n} \right)^2.
\]

Substituting \( R(n) = \sum_k A_k \cos kn \) we have

\[
H = \frac{3k_B T}{2a^2} \int_0^N dn \sum_{k,k'} A_k \cdot A_{k'} \sin kn \sin k'n.
\]

Using the orthogonality of the trigonometric functions, we obtain

\[
H = \frac{3Nk_B T}{4a^2} \sum_k |A_k|^2 k^2.
\]

(b)

Equipartition yields, for each of the components of the vector \( A_k \)

\[
\frac{3Nk_B T}{4a^2} \langle A_{k,\alpha}^2 \rangle k^2 = \frac{1}{2} k_B T
\]

or

\[
\langle |A_k|^2 \rangle = \frac{2a^2}{Nk^2}.
\]
(c) The end-to-end distance is given by

$$ S_N^2 = \langle [\mathbf{R}(N) - \mathbf{R}(0)] \cdot [\mathbf{R}(N) - \mathbf{R}(0)] \rangle. $$

Substituting the Fourier representation of $\mathbf{R}$ and using

$$ \langle \mathbf{A}_k \cdot \mathbf{A}_{k'} \rangle = \delta_{kk'} \left\langle |\mathbf{A}_k|^2 \right\rangle $$

we find

$$ S_N^2 = \frac{2a^2}{N} \sum_k \frac{(\cos kN - 1)^2}{k^2}. $$

Since $k = j\pi/N$, we see that only terms with $j$ an odd integer contribute and, therefore that

$$ S_N^2 = \frac{8Na^2}{\pi^2} \sum_{l=0}^{\infty} \left( \frac{1}{2l+1} \right)^2 = Na^2. $$

8.3

(a) Write the Hamiltonian in the form

$$ H = \frac{3k_BT}{2a^2} \sum_i \mathbf{r}_i^2 - \mathbf{F} \cdot \sum_i \mathbf{r}_i. $$

Then

$$ \langle x_i \rangle = \frac{\int_{-\infty}^{\infty} dx_i x_i \exp\left\{-\frac{3x_i^2}{2a^2} + \beta F x_i \right\}}{\int_{-\infty}^{\infty} dx_i \exp\left\{-\frac{3x_i^2}{2a^2} + \beta F x_i \right\}}. $$

Completing the square in the exponential in both numerator and denominator, we obtain

$$ \langle x_i \rangle = \frac{\int_{-\infty}^{\infty} dx_i x_i \exp\left\{-\frac{3x_i^2}{2a^2} (x_i - \bar{x})^2 \right\}}{\int_{-\infty}^{\infty} dx_i \exp\left\{-\frac{3x_i^2}{2a^2} (x_i - \bar{x})^2 \right\}} $$

where $\bar{x} = \frac{\beta F a^2}{3}$. Clearly,

$$ \langle x_i \rangle = \bar{x} $$
and

$$\langle r_i \rangle = \frac{\beta a^2}{3} F.$$  

Similarly,

$$\langle x_i^2 \rangle = \langle (\bar{x} + (x - \bar{x}))^2 \rangle = \bar{x}^2 + \frac{a^2}{3}$$

and

$$\langle r_i^2 \rangle = \frac{\beta^2 a^4}{9} F^2 + a^2.$$  

The end-to-end distance may be written in the form

$$S_n^2 = \left\langle \left( \sum_i r_i \right)^2 \right\rangle = \sum_i \langle r_i^2 \rangle + \sum_{i \neq j} \langle r_i \cdot r_j \rangle$$

$$= N \left[ a^2 + \frac{1}{9} \beta^2 a^4 F^2 \right] + N(N - 1) \langle r_i \rangle \cdot \langle r_j \rangle$$

$$= N a^2 + \frac{1}{9} N^2 a^4 \beta^2 F^2$$

where we have used the fact that the fluctuations of different vectors $r_i$ are independent.

(b)

The partition function of the chain under tension can be written in the form

$$Z(F) = \prod_i \left[ \int d^3 r_i \exp\left\{ -\frac{3}{2a^2} (r_i - \beta a^2 F / 3)^2 \right\} e^{\beta^2 a^2 F^2 / 6} \right]$$

$$= Z(0) \exp\left\{ -\frac{N \beta^2 F^2 a^2}{6} \right\} = \exp\left\{ -\beta [A(0) + \Delta A] \right\}$$

where $A(0)$ is the free energy if no force is applied. From part (a) we have

$$S_N^2(F) = S_N^2(0) + \frac{N^2 F^2 a^4 \beta^2}{9}$$

or

$$F^2 = \frac{9k_B T^2}{N^2 a^4} \left[ R^2(F) - R^2(0) \right].$$

Substituting into the expression for $\Delta A$ we have

$$\Delta A = -\frac{3k_B T}{2Na^2} \left[ R^2(F) - R^2(0) \right].$$
8.4

(a)

In Figure 8.1 we show how to generate self-avoiding walks of \( N \) steps recursively, beginning with the nearest neighbor walk which can be taken in any one of four equivalent ways. The numbers next to the lines are the number of equivalent ways the line can be added to the lower order graph. For \( N = 3 \), the dashed lines represent different inequivalent possibilities. Clearly, this process can be continued in a straightforward way to \( N = 5 \). In Figure 8.2 we show the last step in obtaining five-step walks from four-step walks, the dashed lines representing the last step. Each dashed line except the vertical one in the second graph enters with a multiplicity of 1 and all four-step graphs except the second one have a multiplicity of 8. There are therefore 4, 12, 36, 100 and 284 self-avoiding walks of 1–5 steps. The average end-to-end distance is given by

\[
S_N^2 = \frac{\sum_j R^2(j)}{N_N}
\]

where \( R(j) \) is the end-point of the \( j \)th walk. Straightforward enumeration yields \( S_1^2 = 1 \), \( S_2^2 = \frac{2}{3} \), \( S_3^2 = \frac{5}{9} \), \( S_4^2 = \frac{7}{25} \) and \( S_5^2 = \frac{40}{71} \).
Figure 8.1: Self-avoiding walks of up to 3 steps.

Figure 8.2: Self-avoiding walks of 5 steps.
Figure 8.3: Plot of the end-to-end distance of self avoiding walks of $N$ steps on the square lattice.

(b)

A plot of $S_N^2$ is shown below along with a fit to a power law. The estimate of the exponent is $\nu \approx 0.7$. 
Chapter 9

Quantum Fluids

9.1

(a)

We have from (9.15) in the text

\[
\Omega(V, T, z) = -PV = \begin{cases} 
-aT^{5/2} g_{5/2}(z) & T > T_c \\
-aT^{5/2} \zeta(5/2) & T < T_c 
\end{cases}
\]

By differentiating we obtain

\[
S = - \left( \frac{\partial \Omega}{\partial T} \right)_{V, \mu} = \begin{cases} 
\frac{5}{2} aT^{3/2} g_{5/2}(z) + aT^{5/2} \frac{dg_{5/2}(z)}{dz} \frac{\partial z}{\partial T} & \text{for } T > T_c \\
\frac{5}{2} aT^{3/2} \zeta(5/2) & \text{for } T < T_c 
\end{cases}
\]

Using the definition (9.6) in the text and integrating by parts we find

\[
\frac{dg_{\nu}}{dz} = -\frac{1}{z^2 \Gamma(\nu)} \int_0^\infty dx \frac{x^{\nu-1} e^x}{(\frac{z}{z} e^x - 1)^2} = \frac{(\nu - 1) \Gamma(\nu - 1)}{z \Gamma(\nu)} g_{\nu-1}(z) = \frac{1}{z} g_{\nu-1}(z) .
\]

We also have

\[
\left( \frac{\partial z}{\partial T} \right)_{V, \mu} = \left( \frac{\partial \exp\{\frac{\mu}{k_B T}\}}{\partial T} \right)_{V, \mu} = -\frac{\mu}{k_B T^2} \exp\{\frac{\mu}{k_B T}\} = -\frac{z \ln z}{T} .
\]
We find for $T > T_c$

$$S = \frac{5}{2} aT^{3/2} g_{5/2}(z) + aT^{3/2} g_{3/2}(z) \ln(z).$$

We have (9.7) in the text for $T > T_c$

$$N = \frac{aT^{3/2}}{k_B} g_{3/2}(z)$$

(9.2)

which finally yields the desired result

$$S = \frac{5}{2} aT^{3/2} g_{5/2}(z) + k_B N \ln z.$$ 

(b)

From

$$C_{V,N} = T \left( \frac{\partial S}{\partial T} \right)_{V,z} + T \left( \frac{\partial S}{\partial z} \right)_{V,T} \left( \frac{\partial z}{\partial T} \right)_{V,N}$$

and (9.1) we find for $T > T_c$

$$C_{V,N} = \frac{15}{4} aT^{1/2} g_{5/2}(z) + \frac{7Nk_B}{2z} \left( \frac{\partial z}{\partial T} \right)_{V,N}.$$ 

(9.3)

By differentiating (9.2) using (9.1) we find

$$\left( \frac{\partial z}{\partial T} \right)_{V,N} = \frac{3gz_{3/2}(z)}{2Tg_{1/2}(z)}$$

(9.4)

Since $g_{1/2}(z) \rightarrow \infty$ as $z \rightarrow 1$ we have

$$\left( \frac{\partial z}{\partial T} \right)_{V,N} \rightarrow 0$$

as $T \rightarrow T_c$ or

$$C_{V,N} \rightarrow \frac{15}{4} aT^{3/2} \zeta_{5/2} = C_{V,N}(T < T_c)$$

i.e. the specific heat is continuous at the transition.
(c) To answer this question we need to find out how $g_{1/2}(z)$ diverges as $z \to 1$. From 5.2.3 in the text we have that if a function diverges as

$$(1 - z)^{-\gamma}$$

and has a power series $z = \sum_{n=0}^{\infty} a_n z^n$, we expect the approximant

$$S_n = 1 + n \left( \frac{a_n}{a_n - 1} - 1 \right)$$

to approach $\gamma$ as $n \to \infty$.

From (9.6) in the text

$$g_{1/2}(z) = \sum_{n=1}^{\infty} \frac{z^n}{\sqrt{n}}$$

we find

$$\gamma = \lim_{n \to \infty} n \left( \frac{\sqrt{n}}{\sqrt{n} - 1} - 1 \right) = \frac{1}{2}.$$  

From (9.3) and (9.4) we find that $C_{V,N}$ above $T_c$ will contain a term $\propto (z - 1)^{1/2}$. When differentiating this term we get a term $\propto (z - 1)^{-1/2}$, while $(\partial z / \partial T)_{N,V}$ gives rise to a cancelling term $\propto (z - 1)^{1/2}$. These terms are absent below $T_c$ but the total temperature derivative of the terms approaches a constant. Therefore, $(\partial C_{V,N} / \partial T)_{N,V}$ will be discontinuous at the transition.

(d) Since $P = -\Omega / V$ we can apply the same arguments as above to the temperature derivatives of $P$ at constant $V$ and $N$. We find that $P$, $(\partial P / \partial T)_{V,N}$, and $(\partial^2 P / \partial T^2)_{V,N}$ will be continuous at the transition, while $(\partial^3 P / \partial T^3)_{V,N}$ will be discontinuous.

9.2

Bose condensation takes place when the concentration reaches a critical value

$$n_c = \left( \frac{mk_B T}{2\pi \hbar^2} \right)^{3/2} \zeta(3/2).$$
Using \( m = 1.67 \times 10^{-27} \text{kg} \), \( k_B = 1.38066 \text{J/K} \), \( \hbar = 1.05459 \times 10^{-34} \text{Js} \), \( T = 0.1 \text{K} \), \( \zeta(3/2) = 2.612 \) we get \( n_c = 1.57 \times 10^{25} \text{m}^{-3} \).

The surface energy is \( 4\pi r^2 \sigma \) where \( r \) is the radius of the bubble and \( \sigma \) is the surface tension. Let the radius change by a small amount \( dr \). Then

\[
dE = 8\pi \sigma r dr = PdV = 4\pi r^2 dr
\]

and we find that the pressure and the surface tension are in mechanical balance if

\[
P = \frac{2\sigma}{r}.
\]

As the bubble shrinks due to hydrogen recombination the pressure increases until we reach the critical pressure

\[
P_c = \left( \frac{m}{2\pi \hbar^2} \right)^{3/2} (k_B T)^{5/2} \zeta(5/2).
\]

At this point the bubble will collapse. Substituting \( \zeta(5/2) = 1.341 \) gives \( P_c = 11 \text{Pa} \). At this pressure the radius of the bubble is \( 6.7 \times 10^{-5} \text{m} \) and there are \( N = 4\pi n_c r^3 / 3 = 1.93 \times 10^{13} \) particles in the bubble.

### 9.3

The gas of phonons and rotons is assumed to be in equilibrium with respect to the laboratory frame, while the superfluid component is moving with velocity \( v \) with respect to this frame. Let \( p \) be the momentum of an elementary excitation in the superfluid frame and \( \epsilon(p) \) the corresponding energy in this frame. In the laboratory frame the energy is \( \epsilon(p) - p \cdot v \). The equilibrium value of the average number of these excitations are thus given by the Bose–Einstein distribution

\[
n(\epsilon - p \cdot v) = \frac{1}{\exp \beta [\epsilon - p \cdot v] - 1}.
\]

(a)

The momentum of the gas of excitations in the superfluid frame is thus given by

\[
P = \sum_p p n(\epsilon - p \cdot v) \approx -\sum_p p(p \cdot v) \frac{dn}{d\epsilon} = \frac{-v}{3} \sum_p p^2 \frac{dn}{d\epsilon}.
\]

(9.5)
Chapter 9. Quantum Fluids

The inertia of this gas is with \( V \) the volume
\[
\frac{P}{V} = -\frac{V}{3} \frac{4\pi}{\hbar^3(2\pi)^3} \int_0^\infty p^2 dp \frac{d^2}{d\epsilon}.
\]
In the case of phonons \( \epsilon = cp \). With \( x = \beta cp \) we find for the phonon inertia
\[
-\frac{V}{\beta^4c^5\hbar^36\pi^2} \int_0^\infty dx x^4 \frac{d}{dx} \left(\frac{1}{e^x - 1}\right) = \frac{2V}{\beta^4c^5\hbar^33\pi^2} \int_0^\infty \frac{x^3}{e^x - 1}.
\]
(9.6)
The integral on the right hand side in (9.6) is equal to \( \pi^4/15 \) giving the desired result for the phonon inertia
\[
M_{ph} = \frac{2\pi^2VT^4k_B^4}{45\hbar^3c^5}.
\]
(b)
In the case of the rotons we assume that
\[
n(\epsilon) = \frac{1}{e^{\beta\epsilon} - 1} \approx e^{-\beta\epsilon}
\]
so that \( dn/d\epsilon = -\beta e^{-\beta\epsilon} \) and using (9.5) we find
\[
M_r \approx \frac{V\beta^4\pi}{\hbar^33(2\pi)^3} \int dp \frac{p^4}{p^0} \exp\left(-\beta[\Delta + \frac{\beta(p-p_0)^2}{m^*}]\right).
\]
With \( x = p - p_0 \) we find the approximate result
\[
M_r \approx \frac{V\beta^4p_0^4e^{-\beta\Delta}}{6\pi^2} \int_{-\infty}^\infty dx \exp\left(-\frac{\beta x^2}{m^*}\right)
\]
or
\[
M_r = \frac{2(m^*)^{1/2}p_0^4\exp\{-\beta\Delta\}}{3(2\pi)^{3/2}(k_BT)^{1/2}\hbar^3} V
\]
which is the desired result.

(c)
Substituting \( m^* = 0.16m_{He} \), \( c = 240m/s \), \( p_0/\hbar = 1.9 \times 10^{10}m^{-1} \), \( \Delta/k_B = 8.7K \) and \( M_{He}/V = 145kg/m^3 \) we find by trial and error that \( M_{He} = M_r + M_{Ph} \) for \( T = 2.85K \). At this temperature \( M_r/V = 144kg/m^3 \), \( M_{ph}/V = 1kg/m^3 \), i.e., the roton gas yields the dominant contribution. The calculated temperature compares favorably with the experimental result \( T_\lambda = 2.2K \).
Yes, the argument works for the Bose gas too. If we substitute $\epsilon = p^2 / 2m$ into (9.5) we find for the critical temperature

$$k_B T_c = \frac{2\pi \hbar^2}{m} \left[ \frac{\langle N \rangle}{\zeta(\frac{5}{2})V} \right]^{2/3}.$$
Chapter 10

Linear Response Theory

10.1

(a)

From

\[ \mu = \mu_0[n(r)] + \phi(r) = \text{constant} \]

we find

\[ \langle \delta n(r') \rangle = -\int \frac{\delta(r' - r)}{\delta n} \phi(r) d^3r. \]

At \( T = 0 \) we have \( \mu_0 = \epsilon_F \). Using

\[ k_F = \sqrt{\frac{2m\epsilon_F}{\hbar^2}} \]

and

\[ n = \frac{k_F^3}{3\pi^2} \]

we find

\[ \chi_0(q) = -\frac{\partial n_0}{\partial \epsilon_F} = -\frac{1}{2\pi^2} \left( \frac{2m}{\hbar^2} \right)^{3/2} \epsilon_F^{1/2}. \]
Substituting
\[ \chi_{MF}(q) = \frac{\chi_0^R(q)}{1 - e^2 \chi_0^R(q)/\varepsilon_0 q^2} \]
and the formula for \( \chi_0 \) we immediately find the desired result
\[ \varepsilon(q) = 1 + \frac{k_{TF}^2}{q^2} \]  \hspace{1cm} (10.1)
where
\[ k_{TF} = \left[ m e^2 k_F / (\pi^2 \varepsilon_0 \hbar^2) \right]^{1/2} . \]

We have \( \phi_{ext}(q) = e^2 / \varepsilon_0 q^2 \) and
\[ \phi_{eff}(r) = \frac{e^2}{\varepsilon_0 (2\pi)^3} \int d^3q \frac{e^{i\mathbf{q} \cdot \mathbf{r}}}{q^2 + k_{TF}^2} = \frac{e^2}{\varepsilon_0 r} e^{-k_{TF}r} . \]

For a classical ideal gas we have for the chemical potential
\[ \mu = k_B T \ln(n_0 \lambda^3) \]
where \( \lambda \) is the thermal wavelength
\[ \lambda = \sqrt{\frac{2\pi \hbar^2}{mk_B T}} . \]

We find
\[ \chi_0(q) = -\frac{\partial n_0}{\partial \mu} = \frac{n_0}{k_B T} \]
and the mean field expression for the dielectric function will be on the form (10.1) except \( k_{TF} \) is replaced by \( \lambda_D^{-1} \) where
\[ \lambda_D = \sqrt{\frac{n_0 e^2}{\varepsilon_0 k_B T}} . \]
10.2

(a)

We have for \( q \neq 0 \)

\[
S(q) = \frac{1}{\langle N \rangle} \left\langle \sum_{\mathbf{k}, \mathbf{p}} b_{\mathbf{k}^- \mathbf{q}}^\dagger b_{\mathbf{k}^+ \mathbf{p}+\mathbf{q}} b_{\mathbf{k}^+ \mathbf{p}} b_{\mathbf{k}^- \mathbf{q}}^\dagger \right\rangle
\]

where \( b, b^\dagger \) are, respectively, boson annihilation and creation operators. Evaluating the matrix element we find

\[
S(q) = \frac{1}{\langle N \rangle} \sum_{\mathbf{p}} \langle n_{\mathbf{p}} \rangle (1 + \langle n_{\mathbf{p}+\mathbf{q}} \rangle)
\]

where \( n_{\mathbf{p}} \) is the occupation number and

\[
\langle n_{\mathbf{p}} \rangle = \frac{1}{\frac{1}{z} e^{\beta \epsilon(\mathbf{p})} - 1}
\]

and

\[
\epsilon(\mathbf{p}) = \frac{\hbar^2 p^2}{2m}.
\]

For \( T > T_c \) we can convert the sum into an integral

\[
S(q) = \frac{V}{\langle N \rangle (2\pi)^3} \int \frac{d^3 p}{\left( \frac{1}{z} e^{\beta \epsilon(\mathbf{p})} - 1 \right)(1 - ze^{-\beta \epsilon(\mathbf{p}+\mathbf{q})})}.
\]

It is relatively straightforward to carry out the angular part of the integration, but since we only need the limit \( q \to 0 \) in the remainder of the problem we skip this step.

(b)

The isothermal compressibility is proportional to \( S(q \to 0) \) which is given by

\[
S(q \to 0) = \frac{V}{2\pi^2 \langle N \rangle z} \int_0^\infty \exp\left( \frac{\beta \hbar^2 p^2}{2m} \right) p^2 dp \left[ \frac{1}{z} \exp\left( \frac{\beta \hbar^2 p^2}{2m} \right) - 1 \right]^2.
\]
Introducing the new variable

\[ x = \frac{\beta \hbar^2 p^2}{2m} \]

we obtain

\[ S(q \to 0) = \frac{V}{4\pi^2 \langle N \rangle z^2} \left( \frac{2m}{\beta \hbar^2} \right)^{3/2} \int_0^\infty \frac{\sqrt{x}e^x \, dx}{\left( \frac{1}{z} e^x - 1 \right)^2} . \]

When the system approaches the condensation temperature from above \( z \to 1 \). If we look at the integrand for small \( x \) we find that the numerator approaches \( \sqrt{x} \) while the denominator is proportional to \( x^2 \) when \( z = 1 \). The integral is thus divergent in the limit \( z \to 1 \) and the compressibility will \( \to \infty \) as \( T \to T_c \).

(c)

Integrating by parts we find

\[ S(q \to 0) = \frac{V}{8\pi^2 \langle N \rangle} \left( \frac{2m}{\beta \hbar^2} \right)^{3/2} \int_0^\infty \frac{dx}{\sqrt{x} \left( \frac{1}{z} e^x - 1 \right)} \cdot \]

If we substitute

\[ \frac{\langle N \rangle}{V} = n = \left( \frac{mk_BT}{2\pi \hbar^2} \right)^{3/2} g_{3/2}(z) \quad T > T_c \]

\[ g_{3/2}(z) = \frac{1}{\Gamma(1/2)} \int_0^\infty \frac{dx}{\sqrt{x} (z^{-1}e^x - 1)} \]

and \( \Gamma(1/2) = \sqrt{\pi} \) we finally find the desired result

\[ S(q \to 0) = \frac{g_{1/2}(z)}{g_{3/2}(z)} . \]

By comparison, for a classical ideal gas we have \( S(q) = 1 \).

10.3

(a)

Taking the imaginary part of (10.70) gives

\[ \text{Im} \chi_R^M(q, \omega) = \frac{\langle N \rangle}{V} \frac{\epsilon_0(q)}{\epsilon(q)} \pi [\delta(\hbar \omega - \epsilon(q)) - \delta(\hbar \omega + \epsilon(q))] . \]
We thus find
\[
\int_{-\infty}^{\infty} \frac{d\omega}{\pi} \operatorname{Im} \chi_{MF}^{R}(q, \omega) = \frac{2\langle N \rangle}{V \hbar^2 \epsilon_0(q)} = \frac{q^2 \langle N \rangle}{mV}
\]
which is the \( f \)-sum rule.

(b)

From (10.71)
\[
S(q, \omega) = 2\pi N \hbar \frac{\epsilon_0(q)}{\epsilon(q)} \delta(\hbar \omega - \epsilon(q))
\]
and from (10.46)
\[
S(q) = \frac{1}{N} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} S(q, \omega) = \frac{\epsilon_0(q)}{\epsilon(q)}
\]
We have from (4.27)
\[
S(q) - 1 = \frac{N}{V} \int d^3r [g(r) - 1] e^{i \mathbf{q} \cdot \mathbf{r}}.
\]
Inverting this expression we find
\[
g(r) = 1 + \frac{V}{(2\pi)^3 N} \int d^3q \left( \frac{\epsilon_0(q)}{\epsilon(q)} - 1 \right) e^{-i \mathbf{q} \cdot \mathbf{r}}
\]
and
\[
g(0) = \frac{V}{2\pi^2 N} \int_0^{\infty} dq \, q^2 \left( \frac{\epsilon_0(q)}{\epsilon(q)} - 1 \right).
\]
The convergence of this integral depends on the behavior of the integrand for large \( q \). We have in the large \( q \) limit
\[
\epsilon(q) = \epsilon_0(q) \sqrt{1 + \frac{2N v_q}{V \epsilon_0(q)}} \approx \epsilon_0(q) \left( 1 + \frac{2N m v_q}{V \hbar^2 q^2} + \cdots \right).
\]
For the integral to be convergent the integrand must fall off faster than \( 1/q \) for large \( q \). This means that \( v_q \) must also fall of faster than \( 1/q \) for \( g(0) \) to be finite.
10.4

From (10.113)

\[
\chi_0^R(q, \omega) = \frac{2}{V} \sum_{k < k_F} \frac{q^2/m}{[\omega - (\hbar/2m)(q^2 + 2k \cdot q)][\omega + (\hbar/2m)(q^2 - 2k \cdot q)]}.
\]

We expand this equation using

\[
\frac{1}{(\omega - a)(\omega + b)} = \frac{1}{\omega^2} \left(1 + \frac{a - b}{\omega} + \frac{a^2 + b^2 - ab}{\omega^2}\right)
\]

to find to order \(q^2\)

\[
\chi_0^R(q, \omega) = \frac{2q^2}{mV\omega^2} \sum_{k < k_F} \left(1 + \frac{\hbar}{m} \cdot 2k \cdot q + \frac{3\hbar^2}{m^2\omega^2} (k \cdot q)^2 + O(q^4)\right).
\]

The second term inside the bracket becomes zero after the angular integration, while the the angular average of \((q \cdot \hat{k})^2 = \frac{1}{3}\). This gives

\[
\chi_0^R(q, \omega) = \frac{2q^2}{mV\omega^2} \sum_{k < k_F} \left(1 + \frac{\hbar^2q^2k^2}{m^2\omega^2}\right).
\]

Carrying out the sum over \(k\) we find

\[
\chi_0^R(q, \omega) = \frac{q^2N}{mV\omega^2} \left(1 + \frac{3q^2\hbar^2k_F^2}{5m^2\omega^2}\right)
\]

and

\[
\Omega_p l(q)^2 = \Omega_p l(0)^2 \left(1 + \frac{3q^2v_F^2}{5\Omega_p l(0)^2}\right)
\]

which finally yields

\[
\Omega_p l(q) = \Omega_p l(0) \left(1 + \frac{3q^2v_F^2}{10\Omega_p l(0)^2}\right).
\]

10.5

(a)

We have

\[
v_q = \frac{e^2}{4\pi\varepsilon_0} \int \frac{d^2r}{r} e^{-i\mathbf{q} \cdot \mathbf{r}} = \frac{e^2}{4\pi\varepsilon_0} \int_0^\infty dr \int_0^{2\pi} d\phi e^{-iqr \cos \phi}.
\]
We carry out the $\phi$ integration first and obtain
\[ v_q = \frac{e^2}{2\epsilon_0 q} \int_0^\infty qdr J_0(qr) = \frac{e^2}{2\epsilon_0 q} \]
which is the desired result.

(b)

The generalization of (10.101) to two dimensions is
\[ \chi_0^R(q, 0) = -\frac{2m}{\pi^2 \hbar^2} \int_0^{k_F} kd \int_0^{2\pi} \frac{d\phi}{q^2 + 2kq\cos\phi}. \]

By transforming the integral over $\phi$ to a contour integral over the unit circle one can show that
\[ P \int_0^{2\pi} \frac{d\phi}{a + \cos \phi} = \begin{cases} \frac{2\pi}{\sqrt{a^2 - 1}} & a > 1 \\ 0 & a < 0. \end{cases} \]

We find
\[ \chi_0^R(q, 0) = -\frac{m}{\pi \hbar^2} \int_0^{2k_F/q} \frac{x dx}{\sqrt{1 - x^2}} = -\frac{m}{\hbar^2 \pi} \left[ 1 - \sqrt{1 - \frac{4k_F^2}{q^2}} \right]. \]

For $q > 2k_F$ the $k$-integration runs from 0 to $k_F$ and we find
\[ \chi_0^R(q, 0) = -\frac{m}{\pi \hbar^2} \int_0^{2k_F/q} \frac{x dx}{\sqrt{1 - x^2}} = -\frac{m}{\hbar^2 \pi} \left[ 1 - \sqrt{1 - \frac{4k_F^2}{q^2}} \right]. \]

For $q < 2k_F$ the upper limit to the $k$-integration will be $q/2$ and thus 1 for $2k/q$. We find
\[ \chi_0^R(q, 0) = \frac{m}{\pi \hbar^2} \int_0^1 \frac{x dx}{\sqrt{1 - x^2}} = -\frac{m}{\hbar^2 \pi}. \]

(c)

We now have (assuming the electron charge is $-e$)
\[ v_q = -\frac{e^2}{4\pi \epsilon_0} \int_0^\infty \frac{r dr}{\sqrt{z^2 + r^2}} \int_0^{2\pi} e^{-q r} = -\frac{e^2}{4\pi \epsilon_0} \int_0^\infty \frac{2\pi r dr}{\sqrt{z^2 + r^2}} J_0(qr). \]

If we carry out the last integration above we get the desired result
\[ v_q = -\frac{e^2}{2\epsilon_0 q} e^{-qz}. \]
(d) The induced charge density in mean field theory will be the two dimensional Fourier transform of

\[ \langle \delta \rho_q \rangle = \frac{-e^2}{2q_0} e^{-qz} \frac{\chi^R_0(q, 0)}{1 - \frac{e^2}{2q_0} \chi^R_{0}(q, 0)} . \]

The in-plane screened potential is

\[ v_{MF}(q) = \frac{-e^2}{2q_0} e^{-qz} \frac{1}{1 - \frac{e^2}{2q_0} \chi^R_{0}(q, 0)} \]

with \( \chi^R_{0}(q, 0) \) given by the expression calculated in (b).

10.6

(a) If each spin reduces the magnetization by \( \hbar \) from its saturation value \( N\hbar S \) we have

\[ M = M_0 \left( 1 - \frac{1}{NS} \sum_q \frac{1}{e^{\beta \epsilon(q)} - 1} \right) . \]

Converting the sum into an integral gives

\[ M = M_0 \left( 1 - \frac{V(k_B T)^3}{NS4\pi^2(J\hbar^2 S a^2)^{3/2}} \int_0^\infty \frac{x^2 dx}{e^{x^2} - 1} \right) \tag{10.2} \]

which can be evaluated to give

\[ M = M(0) \left( 1 - 0.0293218 T^{3/2} \left( \frac{k_B}{J\hbar^2 S} \right)^{3/2} \right) . \]

(b) In two dimensions (10.2) is replaced by

\[ M = M_0 \left( 1 - \frac{A(k_B T)^2}{NS2\pi \left( J\hbar^2 S a^2 \right)^2} \int_0^\infty \frac{xdx}{e^{x^2} - 1} \right) . \]

For small \( x, (e^{x^2} - 1) \to x^2 \), while the numerator of the integrand is \( \propto x \). The integral is therefore divergent!
10.7

(a)

A cubic crystal will remain unchanged after a rotation of 90° about one of the cubic axes. Consider a rotation of 90° about the z-axis. The transport coefficients will transform as

$$L' = R^{-1}LR$$

where

$$L = \begin{pmatrix} L_{11} & L_{12} & L_{13} \\ L_{21} & L_{22} & L_{23} \\ L_{31} & L_{32} & L_{33} \end{pmatrix}$$

and

$$R = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$R^{-1} = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Multiplying out 10.3 we have

$$L' = \begin{pmatrix} L_{22} & -L_{21} & L_{23} \\ -L_{12} & L_{11} & -L_{13} \\ L_{32} & -L_{31} & L_{33} \end{pmatrix}$$

The crystal is unchanged under the 90° rotation so we see that $L_{11} = L_{22}$. Similarly, if we had rotated about the x-axis we would have found $L_{22} = L_{33}$. Therefore all the diagonal components must be the same.

By considering the third row in $L'$ we find that $L_{32} = L_{31}$, but $-L_{31} = L_{32}$ giving $L_{31} = L_{32} = 0$. From the third column we find that $L_{13} = L_{23} = 0$ and by considering rotations about the x- and y-axes it is easy to see that the remaining off-diagonal components are zero. A cubic crystal, therefore, most have a diagonal conductivity tensor with all the diagonal components being equal.
(b) Consider a rotation by $120^\circ$ about the symmetry axis. We require that

$$ R^{-1}LR = L $$

On component form this corresponds to

$$
\begin{pmatrix}
-\frac{1}{2} & -\frac{\sqrt{3}}{2} & 0 \\
\frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 \\
0 & 0 & 1
\end{pmatrix}
\begin{pmatrix}
L_{11} & L_{12} & L_{13} \\
L_{21} & L_{22} & L_{23} \\
L_{31} & L_{32} & L_{33}
\end{pmatrix}
\begin{pmatrix}
-\frac{1}{2} & \frac{\sqrt{3}}{2} & 0 \\
-\frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 \\
0 & 0 & 1
\end{pmatrix}

= \begin{pmatrix}
L_{11} & L_{12} & L_{13} \\
L_{21} & L_{22} & L_{23} \\
L_{31} & L_{32} & L_{33}
\end{pmatrix} . \quad (10.4)
$$

Multiplying out (10.4) we obtain the matrix equation $M = 0$ where

\begin{align*}
M_{11} &= \frac{3}{4}(-L_{11} + L_{22}) + \frac{\sqrt{3}}{4}(L_{12} + L_{21}) \\
M_{12} &= \frac{\sqrt{3}}{4}(-L_{11} + L_{22}) - \frac{3}{4}(L_{12} + L_{21}) \\
M_{13} &= -\frac{3}{2}L_{13} - \frac{\sqrt{3}}{2}L_{23} \\
M_{21} &= \frac{\sqrt{3}}{4}(-L_{11} + L_{22}) - \frac{3}{4}(L_{12} + L_{21}) \\
M_{22} &= \frac{3}{4}(L_{11} - L_{22}) - \frac{\sqrt{3}}{4}(L_{12} + L_{21}) \\
M_{23} &= \frac{\sqrt{3}}{2}L_{13} - \frac{3}{2}L_{23} \\
M_{31} &= -\frac{3}{2}L_{13} - \frac{\sqrt{3}}{2}L_{23} \\
M_{32} &= \frac{\sqrt{3}}{2}L_{13} - \frac{3}{2}L_{23} \\
M_{33} &= 0 .
\end{align*}

We conclude that $L_{11} = L_{22}, \ L_{12} = -L_{21} \text{ and } L_{23} = L_{32} = L_{13} = L_{31} = 0$.

10.8

(a) Since the plane wave solutions to the Schrödinger equation are of the form

$$\psi_k = \frac{1}{\sqrt{V}} e^{i\mathbf{k}\cdot\mathbf{r}}$$
we have
\[ |\langle k | u(x) | k' \rangle|^2 = \frac{1}{V^2} |U_{k-k'}|^2. \]

Therefore,
\[ W(k', k) = \frac{2\pi N_i}{V^2 \hbar} |U_{k-k'}|^2 \delta(e_{k'} - e_k). \]

We have
\[ \frac{g_k}{\tau} = \sum_{k'} (g_k - g_{k'}) W(k, k'). \]

Substitution of
\[ g_k = -\tau eE \cdot v_k \delta(e_k - e_{k_F}) \]

using the fact that the system is isotropic (i.e., independent of the direction of \( E \)) we find with \( k \) restricted to the Fermi surface
\[ \frac{1}{\tau} v_k = \frac{2\pi N_i}{V^2 \hbar} \sum_{k'} (v_k - v_{k'}) \delta(e_{k'} - e_F) |U_{k-k'}|^2. \]

We multiply both sides by \( v_k = \frac{\hbar k}{m} \), and note that both \( k \) and \( k' \) are on the Fermi surface, to obtain
\[ \frac{1}{\tau} = \frac{2\pi N_i}{V^2 \hbar} \sum_{k'} \left( 1 - \frac{k \cdot k'}{k_F^2} \right) \delta(e_{k'} - e_F) |U_{k-k'}|^2. \]

Converting the sum into an integral and using
\[ d^3k = \frac{dS_k d\epsilon_k}{\hbar v_k} \]

and the fact that \( k \) is on the Fermi surface we finally find
\[ \frac{1}{\tau} = \frac{n_i}{4\pi^2 v_F^2 \hbar^2} \int d^2 S_F |U_{k-k'}|^2 \left( 1 - \frac{k \cdot k'}{k_F^2} \right) \]

where \( n_i = N_i/V \).

(b)

In order to do the numerical calculation we assume that the potential is of the form
\[ U_{qk_F} = \frac{e^2}{\epsilon_0 k_F^2 q^2} + \frac{1}{k_F^2 u_{qk_F}} \]
with (see (10.106))
\[
\frac{u_{qk_F}}{k_F^2} = \frac{1}{2} + \frac{4 - q^2}{8q} \ln \left| \frac{q + 2}{q - 2} \right|
\]
\[
q[\mu] = \frac{|k - k'|}{k_F} = \sqrt{2 - 2\mu}
\]
in the case of Lindhard screening and \(u_{qk_F} = 1\) for Thomas–Fermi screening. With \(k_F = 0.92 \times 10^{10} m^{-1}\) we have
\[
\frac{k_{TF}^2}{k_F^2} = \frac{me^2}{\pi^2 \epsilon_0 \hbar^2 k_F} = 2.614
\]
We now write (10.5) as
\[
\frac{1}{\tau} = \frac{n_i e^4}{2 \pi v_F k_F^2 \hbar^2 \epsilon_0^2 I}
\]
where the integral \(I\) is given by \((\mu = k \cdot k'/k_F^2)\)
\[
I = \int_{-1}^{1} \frac{(1 - \mu) d\mu}{(q[\mu]^2 + \frac{k_{TF}^2}{k_F^2} u_{q[\mu]})^2}
\]
If we evaluate \(I\) numerically we find \(I = 0.112\) for Lindhard screening and \(I = 0.081\) for Thomas–Fermi screening. With
\[
n_i = \frac{c_i k_F^3}{3 \pi^2}
\]
where \(c_i = 10^{-3}\) is the concentration of divalent impurities and with \(v_F = \hbar k_F/m\) we find for the prefactor of the integral
\[
\frac{me^4 c_i}{6 \pi^3 \hbar^3 \epsilon_0^2} = 3.505 \times 10^{13} s^{-1}
\]
The relaxation time is thus \(2.55 \times 10^{-13} s\) for Lindhard screening and \(3.52 \times 10^{-13} s\) for Thomas–Fermi screening.

We finally find for the resistivity
\[
\rho = \frac{m}{ne^2 \tau} = \frac{3 \pi^2 m}{k_F^3 e^2 \tau} = \begin{cases} 
1.76 \times 10^{-9} \Omega m & \text{Lindhard screening} \\
1.2810^{-9} \Omega m & \text{Thomas–Fermi screening.}
\end{cases}
\]
10.9

We begin with the basic equations
\[
\begin{align*}
  j_E &= L_{EE} \nabla \left( \frac{1}{T} \right) + L_{EN} \nabla \left( -\frac{\mu'}{T} \right) \\
  j_N &= L_{NE} \nabla \left( \frac{1}{T} \right) + L_{NN} \nabla \left( -\frac{\mu'}{T} \right).
\end{align*}
\]

We next construct the equations for \( j_C = e j_N \) and \( j_Q = j_E - \mu' j_N \). After combining all the terms that contain \( \nabla (1/T) \) we have
\[
\begin{align*}
  j_Q &= (L_{EE} - 2\mu' L_{NE} + \mu'^2) \nabla \left( \frac{1}{T} \right) + \frac{e(L_{EN} - \mu' L_{NN})}{T} \mathcal{E} \\
  j_C &= e (L_{NE} - \mu' L_{NN}) \nabla \left( \frac{1}{T} \right) + \frac{e^2 L_{NN}}{T} \mathcal{E}
\end{align*}
\]
where we have used \( \nabla \mu' = -e \mathcal{E} \). Therefore \( L_{QC} = e(L_{EN} - \mu' L_{NN})/T \) and \( L_{CQ} = e(L_{NE} - \mu' L_{NN}) \). The fundamental Onsager relation \( L_{EN} = L_{NE} \) then produces \( L_{CQ} = TL_{QC} \).
Chapter 11

Disordered Systems

11.1

(a)

For a pure material

\[ T_j = \begin{bmatrix} \frac{\epsilon_A - E}{t} & -1 \\ 1 & 0 \end{bmatrix} \]

for all \( j \). Let \( \phi_N = a\psi_1 + b\psi_2 \) where \( \psi_1, \psi_2 \) are the two right eigenvectors of \( T \). Then

\[ T^N \phi_N = a\lambda_1^N \psi_1 + b\lambda_2^N \psi_2 . \]

Clearly, the right hand site is equal to \( \phi_N \) if and only if \( \lambda_1^N = \lambda_2^N = 1 \). Since \( \lambda_1 \lambda_2 = 1 \), we have

\[ \lambda_1 = e^{i\theta} \quad \lambda_2 = e^{-i\theta} \quad \theta = \frac{2\pi k}{N}, \quad k = 0, 1, \ldots N-1 . \]

Substituting \( \lambda_i \) into the characteristic polynomial yields \( E = \epsilon_A - 2t \cos \theta \).
(b)

An easy way of guaranteeing that the fixed end boundary conditions are satisfied is to define

$$A_j \equiv B_j \sin \frac{m\pi(j-1)}{N-1} \quad m = 1, 2, \ldots$$

which guarantees that $A_1 = A_N = 0$. Substituting into the transfer matrix equation we obtain

$$\phi_n = \begin{bmatrix} B_{n+1} \sin kn \\ B_n \sin k(n-1) \end{bmatrix} = \begin{bmatrix} \frac{\epsilon_A - E}{i} & -1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} B_n \sin k(n-1) \\ B_{n-1} \sin k(n-2) \end{bmatrix}$$

where $k = m\pi/(N-1)$. Clearly, a solution of this equation is $B_j = c$, where $c$ is any constant together with $E = \epsilon - 2t \cos k$ for the values of $k$ given above.

11.2

(a)

The conditions on the wave function are that, at each of the scatterers, $\psi$ must be continuous and the discontinuity in the first derivative must obey

$$\frac{d\psi}{dx}\bigg|_{x_j+\epsilon} = \int_{x_j-\epsilon}^{x_j+\epsilon} dx u\delta(x - x_j)\psi(x) = u\psi(x_j)$$

Using the assumed form of the wave function we obtain

$$A_j + B_j = A'_{j+1} + B'_{j+1}$$
$$A_j - B_j = A'_{j+1} - B'_{j+1} - \frac{u}{ik} (A'_{j+1} + B'_{j+1})$$

Writing these equations in matrix form, we obtain the required relation.

(b)

The previous results yield

$$\begin{bmatrix} A_0 \\ B_0 \end{bmatrix} = M_1 Q M_2 Q \ldots M_N Q \begin{bmatrix} A'_{N+1} \\ 0 \end{bmatrix}$$
and
\[
\left[ \begin{array}{cc}
A^*_0 & B^*_0 \\
A^*_{N+1} & 0 \\
\end{array} \right] = \left[ \begin{array}{c}
Q^\dagger M^\dagger_N \\
\vdots \\
Q^\dagger M^\dagger_1 \\
\end{array} \right].
\]

Taking the inner product of these two vectors, we obtain
\[
|A_0|^2 + |B_0|^2 = V_{11} |A'_{N+1}|^2
\]
where the matrix \( V \) is given by:
\[
V = Q^\dagger M^\dagger_N Q^\dagger M^\dagger_{N-1} \ldots Q^\dagger M^\dagger_1 Q^\dagger Q M_1 Q \ldots M_N Q.
\]

(c)

Writing
\[
V = \begin{bmatrix} a_N & b_N \\ b^*_N & a_N \end{bmatrix}
\]
we immediately have
\[
a_N = \left[ Q^\dagger M^\dagger_N \begin{bmatrix} a_{N-1} & b_{N-1} \\ b^*_{N-1} & a_{N-1} \end{bmatrix} M_N Q \right]_{11}.
\]

Clearly, \( b_N \) is simply the \((12)\) matrix element of the foregoing expression. Substituting for \( Q \) and \( M_N \) we find
\[
a_N = a_{N-1} \frac{1 + |r|^2}{|t|^2} + 2 \text{Re} \frac{b_{N-1} r e^{2i k \Delta_N}}{|t|^2},
\]
\[
b_N = 2a_{N-1} \frac{r^*}{(t^*)^2} + \frac{b^*_{N-1} (r^*)^2 e^{-2i k \Delta_N} + b_{N-1} e^{2i k \Delta_N}}{(t^*)^2}.
\]

(d)

Since the \( \Delta_j \) are independent random variables, the above recursion relations can be averaged at each step. Integrating over \( \Delta_N \), we have
\[
\langle a_N \rangle = \frac{1 + |r|^2}{|t|^2} a_{N-1}.
\]

Carrying out this process over all the \( \Delta \)'s, we find
\[
\langle a_N \rangle = \left[ \frac{1 + |r|^2}{|t|^2} \right]^N.
\]

Since the number in the brackets is greater than 1, we have \( a_N \rightarrow \infty \) as \( N \rightarrow \infty \) which implies that \( T_N \rightarrow 0 \) as \( N \rightarrow \infty \).
11.3

(a)

The recursion relation for majority occupation of the nine-site block is obtained straightforwardly:

\[ p' = p^9 + \binom{9}{1} p^8 (1 - p) + \binom{9}{2} p^7 (1 - p)^2 + \binom{9}{3} p^6 (1 - p)^3 + \binom{9}{4} p^5 (1 - p)^4. \]

Expanding and gathering terms, we have

\[ p' = R_3(p) = 70p^9 - 315p^8 + 540p^7 - 420p^6 + 126p^5. \]

The equation \( p' = p = p^* \) has the nontrivial solution \( p^* = \frac{1}{2} \). Differentiating and writing

\[ \left( \frac{\partial p'}{\partial p} \right)_{p^*} = 3^{1/\nu} \]

we find \( \nu \approx 1.22 \).

(b)

To calculate the recursion relation on the basis that the block is occupied we need to enumerate the configurations of \( 3 \leq n \leq 9 \) particles that produce a connected path from left to right. Clearly for \( n = 3 \) there exist three different combinations that produce a connected path. For \( n = 4 \), we can arrange three of the particles in a straight line and put the fourth anywhere in 6 different positions. As well, we can make 4 different connected paths with a right-angle turn that do not connect straight through. For \( n = 9, 8, 7 \) all configurations connect from left to right. These are the trivial cases. For \( n = 5 \) it is simpler to count configurations that connect, for \( n = 6 \) it is easier to count the number of ways in which three holes can block the connection.

\( n = 5 \): (i) Three particles in a straight line, the other two arbitrary: \( 3 \times \binom{6}{2} \).

(ii) Four different 4-particle connections as for \( n = 3 \) with the fifth particle not allowed to occupy a position that would convert these paths into straight-through paths: \( 3 \times 4 \).

(iii) Two different 4-step walks beginning in one corner and ending in the other, starting with a horizontal step.
$n = 6$: Clearly there must be one hole in each row and there are 27 ways of arranging this. Some of these arrangements do not block a path from left to right. If the holes in any two adjacent rows are two sites apart, a connected path will exist. There are 10 such configurations. Therefore there are $\binom{9}{6} - 17 = 67$ configurations that connect.

Taking all this into account, we have

$$p' = p^9 + 9p^8(1 - 9) + 36p^7(1 - p)^2 + 67p^6(1 - p)^3 + 59p^5(1 - p)^4 + 22p^4(1 - p)^5 + 3p^3(1 - p)^6$$

or

$$p' = p^9 - 6p^8 + 14p^7 - 9p^6 - 6p^5 + 4p^4 + 3p^3.$$  

Solving for $p' = p = p^*$ we find $p^* \approx 0.619$ and $\nu \approx 1.184$. 