Chapter 2: Mean-field theory

In general, computing the values of the relevant thermodynamic quantities of a statistical mechanics model is a very challenging tasks. While one can usually solve such problems by Monte-Carlo simulations [1], analytic solutions are often more desirable, as they allow to develop a deeper understanding of the physical mechanisms that are at play. Even if the analytic solution can only be obtained under drastic approximations, it can serve as a useful starting point, especially if there are systematic ways to improve upon it. Mean-field theory allows for the calculation of such useful solutions, especially since it can be applied with relative ease to any statistical mechanics model under consideration.

I. THE MEAN-FIELD APPROXIMATION

The main reason why statistical mechanics models are hard to solve is the existence of correlations in the system arising from interactions between the particles. Hence, if one can approximate a model by a non-interacting counterpart, solving the latter will be much easier. To this end, we can express any degree of freedom such as a spin variable S_i in terms of its mean value $\langle S_i \rangle$ and its fluctuations $\Delta S_i = S_i - \langle S_i \rangle$, i.e., $S_i = \langle S_i \rangle + \Delta S_i$. An interaction such as the Ising interaction can then be written as

$$S_i S_j = (\langle S_i \rangle + \Delta S_i)(\langle S_j \rangle + \Delta S_j) = \langle S_i \rangle \langle S_j \rangle + \Delta S_i \langle S_j \rangle + \langle S_i \rangle \Delta S_j + \Delta S_i \Delta S_j. \qquad (1)$$

The mean-field approximation now neglects the last term, i.e., it assumes that the *quadratic fluctuations* around the mean value are small. Then, one may write

$$S_i S_j \approx S_i \langle S_j \rangle + \langle S_i \rangle S_j - \langle S_i \rangle \langle S_j \rangle. \qquad (2)$$

II. MEAN-FIELD SOLUTION OF THE ISING MODEL

Let us now apply the mean-field approximation to the Ising model. In addition to the Ising interaction, we also consider an external magnetic field h. Then, the parition function is given by

$$Z = \sum_{\{S_i\}} \exp\left[\beta\left(h\sum_i S_i + J\sum_{\langle ij \rangle} S_i S_j\right)\right]. \qquad (3)$$

Following the mean-field approximation, the partition function becomes

$$Z_{MF} = \sum_{\{S_i\}} \exp\left[\beta(h + zJm)\sum_i S_i - \frac{zJ}{2}m^2\right], \tag{4}$$

where z the coordination number of the lattice and $m = \langle S_i \rangle$ is the magnetization of the system. Since the sites i are identical, the sum involves only the two spin states $S_i = \{-1, 1\}$, yielding

$$Z_{MF} = \left[2\exp\left(-\frac{zJ}{2}\beta m^2\right)\cosh\beta(h + zJm)\right]^N. \tag{5}$$

Since the magnetization m is given by $m = (\beta N)^{-1}\partial/\partial h \log Z$ [2], we obtain the mean-field equation of state

$$m = \tanh\beta(zJm + h). \tag{6}$$

III. PHASE TRANSITIONS IN THE ISING MODEL

Let us first have a closer look at the case where the external field h vanishes. Then, we can perform a Taylor expansion for small values of m,

$$m = \beta zJm - \frac{1}{3}(\beta zJm)^3 + O(m^5). \tag{7}$$

This equation has three solutions,

$$m_0 = 0, \quad m_{1/2} = \pm\sqrt{-3\tau}, \tag{8}$$

where we have introduced the reduced temperature

$$\tau = \frac{T - T_c}{T_c} \tag{9}$$

that is defined in terms of the critical temperature $T_c = zJ/k_B$.

Above T_c, we have only one real solution, but below T_c, there are three. Which of the three solutions is then the correct one? Fortunately, we know that in thermal equilibrium, the free energy F will be at a minimum. We can readily calculate the free energy according to the mean-field partition function (5), which we again expand for small m,

$$F = -\beta^{-1}\log Z_{MF} = Nk_B(T - T_c)m^2 + Nk_B\frac{T_c}{12}m^4 + O(m^6) + \text{const.} \tag{10}$$

Hence, we see that below T_c, the solutions with a finite m have a lower free energy. Consequently, the system will exhibit a finite magnetization m, which can be either positive or negative. From the $m \sim |\tau|^{1/2}$ behavior of (8) we can also read off the mean-field critical exponent $\beta = 1/2$.

Furthermore, we can expand the mean-field equation of state (6) for small h and m, leading to

$$m = \beta(zJm + h) - \frac{1}{3}(\beta zJm)^3. \tag{11}$$

At the critical temperature given by $\beta_c = 1/(zJ)$, the linear term in m cancels, so we are left with

$$m = \left(\frac{3h}{k_B T_c}\right)^{1/3}, \tag{12}$$

from which we obtain the second critical exponent $\delta = 3$.

These calculations show that according to the mean-field solution, the Ising model has a phase transition from a paramagnet ($m = 0$) to a ferromagnet ($m \neq 0$) occuring at the critical temperature $T_c = zJ/k_B$. Just below the critical point, the free energy is given by

$$F = -\frac{3}{4} N k_B T_c \left(\frac{T - T_c}{T_c}\right)^2, \tag{13}$$

which continuously but non-analytically connects to $F = 0$ for $T > T_c$. Note that the free energy (10) is symmetric under the transformation $m \to -m$, which is a manifestation of the $\mathbb{Z}_2$ symmetry of the Ising model. Since any finite magnetization will no longer respect that symmetry, we have found an example of spontaneous symmetry breaking.

However, the situation is very different when considering a small external field h as well. Then, the free energy picks up an additional term $-hm$ that is linear in the magnetization, i.e., the $\mathbb{Z}_2$ symmetry is broken. For $T > T_c$, we can find the minimum of the free energy simply by looking at the terms up to m^2 in the expansion. Then, we obtain for the magnetization

$$m = \frac{h}{2k_B(T - T_c)}. \tag{14}$$

Since the free energy is always an analytic function in this case, there is no phase transition.

Below T_c, we obtain the following picture. We can expand the free energy around the two minima of the solution without the external field. Denoting, the magnetization by $m = m_0 + \delta m$, where m_0 follows from the field free solution (8), we obtain up to second order in δm

$$F = -\frac{3}{4} N k_B T_c \left(\frac{T - T_c}{T_c}\right)^2 - N k_B (T - T_c)\delta m^2 - N k_B h m_0. \tag{15}$$

Crucially, the sign of the last term depends on the sign of m_0 and on the sign of h. For $h < 0$, the solution with $m_0 < 0$ will lower the free energy, whereas for $h > 0$ the solution with positive magnetization is the correct one. This means that at $h = 0$ the magnetization will abruptly change from $m = -|m_0|$ to $m = +|m_0|$, i.e., we have found a first order transition.

IV. VARIATIONAL MEAN-FIELD THEORY

In the previous section, we arrived at the mean-field equation of state for the Ising model by relating the magnetization m to a thermodynamic derivative of the partition function. However, can we also compute the equation of state in a more general way? This would be useful in cases where such a relationship is not obvious. Additionally, such an approach would be more general, since it does not rely on model-specific properties.

To this end, we construct a variational formulation of the problem. Variational techniques can be extremely powerful, as can be seen from Hamiltonian's principle of stationary action or Fermat's principle in geometric optics. Here, we will construct a variational principle for statistical mechanics problems, based on the notion that the solution of the problem should minimize the free energy.

Specifically, we consider product states of the form

$$p_{\{S_i\}} = \prod_i p_i(S_i). \tag{16}$$

Crucially, these states do not have any correlations between the different S_i, so they are relatively easy to work with. Of course, the assumption that the equilibrium state of a statistical mechanics problem is at least approximately described by a product state is a drastic assumption. And, even with a powerful variational principle at hand, the results can only be as good as the variational manifold of states that one allows for.

If we now turn to the Ising model, we can assume that all the sites are identical, i.e., $p_i(S_i = +1) = 1 - p_i(S_i = -1) \equiv p = (m+1)/2$. In the following, we regard m as our single variational parameter, which we will optimize such that the free energy becomes minimal. For such a product state. the mean value of the energy E can be calculated exactly since there are no correlations that we need to account for. In the absence of an external field ($h = 0$), we obtain

$$E = \frac{NzJ}{2}\left[-p^2 + 2p(1-p) - (1-p)^2\right] = -\frac{NzJ}{2}m^2. \tag{17}$$

In thermal equilibrium, the entropy of the system is given by the Shannon entropy $S = -k_B \sum_j p_j \log p_j$, where j runs over all possible configurations of the system. Here, we have N spins that can take two possible values with probabilties p and $1-p$, respectively, so the entropy is given by

$$S = -k_B N \left[p \log p + (1-p) \log(1-p) \right]. \tag{18}$$

Consequently, the free energy can be expressed in terms of our variational parameter as

$$F = E - TS = -\frac{NzJ}{2} m^2 + \frac{N k_B T}{2} \left[(1+m) \log(1+m) + (1-m) \log(1-m) - 2 \log 2 \right]. \tag{19}$$

Minimizing with respect to m leads to

$$\frac{\partial F}{\partial m} = -NzJm + \frac{N k_B T}{2} \log \frac{1+m}{1-m} = 0. \tag{20}$$

The resulting transcendental equation may be written as

$$m = \frac{\exp(2\beta zJm) - 1}{\exp(2\beta zJm) + 1}. \tag{21}$$

Since $\tanh x = (e^{2x} - 1)/(e^{2x} + 1)$, we finally obtain

$$m = \tanh \beta zJm, \tag{22}$$

which is exactly the same as the equation of state (6) obtained in the mean-field approximation.

[1] N. Metropolis, A. W. Rosenbluth, M. N. Rosenbluth, A. H. Teller, and E. Teller, J. Chem. Phys. **21**, 1087 (1953).

[2] F. Schwabl, *Statistical Mechanics* (Springer, Berlin, 2006).