Problem 15: (Anti-)Ferromagnetism (7 points)

An (anti-)ferromagnet can be approximated by the Ising model, i.e. by a Hamiltonian

$$H = -\frac{1}{2}\sum_{i,j=1}^{N} J_{ij}\, s_i\, s_j + \mu_B\, B_0 \sum_{i=1}^{N} s_i$$

with $s_i = \pm 1$ (Spin up/down). The factor $\frac{1}{2}$ compensates double counting of pairs $s_i\, s_j$ in the double sum. J_{ij} are the exchange integrals between the spins ($J > 0 \leftrightarrow$ ferromagnetic, $J < 0 \leftrightarrow$ antiferromagnetic), and B_0 denotes an external magnetic field (the orientation of the magnetic field defines the quantization axis of the spins). Consider nearest-neighbour interactions only, which may be all equal: $J_{ij} = J$. For simplicity we focus on linear chains / quadratic patterns / cubic lattices, i.e. each spin has $2D$ neighbours ($D = 1, 2, 3$: spatial dimension of the problem). Consider the system in the canonical ensemble, in the thermodynamic limit ($N \to \infty$).

a) Reformulate H by using the mean-field approximation, i.e. by neglecting the last term in the equation
$$s_i\, s_j = s_i \langle s_j \rangle + \langle s_i \rangle s_j - \langle s_i \rangle \langle s_j \rangle + (s_i - \langle s_i \rangle)(s_j - \langle s_j \rangle) \; .$$

b) Derive (for the ferromagnetic case), within the mean-field approximation, the relationship between the spin expectation value $\langle s \rangle$, the exchange integral J, and the external magnetic field B_0.

c) The relationship of a) must be solved self-consistently. Without external field ($B_0 = 0$) one obtains (below a critical temperature T_C) spontaneous magnetization ($\langle s \rangle \neq 0$: ferromagnetic phase). $\langle s \rangle = 0$ is also a possible solution below T_C, but not stable: Demonstrate its thermodynamical instability by showing that the free energy is higher than for the solution with non-zero $\langle s \rangle$. Show that above T_C one obtains $\langle s \rangle = 0$ (paramagnetic phase). Determine the value of T_C. Determine the spin expectation value for very small temperature ($T \ll T_C$) and slightly below T_C (i.e. $|T - T_C| \ll T_C$).

d) Now include the external magnetic field (i.e. $B_0 \neq 0$). Determine (for the limit $B_0 \to 0$) the magnetic susceptibility slightly above and slightly below T_C.

e) Now consider the same system for the antiferromagnetic case, i.e. $J < 0$. Show (again within mean-field approximation) that there exists again a transition temperature T_N (Néel-Temperatur) between an antiferromagnetic and a paramagnetic phase. Determine T_N. Determine the magnetic susceptibility slightly above T_N.

   Hint: Since neighbouring spins now tend to be anti-parallel to each other, it is necessary to consider (for the ordered phase) alternating spins on two sublattices (with *two* spin expectation values $\langle s_1 \rangle$ and $\langle s_2 \rangle$).

Problem 16: Exact solution of the Ising model in one dimension (3 points)

Consider an Ising model of a one-dimensional chain of N sites with nearest-neighbour interaction, without external magnetic field, i.e.

$$H = -\sum_{i=1}^{N-1} J_i\, s_i\, s_{i+1} \ .$$

For the calculation it is convenient to consider individual values for J_i. At the end, they all take the same value, $J_i = J$.

a) Show (e.g., by complete induction) that the canonical partition sum (Zustandssumme) is given by

$$Z_N = 2^N\, [\cosh(\beta J)]^{N-1} \ .$$

b) Calculate the expectation value

$$\langle s_j\, s_{j+k}\rangle = \frac{1}{Z_N} \sum_{s_1=\pm 1} \ldots \sum_{s_N=\pm 1} s_j\, s_{j+k}\, \mathrm{e}^{-\beta H}$$

and show that

$$\langle s_j\, s_{j+k}\rangle = [\tanh(\beta H)]^k \ .$$

Hints: prove first that

(1) $\quad s_j\, s_{j+k} = s_j\, s_{j+1}\, s_{j+1}\, s_{j+2}\, s_{j+2} \ldots s_{j+k-1}\, s_{j+k-1}\, s_{j+k}\ ,$

(2) $\quad s_j\, s_{j+1}\, \mathrm{e}^{-\beta H} = \dfrac{1}{\beta} \dfrac{\partial}{\partial J_j}\, \mathrm{e}^{-\beta H} \ .$

c) $\langle s_j\, s_{j+k}\rangle$ contains „correlation“ between spins j and $j + k$, but at large distance ($k \to \infty$) this should vanish and the non-correlated result $\langle s_j\rangle \cdot \langle s_{j+k}\rangle$ must emerge. In the limit of an infinitely long chain, all $\langle s_j\rangle$ should be the same ($= \langle s\rangle$), which leads to

$$\langle s\rangle^2 = \lim_{k\to\infty} \langle s_j\, s_{j+k}\rangle \ .$$

What do you obtain for $\langle s\rangle$ (as a function of T)? Is there a critical temperature between two phases?

d) Compare $\langle s\rangle$ (as a function of T) and the critical temperature (if any) with the mean-field result (e.g., problem 15). Differences would indicate that the mean-field approximation is not exact.

Remark: Also for 2D, an exact solution of the Ising model exists ($\to$ Onsager solution). In 3D, no exact solution has been found so far.