1. The Bragg-Williams approximation gives the Gibbs free energy for the Ising model as a sum of a mean field energy and an entropy of an ideal mixture:

\[ G(m, h, T) = -\frac{qJN}{2}m^2 - Nhm + Nk_B T \left[ \frac{1+m}{2} \ln \frac{1+m}{2} + \frac{1-m}{2} \ln \frac{1-m}{2} \right] \]

Derive from this an equation that determines the magnetization, \( m \), in the mean field approximation! Show that without an applied field, this equation has only one solution \( m = 0 \) above a certain temperature and determine this temperature. Discuss qualitatively what solutions one has depending on temperature and applied field.

2. The Bethe approximation is an improved mean field approximation to the Ising model. For a three dimensional simple cubic lattice, a cluster consisting of seven spins (a central one and 6 nearest neighbours) is treated explicitly, while the surrounding spins are treated as a mean field. Derive the critical temperature of the three dimensional Ising model in this approximation!

3. In a fluid with pair interactions, the Hamiltonian can be written:

\[ H = \frac{1}{2m} \sum_{i=1}^{N} |\vec{p}_i|^2 + \sum_{i<j} u(r_{ij}). \]

The pair correlation function \( g(r, T, N/V) \) or \( h(r, T, N/V) = g(r, T, N/V) - 1 \) is useful to describe the properties such a fluid. Express the pressure in terms of the pair correlation function, the pair potential \( u(r) \), \( N \), \( V \) and \( T \!\).  

4. Start from the scaling relation for the singular part of the free energy:

\[ f_s(t, h) \propto L^{-d} f_s(L^y t, L^y h) \]

were \( t = (T - T_c)/T_c \) and show that this implies the Rushbrooke scaling relation

\[ \alpha + 2\beta + \gamma = 2 \]
between the critical exponents.

5. An infinite range Ising model is described by the Hamiltonian:

\[ H = - \frac{J}{2N} \sum_{i,j=1}^{N} S_i S_j = - \frac{J}{2N} S^2 \quad \text{with} \quad S = \sum_{i=1}^{N} S_i \]

were the sum goes over all \( N \) spins of the system. Show that this model in the limit of large \( N \) in arbitrary dimensionality gives the mean field equation for the magnetization. The mathematical identity:

\[ e^{KS^2/2} = \frac{1}{\sqrt{2\pi K}} \int_{-\infty}^{+\infty} e^{-x^2/(2K)} dx \]

might be of some help.

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**SUGGESTED SOLUTIONS**

**Solution, problem 1:**

The actual magnetization \( m \) is the one that minimizes \( G \) at fixed \( h \) and \( T \). This gives:

\[ \frac{\partial G}{\partial m} = 0 = -qJm - h - \frac{1}{2} k_B T \ln \frac{1 + m}{1 - m} \]

This gives after some algebra the equation for \( m \):

\[ m = \tanh[(qJm + h)/k_B T] \]

For \( h = 0 \), this equation will only have the solution \( m = 0 \) if the slope of the \( \tanh \)-function is smaller than 1 at \( m = 0 \). This means if \( T > qJ/k_B \). For lower temperatures, there will also be two symmetric solutions with finite magnetization.

**Solution, problem 2:**

See Bergersen and Plischke 3:rd ed. p.71-73. The derivation is independent of dimensionality. It is just the number of nearest neighbours \( (q) \) that matters. The final equation becomes:

\[ \cotanh \left( \frac{J}{k_B T_c} \right) = q - 1 = 5 \]

This has the solution:

\[ \frac{k_B T_c}{J} = \frac{2}{\ln 3/2} \approx 4.933 \]

which is slightly higher than the value obtained in numerical simulations (4.511..).

**Solution, problem 3:**

The pressure is defined as:

\[ p = - \left( \frac{\partial F}{\partial V} \right)_T = k_B T \left( \frac{\partial \ln Z}{\partial V} \right)_T = k_B T \left( \frac{\partial \ln \int ... \int e^{-\Phi(r_1,..,r_N)/k_B T} d^3N_r}{\partial V} \right)_T. \]
Here we have excluded the momentum part of the partition function since this is independent of volume. Now, we change to new dimensionless integration variables \( \xi_i = \bar{r}_i / V^{1/3} \) that do not depend upon the volume of the system. This gives the pressure as:

\[
p = k_B T \left[ \left( \frac{\partial \ln V^N}{\partial V} \right)_T - \frac{1}{3V} \int \cdots \int \frac{\left( \xi_i \Phi \right)}{N} \frac{e^{-\Phi(V^{1/3} \xi_i, \ldots, V^{1/3} \xi_N) / k_B T}}{d^3N \xi} \right].
\]

Reintroducing the old variables we may write this as:

\[
p = \frac{N k_B T}{V} - \frac{1}{3V} \int \cdots \int \frac{\left( \bar{r}_i \cdot \nabla_i \Phi \right)}{k_B T} \frac{e^{-\Phi(r_1, \ldots, r_N) / k_B T}}{d^3N r} = \frac{N k_B T}{V} - \frac{1}{3V} \sum_i (\bar{r}_i \cdot \nabla_i \Phi).
\]

Now we introduce that \( \Phi = 1 / T \) which after some algebra gives:

\[
p = \frac{N k_B T}{V} - \frac{N}{6V} \sum_{ij} \langle r_{ij} u'(r_{ij}) \rangle = \frac{N k_B T}{V} - \frac{N^2}{6V^2} \int g(r, N/V, T) u'(r) 4\pi r^3 dr
\]

**Solution, problem 4:**

\[
f_s(t, h) \propto L^{-d} f_s(L^{y_1} t, L^{y_2} h)
\]

\[
m(t, h) = - \frac{\partial f_s}{\partial h} \equiv L^{y_2 - d} m(L^{y_1} t, L^{y_2} h)
\]

\[
\chi(t, h) = \frac{\partial m}{\partial h} \equiv L^{2y_2 - d} \chi(L^{y_1} t, L^{y_2} h)
\]

Choose \( h = 0 \) and \( L = |t|^{-1/y_2} \) and we get

\[
m(t, 0) \propto |t|^{-(y_2 - d)/y_2} m(-1, 0) \equiv |t|^{\beta} \text{ which gives } \beta = (d - y_2) / y_t
\]

Similarly we get

\[
\chi(t, 0) \propto |t|^{(2y_2 - d)/y_2} \chi(1, 0) \equiv |t|^{-\gamma} \text{ which gives } \gamma = (2y_2 - d) / y_t
\]

and

\[
f_s(t, 0) \propto |t|^{d/y_2} f_s(t / |t|, 0) \equiv |t|^d / y_t \text{ which gives } c \propto |t|^{d/y_2 - 2} \equiv |t|^{-\alpha} \text{ and } \alpha = 2 - d / y_t.
\]

This gives

\[
\alpha + 2\beta + \gamma = 2 - d / y_t + 2(d - y_2) / y_t + (2y_2 - d) / y_t = 2
\]

**Solution, problem 5:**

We have the partition function:

\[
Z = \sum_{S_1 = \pm 1} \cdots \sum_{S_N = \pm 1} e^{-\beta H} = \sum_{S_1 = \pm 1} \cdots \sum_{S_N = \pm 1} e^{\beta JS^2 / 2N} = \sum_{S_1 = \pm 1} \cdots \sum_{S_N = \pm 1} e^{KS^2 / 2}
\]

with \( K = \beta J / N \). Thus we get:

\[
Z = \frac{1}{\sqrt{2\pi K}} \int_{-\infty}^{+\infty} e^{-x^2 / 2K} \sum_{S_1 = \pm 1} \cdots \sum_{S_N = \pm 1} e^{xS} dx = \frac{1}{\sqrt{2\pi K}} \int_{-\infty}^{+\infty} e^{-x^2 / 2K}[2\cosh(x)]^N dx = \]
\[
\frac{1}{\sqrt{2\pi K}} \int_{-\infty}^{+\infty} e^{-x^2/2K+N\ln(2\cosh(x))} \, dx
\]

In the limit of very large \( N \), this integrand is sharply peaked (since both terms in the exponential are proportional to \( N \)) and the integrand can be estimated from the value at this maximum. We get:

\[
\frac{d}{dx} \left( -\frac{x^2}{2K} + N \ln [2\cosh(x)] \right) = -\frac{x}{K} + N \tanh(x) = -\frac{N}{\beta J} + N \tanh(x) = 0,
\]

which gives the equation:

\[
x = \beta J \tanh(x)
\]

for \( x \). From the definition of the magnetization, the parameter \( x \) can be identified as \( x = \beta J m \) and we do obtain the mean field equation

\[
m = \tanh(\beta J m)
\]

for the spontaneous magnetization.