

Phase Transitions

Homework Sheet 5

Due 10am Tue 11 April 2017, in the 563 box.

Question 5–1.

This question concerns scaling near the phase transition of the one-dimensional Ising model, using the exact results derived previously from transfer matrix calculations.

- Usually, in writing down the scaling form of (*e.g.*) the singular part of the free energy density, we use the variables t and h , defined by $t \equiv (T - T_c)/T_c$ and $h \equiv H/k_B T$. This does not apply for one-dimensional Ising model, which has a zero temperature phase transition with essential singularity behaviour, as discussed in class. What will be the appropriate definition of these variables for the one-dimensional Ising model?
- Show that for small t and h , the free energy and magnetisation can be written in scaling form, and determine the exponents y_t and y_h defined in class.
- Show that for small t and h the correlation function also has the expected scaling form.

Question 5–2.

This question is a continuation of HW 4–1, in which the mean field theory for the Ising universality class was derived from the Hubbard-Stratonovich transformation. Here, we use the mean field theory calculation of the Gibbs free energy to present the analogue of the Maxwell construction for magnetic systems, and to motivate the Landau free energy. The notation is given in HW4–1.

- Consider the case of uniform magnetisation $m_i = m$ on a d -dimensional hypercubic lattice, with coordination number $z = 2d$. Expand Γ to quartic order in m and show that there is a second order (continuous) transition at $T_c = 2dJ/k_B$. From the equation of state, check the values of the critical exponents β and δ and verify they are what we expect in MFT.
- Sketch the form of $H(m)$ and $m(H)$ above and below the transition, *as given by the mean field theory*. Notice that your answer contains an unphysical portion below T_c . Explain what this region is, and why it is unphysical.
- Consider the function given by

$$L'(m, \hat{H}) \equiv \Gamma(m) - mN(\Omega)\hat{H}$$

where \hat{H} is a parameter and not the function $H(m)$, and $m(H)$ is given by the mean field theory. Show that the condition that L' be minimised with respect to m implies the equation of state $\hat{H} = H(m)$. Sketch the form of $L'(m)$ above and below the transition for \hat{H} positive, negative and zero. Hence show that the condition that L' be globally minimised removes the unphysical portion of the curve $m(H)$.

Question 5–3.

The spontaneous magnetisation m per spin of the two-dimensional Ising model below T_c is given by

$$m^8 = 1 - (\sinh 2J/k_B T)^{-4}.$$

This result was written down by L. Onsager in 1949 at a conference, but he did not give a proof. A proof was eventually provided by C.N. Yang in 1952. According to our discussion in class, we expect that near the critical point, we can write

$$m = A(-t)^\beta [1 + B(-t)^\Delta + \dots]$$

where $t \equiv (T - T_c)/T_c$ and A and B are constants. The term proportional to B is known as a correction to scaling, and describes behavior that is sub-dominant to the leading asymptotics near T_c given by the term $(-t)^\beta$.

- (a) Determine β and Δ from Onsager's formula.
- (b) Express A and B in terms of $K_c \equiv J/k_B T_c$.
- (c) Investigate over what range of temperatures it is acceptable to ignore the correction to scaling. You may use Matlab or Mathematica or Python etc...

Question 5–4.

On the web page I have deposited a data file for the dependence on temperature T of the electromagnetic penetration depth $\lambda(T)$ in the high temperature superconductor $\text{YBa}_2\text{-Cu}_3\text{O}_{7-\delta}$. Analyse these data to find the critical temperature T_c , λ_0 and the exponent y describing how the penetration depth diverges near the critical temperature:

$$\lambda = \lambda_0 t^{-y}$$

where $t \equiv (T_c - T)/T_c$. Estimate the size of the critical region. Make sure that you generate plots of your analyses, and in your write-up try to determine error bars on the various quantities you were asked to find. As in the atom bomb problem, you will probably need to do several different plots to get reliable and consistent results.

Question 5–5.

Here we will use our mean field solution of the Ising model to solve the lattice gas model of a fluid. Please refer to section 12.2.1 of my book to remind yourself of the detailed basis for the correspondence between the Ising model and fluid models. The relevant section is attached to this PDF. The goal is to make a simple theory of the critical behaviour of a fluid. Set $U_1 = 0$, and check that you understand the correspondence between the lattice gas variables and the Ising variables. In particular, write down the relation between the pressure and the free energy of the Ising model. Also, write down the relation between the mean density ρ of the lattice gas and the mean value of the magnetisation of the Ising model.

- (a) Express E_0 in terms of H and J . Using the result of HW 4–1, rewrite this in terms of H and T_c . Write down the relation between the pressure p , $H(m)$ and $S(m)$, using the results from 4–1 for the uniform magnetisation case. Hence show that the equation of state in the mean field approximation is

$$p = k_B T \log \left(\frac{1}{1 - \rho} \right) - 2k_B T_c \rho^2$$

- (b) Show that at the critical point for the fluid (p^*, ρ^*, T^*) ,

$$p^* = k_B T_c (\log 2 - 1/2),$$

and $T^* = T_c$, $\rho^* = 1/2$. This corresponds to the critical point $H = 0$, $T = T_c$ in the Ising model.

As in the magnetic case, a variety of analytic properties may be proven, many of which derive from the convexity of f_b :

- (a) $p(T, \mu) \geq 0$.
- (b) $p(T, \mu)$ is continuous.
- (c) $\partial p / \partial T$, $\partial p / \partial \mu$ exist almost everywhere.
- (d) $\partial p / \partial \mu = \rho \geq 0$.
- (e) $\partial p / \partial T = \sigma \geq 0$ (True in quantum statistical mechanics only, but false for classical systems).
- (f) $\partial p / \partial T$ is monotonic non-decreasing, which implies that the heat capacity $C_\mu \geq 0$.
- (g) $\partial p / \partial \mu$ is monotonic non-decreasing, which implies that the isothermal compressibility K_T is non-negative.

2.12 LATTICE GASES

One of the reasons for the importance of the Ising model is that a variety of other statistical mechanical systems can be simulated by it. This is the topic of **equivalence** between models, or more precisely **exact equivalence** or **mapping**. Now we discuss a simple model for the statistical mechanics of a fluid — the **lattice gas**, due to Lee and Yang. The basic idea is to relate the local density of particles in a fluid to the local up-spin density of a magnet: We will demonstrate the equivalence in two steps, and in so doing, we will, incidentally, expose the advantage of the grand canonical ensemble over the canonical ensemble.

As a preliminary step, recall that the potential terms in the Hamiltonian (2.123) may be re-written in terms of the microscopic density of the fluid

$$\rho(\mathbf{r}) \equiv \sum_{i=1}^N \delta(\mathbf{r} - \mathbf{r}_i). \quad (2.136)$$

This expression is the microscopic density, because

$$\int_V \rho(\mathbf{r}) d^3\mathbf{r} = N(V) \quad (2.137)$$

where $N(V)$ is the number of particles in the arbitrary volume V . Then, using the property of the delta function that

$$\int f(x) \delta(x - a) dx = f(a), \quad (2.138)$$

we write

$$\sum_i U_1(\mathbf{r}_i) = \sum_i \int_\Omega U_1(\mathbf{r}) \delta(\mathbf{r} - \mathbf{r}_i) d^d\mathbf{r} = \int_\Omega d^d\mathbf{r} U_1(\mathbf{r}) \rho(\mathbf{r}) \quad (2.139)$$

2.12 Lattice Gases

and

$$\begin{aligned} \sum_{i \neq j} U_2(\mathbf{r}_i - \mathbf{r}_j) &= \sum_{i \neq j} \int_\Omega U_2(\mathbf{r}_i - \mathbf{r}') \delta(\mathbf{r}' - \mathbf{r}_j) d^d\mathbf{r}' \\ &= \sum_{i \neq j} \int_\Omega \int_\Omega U_2(\mathbf{r} - \mathbf{r}') \delta(\mathbf{r} - \mathbf{r}_i) \delta(\mathbf{r}' - \mathbf{r}_j) d^d\mathbf{r} d^d\mathbf{r}' \\ &= \int_\Omega \int_\Omega U_2(\mathbf{r} - \mathbf{r}') \rho(\mathbf{r}) \rho(\mathbf{r}') d^d\mathbf{r} d^d\mathbf{r}'. \end{aligned} \quad (2.140)$$

These expressions are not directly useful as they stand, because the degrees of freedom in the grand canonical trace operation are the co-ordinates, not the microscopic density. We will shortly see how we can effectively make a change of variables to the density co-ordinates; but first, we need to discuss how to represent a fluid system by a spin system.

2.12.1 Lattice Gas Thermodynamics from the Ising Model

Consider a d -dimensional lattice, with co-ordination number z . Each site can be occupied by a single molecule or not at all. The occupation number of the i^{th} site, n_i , takes the values 0 and 1 only. The total number of particles in the system is

$$N = \sum_{i=1}^{N(\Omega)} n_i. \quad (2.141)$$

The occupation number n_i is rather like the microscopic density $\rho(\mathbf{r})$ in the continuum fluid. Thus we might guess a suitable Hamiltonian for the lattice gas of the form

$$H_\Omega = \sum_{i=1}^{N(\Omega)} U_1(i) n_i + \frac{1}{2} \sum_{i,j=1}^{N(\Omega)} U_2(i,j) n_i n_j + O(n_i n_j n_k), \quad (2.142)$$

so that, in the grand canonical ensemble,

$$H_\Omega - \mu N = \sum_i (U_i - \mu) n_i + \frac{1}{2} \sum_{ij} U_2(i,j) n_i n_j + \dots \quad (2.143)$$

The factor of 1/2 in the above equations avoids double counting the contribution to the energy from the interaction between two particles. The Hamiltonian (2.142) only represents the potential energy of the gas; but

this does not matter, since as we have seen, the kinetic energy only contributes to the fugacity. In the following, we will actually model the configurational sum Q_N , rather than the full partition function.

To make contact with the Ising model, define

$$n_i = \frac{1}{2}(1 + S_i), \quad S_i = \pm 1 \quad (2.144)$$

$$n_i = 0 \iff S_i = -1 \quad (2.145)$$

$$n_i = 1 \iff S_i = +1. \quad (2.146)$$

Substitution into eqn. (2.143) gives

$$\sum_i (U_1(i) - \mu) \frac{1}{2}(1 + S_i) = \frac{1}{2} \sum_i (U_1(i) - \mu) + \frac{1}{2} \sum_i (U_1(i) - \mu) S_i \quad (2.147)$$

and

$$\begin{aligned} \frac{1}{2} \sum_{ij} U_2(i, j) n_i n_j &= \frac{1}{2} \cdot \frac{1}{4} \sum_{ij} U_2(i, j) (1 + S_i)(1 + S_j) \\ &= \frac{1}{2} \cdot \frac{1}{4} \sum_{ij} U_2(i, j) + \frac{1}{2} \cdot \frac{1}{4} \sum_{ij} U_2(i, j) S_i \cdot 2. \quad (2.148) \\ &\quad + \frac{1}{2} \cdot \frac{1}{4} \sum_{ij} U_2(i, j) S_i S_j \end{aligned}$$

If the forces between fluid particles are short-ranged and the density is sufficiently low, then we can ignore three and higher body potentials, and model the two-body potential by

$$U_2(i, j) = \begin{cases} U_2 & i \text{ and } j \text{ nearest neighbors;} \\ 0 & \text{otherwise.} \end{cases} \quad (2.149)$$

Then the right hand side of eqn. (2.148) becomes

$$\frac{1}{4} U_2 \cdot N(\Omega) z \cdot \frac{1}{2} + \frac{2}{2} \cdot \frac{1}{4} U_2 \cdot z \cdot \sum_i S_i + \frac{U_2}{4} \cdot \sum_{\langle ij \rangle} S_i S_j. \quad (2.150)$$

Setting $U_1 = 0$, we find that

$$H_\Omega - \mu N = E_0 - \sum_i S_i H_i - J \sum_{\langle ij \rangle} S_i S_j \quad (2.151)$$

with

$$E_0 = -\frac{1}{2} N(\Omega) \mu + U_2 N(\Omega) z / 8 \quad (2.152)$$

$$-H = -\frac{1}{2} \mu + \frac{1}{4} U_2 z \quad (2.153)$$

$$-J = \frac{U_2}{4}. \quad (2.154)$$

Thus

$$\begin{aligned} \Xi_{\text{lattice gas}} &= \text{Tr } e^{-\beta(H_\Omega - \mu N)} \\ &= \left(\prod_{i=1}^{N(\Omega)} \sum_{n_i=0,1} \right) e^{-\beta(H_\Omega - \mu N)} \quad (2.155) \\ &= e^{-\beta E_0} Z_{\text{Ising}}(H, J, N(\Omega)) \end{aligned}$$

This is our desired result — the thermodynamic properties of the lattice gas may be obtained from the thermodynamics of the Ising model. The reader is invited to investigate this in a subsequent example, which shows that the ideal gas law and corrections to it, the equation of state *etc.* may all be derived from the lattice gas model.

2.12.2 Derivation of Lattice Gas Model from the Configurational Sum

In the previous section, we showed that the lattice gas model is related to a spin system. In this section, we derive the lattice gas model directly from the configurational sum for a fluid. These two results together serve to illustrate an equivalence between fluid and magnetic systems.

We approximate Q_N by dividing space Ω up into cells of linear dimension a , such that probability of finding more than one molecule per cell is negligible: *i.e.* $a \leq$ hard core radius. Then, the measure in Q_N may be replaced heuristically by

$$\int_\Omega \prod_{i=1}^N d^d \mathbf{r}_i \approx a^{dN(\Omega)} \sum_{\alpha=1}^{N(\Omega)}, \quad (2.156)$$

where α labels the cells and

$$1 \leq \alpha \leq N(\Omega) \equiv \frac{V(\Omega)}{a^d}. \quad (2.157)$$

Note the distinction between N , the number of particles, and $N(\Omega)$, the number of cells. Next, we replace the interaction $U\{\mathbf{r}_i\}$ between the particles by the interaction energy between occupied cells:

$$U_2(\mathbf{r}_i, \mathbf{r}_j) = U_2(\alpha, \beta) \quad \text{if } \mathbf{r}_i \in \text{cell } \alpha \text{ and } \mathbf{r}_j \in \text{cell } \beta. \quad (2.158)$$