

Exercise 11.1 The Ising Model in the High-Temperature Limit

Consider the Ising model with nearest neighbor interactions in the presence of a homogeneous magnetic field h ,

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} S_i S_j - h \sum_i S_i, \quad J > 0, \quad (1)$$

where the spins assume the values $S_i = \pm S$ along the magnetic field and the sum $\sum_{\langle i,j \rangle}$ runs over nearest neighboring sites on the lattice. The number of spins is very large, $N \gg 1$, such that surface effects may be neglected.

- a) Determine the partition function in the high-temperature limit $\beta J \ll 1$.

Hint: Note that for $\beta J \ll 1$, one may neglect bond-bond correlations and the partition function simplifies to

$$Z \approx \sum_{\{S_i\}} e^{\beta h \sum_i S_i} \left(1 + \frac{\beta J}{2} \sum_j \sum_{m \in \Lambda_j} S_j S_m \right), \quad (2)$$

where Λ_j represents the set of nearest neighbors of site j such that $|\Lambda_j| = z$ with the coordination number z .

- b) Calculate the spin susceptibility at $h = 0$. In analogy to the lecture notes (Section 3.4.6), plot $1/\chi_0$ as a function of temperature and extrapolate the high- T limit to lower temperatures to find the intersection on the T -axis. What is the physical interpretation of the intersection temperature?

Exercise 11.2 The Lattice Gas model

The lattice gas model is obtained by dividing the volume V into microscopic cells which are assumed to be small such that they contain at most one gas molecule. We neglect the kinetic energy of a molecule and assume that only nearest neighbours interact. The total energy is given by

$$H = -\lambda \sum_{\langle i,j \rangle} n_i n_j \quad (3)$$

where the sum runs over nearest-neighbour pairs and $\lambda > 0$ is the nearest-neighbour attraction. There is at most one particle in each cell ($n_i = 0$ or 1). This model is a simplification of hard-core potentials, like the Lennard-Jones potential, characterized by an attractive interaction and a very short-range repulsive interaction that prevents particles from overlapping.

- a) Show the equivalence of the grand canonical ensemble of the lattice gas model with the canonical ensemble of an Ising model in a magnetic field.

In the following we will use the mean-field solution of the Ising model discussed in Chapter 5.2 of the lecture notes and the equivalence stated in a) in order to discuss the liquid-gas transition in the lattice gas model.

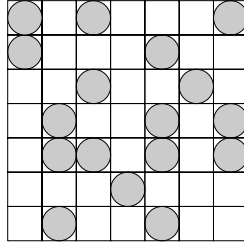


Figure 1: Schematic view of the lattice gas model.

- b) Derive a self-consistence equation for the density $\rho = \langle n_i \rangle$ and discuss its solutions as a function of the temperature T and chemical potential μ .
- c) Find the equation of state $p = p(T, \rho)$ or $p = p(T, v)$ and discuss the liquid-gas transition in the $p - v$ diagram. Thereby, $v = 1/\rho$ is the specific volume. Compare with the van der Waals equation of state:

$$\left(p + \frac{\tilde{a}}{v^2} \right) (v - \tilde{b}) = k_B T.$$

- d) Find the phase diagram ($T - p$ diagram). Determine the phase boundary ($T, p_c(T)$) and, in particular, compute the critical point ($T_c, p_c(T_c)$).

Office Hours: Monday, December 3rd, 8:00-10:00 HIT K 23.7 (Evert van Nieuwenburg)