Exercise 1. ***Condensation and crystallization in the lattice gas model.***

The lattice gas model is obtained by dividing the volume V into microscopic cells which are assumed to be small enough such that they contain at most one gas molecule. In two and three dimensions, the result is a square and a cubic lattice, respectively. We neglect the kinetic energy of a molecule and assume nearest neighbors interactions. The total energy is given by

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

where the sum runs over nearest-neighbor pairs and λ is the nearest-neighbor coupling. 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.

In order to study the case of a repulsive interaction, $\lambda < 0$, we assume that we can divide the lattice into two alternating sublattices A and B. For square or cubic lattices (these are bipartite lattices), we find that all lattice sites A only have points B as their nearest neighbors.

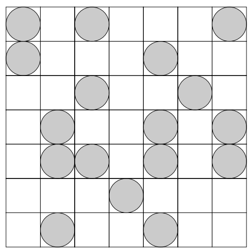

Figure 1: Schematic view of the lattice gas model.

(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.

(b) Introduce two mean-field parameters m_{A} and m_{B}, corresponding to the two sublattices A and B, and adapt the mean-field solution of the Ising model discussed in Sec. 5.2 of the lecture notes for these two parameters. What are the self-consistency conditions for m_{A} and m_{B}?

(c) Use your results from parts (a) and (b) to calculate the grand potential for the lattice gas and determine the self-consistency relations for the two mean-field parameters $\rho_{\mathrm{A}} = \langle n_i \rangle_{i \in \mathrm{A}}$ and $\rho_{\mathrm{B}} = \langle n_i \rangle_{i \in \mathrm{B}}$.

In the following we will use the mean-field solution of the lattice gas model in order to discuss the liquid-gas transition for an attractive interaction $\lambda > 0$.

(d) Argue, why in this case the mean-field results can be simplified as the two densities must be equal, $\rho_{\mathrm{A}} = \rho_{\mathrm{B}} = \rho$. Use your knowledge of the Ising model to define a critical temperature T_{c}, below which there are multiple solutions to the self-consistency equations, and discuss the solutions of ρ for temperatures above or below T_{c}. Define also the critical chemical potential μ_0 corresponding to $h = 0$ in the Ising model and use this for a distinction of cases.

(e) 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:

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

What is different in our model?

Hint. For the lattice gas, we have $\tilde{b} = 1$.

(f) Find the phase diagram ($T - p$ diagram). Determine the phase boundary $(T, p_{\mathrm{c}}(T))$ and, in particular, compute the critical point $(T_{\mathrm{c}}, p_{\mathrm{c}}(T_{\mathrm{c}}))$.

Instead of the liquid-gas transition, which we have observed for an attractive interaction $\lambda > 0$, a crystallization transition (sublimation) can be observed for nearest-neighbor repulsion, $\lambda < 0$. In this case, we will find that the two mean-field parameters are different, $\rho_{\mathrm{A}} \neq \rho_{\mathrm{B}}$, below some critical temperature T_{c}.

(g) Discuss the solutions below the critical temperature for $\lambda < 0$. Plot the densities ρ_{A} and ρ_{B}, as well as the average, $(\rho_{\mathrm{A}} + \rho_{\mathrm{B}})/2$ for both attractive and repulsive nearest-neighbor interaction at low temperature, $T < T_{\mathrm{c}}$.

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