

Exercise 11.1 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

$$H = -\lambda \sum_{\langle i,j \rangle} n_i n_j \quad (1)$$

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.

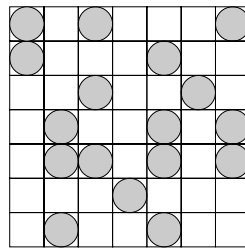


Figure 1: Schematic view of the lattice gas model.

- 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.

- 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 ($T_c, p_c(T_c)$).

Exercise 11.2 Magnetic domain wall

We want to calculate the energy of a magnetic domain wall in the framework of the Ginzburg-Landau (GL) theory. We assume translational symmetry in the (y, z) -plane in which case the GL functional in zero field reads

$$F[m, m'] = F_0 + \int dx \left\{ \frac{A}{2} m(x)^2 + \frac{B}{4} m(x)^4 + \frac{\kappa}{2} [m'(x)]^2 \right\}. \quad (2)$$

- a) Solve the GL equation with boundary conditions

$$m(x \rightarrow \pm\infty) = \pm m_0, \quad m'(x \rightarrow \pm\infty) = 0. \quad (3)$$

Here, m_0 is the magnetization of the uniform solution.

- b) Compute the energy of the solution in a) as compared to the uniformly polarized solution. Use the coefficients A and B according to the expansion of the mean-field free energy of the Ising model [see Eq. (5.65)]. Compare the energy of the domain wall with the energy of a sharp step in the magnetization.

Office Hours: Monday, December 5th, 8:00-10:00 K12.2 (Jonathan Buhmann)