1. Derive an equation that expresses the mean square fluctuations in energy in a canonical ensemble as a function of heat capacity, temperature and system size! Show how the relative energy fluctuations depend on the system size! What will happen for a very large system?

2. In a Landau theory, the coefficient for the fourth order term happens to be zero which gives the free energy
\[ f(T, m) = \frac{a}{2}(T - T_c)m^2 + \frac{b}{6}m^6, \]
with \( a \) and \( b \) being positive constants. Show that there is a phase transition, determine its order, the magnetisation in the different phases and the exponent \( \beta \)!

3. Start from the scaling relation for the singular part of the free energy:
\[ f_s(t, h) \propto L^{-d}f_s(L^{y_t}t, L^{y_h}h) \]
were \( t = (T - T_c)/T_c \) and show that \( m(t, h) \) can be written as \( |t|^\beta m(\pm 1, h|t|^{-\Delta}) \)! Determine the exponents \( \beta \) and \( \Delta \) in terms of \( y_t \) and \( y_h \) and the dimensionality, \( d \)!

4. A one-dimensional hard-core gas consists of \( N \) particles with the linear size \( a \) that are confined to a line of length \( L \). Determine the one-dimensional pressure \( -\partial F/\partial L \) as a function of \( k_BT, N, L \) and \( a \)! Taylor expand the equation of state and obtain all virial coefficients! When doing the last part, you may assume that \( N \gg 1 \).

5. For a one-dimensional Ising model with nearest neighbour interactions and no external field, the Hamiltonian is
\[ H = -J \sum_{i=1}^{N-1} S_i S_{i+1}, \]
with \( S_i = \pm 1 \). Determine the two-spin correlation function \( g_{ij} = \langle S_i S_j \rangle \) as a function of \( J/k_BT \) and \( |i - j| \)!

GOOD LUCK!

turn
Definition of some critical exponents:

\[ c(t, h = 0) = -T \frac{\partial^2 f}{\partial T^2} \propto |t|^{-\alpha} \]
\[ m(t, h = 0) = -\frac{\partial f}{\partial h} \propto (t)^\beta \]
\[ \chi(t, h = 0) = \frac{\partial m}{\partial h} \propto |t|^{-\gamma} \]
\[ \xi(t, h = 0) \propto |t|^{-\nu} \]

**SUGGESTED SOLUTIONS**

**Solution, problem 1:**
The average energy is obtained as

\[ \langle E \rangle = \frac{\sum_i E_i e^{-E_i / k_B T}}{\sum_i e^{-E_i / k_B T}}, \]

with the sum going over all states of the \( N \)-particle system. The heat capacity at constant volume is obtained as the derivative of the average energy with respect to \( T \)

\[ C_V = \frac{\partial \langle E \rangle}{\partial T} = \frac{1}{k_B T^2} \left[ \frac{\sum_i E_i^2 e^{-E_i / k_B T}}{\sum_i e^{-E_i / k_B T}} - \left( \frac{\sum_i E_i e^{-E_i / k_B T}}{\sum_i e^{-E_i / k_B T}} \right)^2 \right] = \]

\[ = \frac{1}{k_B T^2} \left( \langle E^2 \rangle - \langle E \rangle^2 \right) = \frac{\sigma_E^2}{k_B T^2}. \]

Thus the relative fluctuations in energy are

\[ \frac{\sigma_E}{\langle E \rangle} = \sqrt{\frac{k_B T^2 C_V}{\langle E \rangle}} = \sqrt{\frac{k_B T^2 c_V}{\langle e \rangle}} \frac{1}{\sqrt{N}}, \]

with \( c_V = C_V / N \) being the heat capacity per particle (atom) and \( \langle e \rangle = \langle E / N \rangle \) being the average energy per particle (atom). Thus the relative energy fluctuations will go to zero when system size goes to infinity.

**Solution, problem 2:**
The free energy is a sixth:es degree polynomial in the magnetisation. The sign of the second degree term will be negative for \( T < T_c \) and positive for \( T > T_c \). The maxima and minima are obtained from

\[ \frac{\partial f}{\partial m} = m[a(T - T_c) + bm^4] = 0. \]

For \( T > T_c \) this equation has one single real solution, \( m = 0 \), giving a minimum in the free energy corresponding to a state without spontaneous magnetisation. For \( T < T_c \), \( m = 0 \) will be a maximum an there are in addition two symmetric minima at \( m = \pm (a/b)^{1/4}(T_c - T)^{1/4} \). These minima correspond to spontaneous magnetisation. When \( T \) approaches \( T_c \) from below, the magnetisation goes continuously to zero an we have thus a second order phase transition.
at $T = T_c$. The exponent $\beta$ by which $m(t)$ approaches zero is thus $1/4$.

**Solution, problem 3:**

With

$$f(t, h) = L^{-d} f(tL^y, hL^y),$$

The magnetisation is then obtained as

$$m(t, h) = \frac{\partial f(t, h)}{\partial h} = L^{yn-d} m(tL^y, hL^y).$$

Now we may chose the scaling factor $L$ in different ways. The choice $|t|^{-1/y}$ gives the desired result

$$m(t, h) = |t|^{(d-yh)/yt} m(\pm 1, h|t|^{-yh/yt}),$$

from which the exponents could be identified as $\beta = (d - yh)/yt$ and $\Delta = yh/yt$.

**Solution, problem 4:**

The configurational part of the partition function is:

$$Q(N, L, a) = \int_{L-Na}^{L-Na} dx_1 \int_{x_1 + a}^{L-(N-1)a} dx_2 \ldots \int_{x_{N-2} + a}^{L-a} dx_{N-1} \int_{x_{N-2} + a}^{L} dx_N$$

The integrals can be performed successively starting from the end with the one over $x_N$. This gives

$$Q(N, L, a) = \frac{1}{N!} (L - Na)^N$$

Thus, we have

$$F(N, L, a, T) = -k_BT \ln Q = k_BT [N \ln (L - Na) - \ln N!],$$

which gives the one dimensional pressure as

$$p = -\frac{\partial F}{\partial L} = \frac{Nk_BT}{L-Na} = \frac{Nk_BT}{L} \frac{1}{1 - \frac{N}{L}a}.$$

The virial expansion is an expansion in $N/L$, and is the geometric series

$$p = \frac{Nk_BT}{L} \left[ 1 + \frac{N}{L} a + \left( \frac{N}{L} \right)^2 a^2 + \ldots \right].$$

**Solution, problem 5:**

We want to calculate

$$g_{ij} = \langle S_i S_j \rangle = \frac{1}{Z} \sum_{S_1 = \pm 1, \ldots, S_N = \pm 1} S_i S_j e^{\frac{J}{k_BT} \sum_{k=1}^{N-1} S_k S_{k+1}},$$

with the partition function $Z$ being

$$Z = \sum_{S_1 = \pm 1, \ldots, S_N = \pm 1} e^{\frac{J}{k_BT} \sum_{k=1}^{N-1} S_k S_{k+1}} = 2^N \left[ \cosh \left( \frac{J}{k_BT} \right) \right]^{N-1}.$$
This can be slightly generalised by letting the coupling constant be a function of position, \( k \), giving

\[
Z(J_1, \ldots J_{N-1}) = \sum_{S_1 = \pm 1, \ldots, S_N = \pm 1} \frac{1}{e^{k_B T}} \sum_{k=1}^{N-1} J_k S_k S_{k+1} = 2^N \prod_{k=1}^{N-1} \cosh \left( \frac{J_k}{k_B T} \right).
\]

Since the average is symmetric in \( i \) and \( j \) we could choose the order in which way we like, e.g., with \( j > i \). Since \( S_k^2 = 1 \) we may then write

\[
S_i S_j = S_i S_{i+1} S_{i+1} S_{i+2} S_{i+2} \ldots S_{j-1} S_{j-1} S_j.
\]

We note now, that if we take the derivative of the partition function with respect to \( J_k \) we will get out a factor \( S_k S_{k+1}/k_B T \). Thus, the desired average could be written as a logarithmic derivative of the generalised partition function

\[
\langle S_i S_j \rangle = (k_B T)^{j-i} \frac{\partial^{j-i} \ln (Z(J_1, \ldots J_{N-1}))}{\partial J_i \ldots \partial J_{j-1}},
\]

which easily is calculated from the partition function above. After this all the \( J_k \)'s can be put equal again and the final result may be written as

\[
g_{ij} = \langle S_i S_j \rangle = \left[ \tanh \left( \frac{J}{k_B T} \right) \right]^{i-j}.
\]

It might be worthwhile to check a few special cases. For \( i = j \) the correlation function is 1 as it should be. For large temperatures, the correlation function will go to zero, for low temperatures it will go to one. At any finite temperature \( 0 < \tanh \left( \frac{J}{k_B T} \right) < 1 \) and the correlation function will thus be a continuously decaying function of \( |i - j| \).