

8.1 Equilibrium of ideal gas with traps

A closed container of volume V is filled with an ideal monoatomic classical gas. The molecules can stick to the walls of the container: there are $N_T \gg 1$ traps on the walls that can bind one molecule each with binding energy Δ . Each trap can be in only two states, empty or filled, independently from all the other traps; the traps are distinguishable from each other.

- Calculate the entropy and the free energy of the gas bound by the traps if there are $N_b \leq N_T$ bound molecules.
- Write the condition for the equilibrium of bound and unbound parts of the gas; what plays the role of the chemical potential for the bound gas?
- Find the relation between the number of filled traps $x_b = N_b/N_T$ and the density of the unbound gas $n = N/V$.

8.2 Mean-field theory of the Ising model

In the class we have studied the Ising model of N spins on a d -dimensional square (cubic) lattice with the Hamiltonian

$$\mathcal{H} = -J \sum_{\langle ij \rangle} s_i s_j - h \sum_i s_i, \quad s_i = \pm 1 \quad (1)$$

using mean-field theory with an order parameter $\eta = \langle s_i \rangle$ assuming that the correlation $\langle (s_i - \eta)(s_j - \eta) \rangle$ is negligible, which led to the Hamiltonian

$$\mathcal{H} = dJN \eta^2 - (h + 2dJ\eta) \sum_i s_i = dJN \eta^2 - h_{eff} \sum_i s_i$$

with a self-consistent solution $\eta = \langle s_i \rangle = \tanh \frac{h_{eff}}{T}$. Assuming that the temperature T is close to the critical $T_c = 2Jd$ and $\eta \ll 1$, find the matching between the parameters of the Ising model (1) and the mean-field free energy density

$$f = \frac{F}{N} = a\tau\eta^2 + \frac{1}{2}b\eta^4 - h\eta.$$

8.3 First-order phase transition

Assume that the density of the thermodynamic potential is given by the following expansion in the order parameter η and temperature parameter $\tau = T/T_0 - 1$,

$$\phi(\eta) = a\tau\eta^2 - c\eta^3 + \frac{1}{2}b\eta^4, \quad a, b, c > 0, \quad 0 < \tau < \frac{9c^2}{16ab}.$$

- Plot or sketch the dependency of the thermodynamic potential $\phi(\eta)$ for $\tau > 0$ and find the values of η corresponding to (meta)stable equilibrium.
- Suppose that the metastable value of η cannot be maintained (i.e. the system always chooses the global minimum of ϕ). Find the temperature at which the value of the order parameter changes discontinuously (i.e., the temperature of the first-order phase transition).
- * Calculate the latent heat of the first-order phase transition (*hint* : the entropy density is $s = -(\partial\phi/\partial T)$).