Exercises
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Exercises
Spontaneous Symmetry Breaking and Field Theory 1

Sheet 2

2/1 Statistical mechanics of binary alloys

The nearest-neighbour interaction model of a binary alloy may be represented by the Hamiltonian

$$\widehat{H}_L = \frac{1}{2} \sum_{ij}{}' \left[E^{AA} t_i^A t_j^A + E^{BB} t_i^B t_j^B + E^{AB} (t_i^A t_j^B + t_i^B t_j^A) \right] \tag{1}$$

where the sum runs over all nearest-neighbour pairs and where $t_i^A = 1$, $t_i^B = 0$ if site i is occupied by an A atom and $t_i^A = 0$, $t_i^B = 1$ if site i is occupied by a B atom. The nearest-neighbour Ising model of magnetism may be represented by the Hamiltonian

$$\widehat{H}_I = - \sum_{ij}{}' J S_i S_j \tag{2}$$

where again the sum runs over all nearest-neighbour spins and where $S_i = \pm 1$.

a) Express the variables t_i^A and t_i^B by the Ising variable S_i and transform $\widehat{H}_L(t_i^A, t_i^B)$ into $\widehat{H}_L(S_i)$.

b) Show that the grandcanonical partition function for the alloy with the interaction energy $\widehat{H}_L(S_i)$ can be mapped on the Gibbs partition function $Y(T, H)$ of the Ising model with the interaction energy $\widehat{H}_I(S_i)$ which is in an external magnetic field H.

c) Having obtained this mapping of the alloy model on the Ising model we can transfer directly the results for the Ising model to those of the alloy model, i.e., we have to solve the statistical mechanics problems just for one model. Illustrate this by discussing the alloy configurations for $T > T_c$ and $T < T_c$ for the cases $J > 0$ (ferromagnetic coupling) and $J < 0$ (antiferromagnetic coupling) from the analogy to the corresponding magnetic configurations.

2/2 Ising model with infinite interaction range

Calculate the partition function for an Ising model where each spin pair interacts with the same strength which is independent of the distance between the spins. The Hamiltonian of this system is given by

$$\widehat{H} = -\frac{J}{N} \sum_{ij} S_i S_j \ , \tag{3}$$

where the sum runs over all spin pairs.

a) Show that the partition function may be written as

$$Z_N = \left(\frac{N}{2\pi}\right)^{1/2} \exp\left(-\frac{J}{kT}\right) \ 2^N \int_{-\infty}^{+\infty} \left\{ \ \exp(-y^2/2) \ \cosh\left((2J/kT)^{1/2} \ y\right) \ \right\}^N dy \ . \tag{4}$$

Use the identity

$$\exp\left(a^2\right) = (2\pi)^{-1/2} \int_{-\infty}^{+\infty} \exp\left(-\frac{1}{2}x^2 + 2^{1/2}ax\right) dx \tag{5}$$

(prove this identity).
Discuss the behaviour of the function

$$f(y) = \left\{ \ \exp(-y^2/2) \ \cosh\left((2J/kT)^{1/2} \ y\right) \ \right\}^N \tag{6}$$

for $N \to \infty$. Use the knowledge which you got from this discussion for the calculation of the magnetic free enthalpy per spin

$$\frac{G_{\text{magn}}(T, \mathbf{H} = 0)}{N} = -\frac{kT \ln Z_N}{N}. \tag{7}$$

Thereby distinguish the cases $J/kT > 1/2$ and $J/kT < 1/2$.
Hint: In the procedure you must determine the maximum of $f(y)$. For $J/kT > 1/2$ this is facilitated by recognizing that the maximum of $f(y)$ is a maximum also of $\ln(f(y))$.

b) Calculate the thermal average of $\overline{S}_n$ for the Ising spin at an arbitrary site n.
Hint: Use again the identity (5) to represent $\overline{S}_n$ by an integral over a second function $f_2(y)$. Use the same arguments as in part (a) to calculate this integral for $N \to \infty$. Compare the result for $\overline{S}_n$ with the one from the molecular field theory.