

Please encircle the questions you have solved and are able to present/discuss in class.

2.1 (a)   2.1 (b)   2.1(c)   2.1(d)   2.1(e)   2.1(f)

## Problem 2.1: Condensation transition in the lattice gas model (10 points)

The lattice gas model is obtained by dividing the volume  $V$  into microscopic cells — lattice sites — which are occupied by gas molecules. In two and three dimensions, the result is a square and cubic lattice, respectively. We neglect the kinetic energy of a molecule and we assume nearest neighbors interactions. The total energy is then given by

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

where  $n_j$  is the number of gas particles on site  $j$ . The sum runs over nearest-neighbor pairs, denoted as  $\langle ij \rangle$  and  $\lambda$  is the nearest-neighbor coupling constant. We assume that the gas particles experience a so-called *hard-core* interaction, i.e., on each lattice site  $i$  there can be at most one particle. As a consequence  $n_j = 0$  or  $1$  for every lattice site  $j$ . This is a simplified model of gases in which particles interact with a Lennard-Jones potential, which is characterized by an attractive interaction and a very short range repulsive interaction that prevents particles from overlapping.

For the first part of the exercise it is instructive to consider the case where the lattice can be divided into two alternating sublattices  $A$  and  $B$  (these are called bipartite lattices). All the lattice sites of  $A$  have then only points of  $B$  as their nearest neighbors. This is shown in Fig. 1 for a square lattice in two dimensions. We will denote henceforth with  $L = A \cup B$  the whole lattice obtained from the union of  $A$  and  $B$ , with  $|L| = N$  the total number of lattice sites (the volume) and with  $\gamma$  the coordination number, i.e., the number of nearest neighbors. For square (dimension  $d = 2$ ) and cubic ( $d = 3$ ) lattices, as in Fig. 1,  $\gamma = 2d$ .

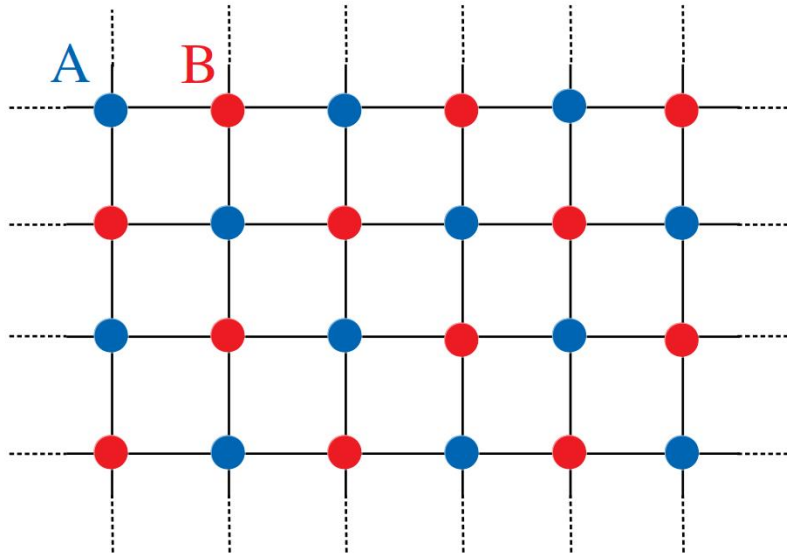


Figure 1: A square lattice is a bipartite lattice since it can be divided into the sublattices  $A$  and  $B$ . Lattice sites belonging to  $A$  are colored in blue, while the ones belonging to  $B$  are red. The union between the sublattice  $A$  and  $B$  generates the whole lattice  $L$ :  $L = A \cup B$ . In the case depicted we have  $d = 2$  and thus  $\gamma = 2d = 4$ .

- (a) Show that the partition function  $Z_G$  of the lattice gas in the *grand-canonical ensemble* is equal, up to a constant factor, to the partition function of the Ising model  $Z_I$  in a magnetic field in the *canonical ensemble*. (1 point)

*Hint:* Remember that the Hamiltonian  $H_G$  in the grand-canonical ensemble is given by

$$H_G = H - \mu \sum_i n_i, \quad (2)$$

with  $\mu$  being the chemical potential and  $H$  given in Eq. (1).

*Hint:* You should obtain the following relation

$$Z_G = Z_I e^{\beta(\frac{\lambda\gamma}{8} + \frac{\mu}{2})N}, \quad (3)$$

with  $\beta = 1/(k_B T)$  the inverse temperature and the Hamiltonian  $H_I$  of the Ising model is

$$H_I = -J \sum_{\langle ij \rangle} s_i s_j - H \sum_i s_i. \quad (4)$$

- (b) Consider the Ising model in Eq. (4) on a bipartite lattice in dimension  $d$  (in  $d = 2$  the lattice is as in Fig. 1), for which we now want to construct the *mean-field solution*. Mean-field is an approximation which replaces the interaction between spins by an “effective” magnetic field. This magnetic field is given by the magnetization of the neighbors of each spin. To understand this we first define two mean field order parameters (one for each sublattice) as

$$m_A = \langle s_i \rangle_{i \in A}, \quad m_B = \langle s_i \rangle_{i \in B}. \quad (5)$$

Then we write down the spin degrees of freedom as

$$s_i = m_{A,B} + \delta_i, \quad \text{with } i \in A \text{ or } B. \quad (6)$$

Here  $\delta_i$  represents the (small) fluctuations of the spin variables  $s_i$  around their mean-field expectation value  $m_{A,B}$ . Insert Eq. (6) into Eq. (4) and expand up to first order in  $\delta_i$ . Verify that the Ising Hamiltonian in Eq. (4) in the mean-field approximation reduces to

$$H_I \approx \frac{\gamma N}{2} J m_A m_B - \sum_{i \in A} (\gamma J m_B + h) s_i - \sum_{j \in B} (\gamma J m_A + h) s_j, \quad (7)$$

where we have set

$$\delta_i = s_i - m_{A,B}, \quad \text{with } i \in A \text{ or } B, \quad (8)$$

according to Eq. (6). Note that in the Hamiltonian  $H_I$  in Eq. (7) the sublattices  $A$  and  $B$  behave as *non-interacting* paramagnets subject to the *effective magnetic fields*

$$h_{\text{eff}}^A = \gamma J m_B + h, \quad \text{for lattice } A, \quad h_{\text{eff}}^B = \gamma J m_A + h, \quad \text{for lattice } B. \quad (9)$$

Compute the partition function  $Z_I$  of the Ising model associated to the mean-field Hamiltonian in Eq. (7). Write down the self-consistency equations determining  $m_A$  and  $m_B$  (**2 points**).

- (c) Use the result obtained in points (a) and (b) to calculate the grand-canonical potential  $\Omega(\beta, \mu, N)$  of the lattice gas and determine the self-consistency equations for  $\rho_A = \langle n_i \rangle_{i \in A}$  and  $\rho_B = \langle n_i \rangle_{i \in B}$ . (**1 point**)

You should obtain the following two equations

$$\rho_A = \frac{1}{1 + e^{-\beta(\lambda\gamma\rho_B + \mu)}}, \quad \text{and} \quad \rho_B = \frac{1}{1 + e^{-\beta(\lambda\gamma\rho_A + \mu)}}. \quad (10)$$

*Hint:* The grand-canonical potential  $\Omega(\beta, \mu, N)$  is defined as

$$\Omega(\beta, \mu, N) = -\frac{1}{\beta} \ln Z_G, \quad (11)$$

and  $Z_G$  is known from point (a) in Eq. (3) with  $Z_I$  computed at point (b) in the mean-field approximation.

In the following we will use the mean-field solution of the lattice gas in order to discuss the liquid-gas transition for attractive interactions  $\lambda > 0$ . In the following points we therefore assume that  $\lambda > 0$ .

- (d) Argue why for  $\lambda > 0$  the mean-field solution can be simplified as the two densities must be equal  $\rho_A = \rho_B = \rho$ . Use your knowledge of the mean-field solution of the Ising model for zero magnetic field  $H = 0$  to define a critical temperature  $T_c$ , below which there are multiple solutions to the self-consistency equations. Discuss the solutions for  $\rho$  for temperatures above and below  $T_c$ . Define also the critical chemical potential  $\mu_0$  corresponding

to  $H = 0$  in the Ising model and use this for a distinction of cases. **(2 points)**

*Hint:* The two self-consistency equation (10) are of the form

$$\rho_A = \phi(\rho_B) \quad \text{and} \quad \rho_B = \phi(\rho_A), \quad \text{with} \quad \phi(x) = \frac{1}{1 + e^{-\beta(\lambda\gamma x + \mu)}}. \quad (12)$$

Note that the function  $\phi(x)$  is monotonically increasing for  $\lambda > 0$ .

*Hint:* For  $T < T_c$  and  $\mu = \mu_0$  you have three solutions:  $\rho = \rho_l(T) > 1/2$ ,  $\rho = \rho_g(T) < 1/2$  and  $\rho = 1/2$ . For  $T < T_c$  the solution  $\rho = 1/2$  has no physical meaning (it is unstable) and therefore we will refer henceforth to  $\rho_l(T)$  and  $\rho_g(T)$  only, which correspond to the liquid and gas phases, respectively.

- (e) Find the equation of state  $p = p(T, \rho)$  or  $p = p(T, v)$  (thereby  $v = 1/\rho$  is the specific volume and  $p$  is the pressure) and discuss the liquid-gas transition in the  $p - v$  diagram. Compare the equation of state you have obtained with the Van Der Waals equation of state

$$\left(p + \frac{a}{v^2}\right)(v - b) = k_B T. \quad (13)$$

What is different in our model ? Is there a limit where the two equations coincide? Explain and interpret the physical meaning of the result.

Note that for  $T < T_c$ , on the basis of the analysis of point (d), you have two solutions of the mean-field self-consistency equation for  $\rho$ . In the case of  $\mu = \mu_0$  these solutions are  $\rho_l(T)$  and  $\rho_g(T)$  defined above. Physically, this corresponds to the fact that for  $T < T_c$  one can have *coexistence* of the liquid and gas phase. In this case to get the correct equation of state you have to set  $\rho = \rho_{l,g}(T)$  into the equation of state  $p(T, \rho_{l,g}(T))$ . The pressure  $p$  is, as a consequence, constant in the coexistence region (this is equivalent to the Maxwell equal area construction). Write down the equation of state for  $T < T_c$  to account for the phase coexistence of the liquid and gas phase. **(2 points)**

*Hint:* For the lattice gas we have  $b = 1$ .

- (f) Determine the phase boundary  $(T, p_c(T))$  and, in particular, compute the critical point  $(T_c, p_c(T_c))$ . **(2 points)**