Unit 4-3: The Mean-Field Approximation for the Ising Model

We now discuss the solution of the Ising model within the *mean-field* approximation. This is also sometimes known as the *Curie-Weiss molecular field* approximation.

The Hamiltonian is,

$$\mathcal{H} = -J\sum_{\langle ij\rangle} s_i s_j - h\sum_i s_i = -\sum_i s_i \left[h + \frac{J}{2}{\sum_j}' s_j\right] \tag{4.3.1}$$

where the sum on j in the right most term is over only the z nearest neighbors of i. The coupling in the right most term is $J/2$ since when we sum this way we are summing over all nearest neighbor pairs $\langle ij\rangle$ twice.

Consider spin s_i. The interaction of s_i with its neighbors s_j, and with the applied magnetic field h, looks just like the interaction with an applied field $\tilde{h}_i = h + \frac{J}{2}\sum_j' s_j$. This $\tilde{h}_i$ fluctuates as the spins s_j fluctuate in thermal equilibrium.

In the mean-field approximation, we replace this fluctuating $\tilde{h}_i$ by its thermal average, hence the name *mean-field*. Since the Hamiltonian has translational invariance, the average of each spin is the same, $\langle s_j\rangle = m = \frac{1}{N}\sum_i \langle s_i\rangle$. We therefore have,

$$h_{MF} \equiv \langle \tilde{h}_i\rangle = h + \frac{J}{2}{\sum_j}'\langle s_j\rangle = h + \frac{J}{2}zm \qquad \text{where } z \text{ is the coordination number} \tag{4.3.2}$$

Note, h_{MF} is the same for all spins.

With this approximation, the Hamiltonian for the N-spin system decouples into the sum of N single-spin Hamiltonians,

$$\mathcal{H}_{MF}[\{s_i\}] = -\sum_i s_i\, h_{MF} = \sum_i \mathcal{H}^{(1)}_{MF}[s_i], \qquad \text{with} \quad \mathcal{H}^{(1)}_{MF} = -s_i\, h_{MF} \tag{4.3.3}$$

To complete the solution, within the mean-field approximation, we need to compute the average spin $m = \langle s_i\rangle$ using $\mathcal{H}_{MF}$, and then self-consistently solve for m from the resulting equation.

Since the N-spin mean-field Hamiltonian is a sum of N single-spin Hamiltonians, the Boltzmann exponential factors into a product of single-spin terms, and so the probability to have any given spin configuration factors into independent probabilities for each s_i. We can therefore write for the probability that s_i has a particular value,

$$\mathcal{P}(s) = \frac{\mathrm{e}^{-\beta\mathcal{H}^{(1)}_{MF}[s]}}{\sum\limits_{s=\pm 1}\mathrm{e}^{-\beta\mathcal{H}^{(1)}_{MF}[s]}} \tag{4.3.4}$$

and so

$$m = \langle s\rangle = \sum_{s=\pm 1} P(s)s = P(1)(1) + P(-1)(-1) = \frac{\mathrm{e}^{\beta h_{MF}} - \mathrm{e}^{-\beta h_{MF}}}{\mathrm{e}^{\beta h_{MF}} + \mathrm{e}^{-\beta h_{MF}}} = \tanh\left[\beta h_{MF}\right] \tag{4.3.5}$$

$$\boxed{m = \tanh\left[\beta\left(\frac{zJm}{2} + h\right)\right]} \tag{4.3.6}$$

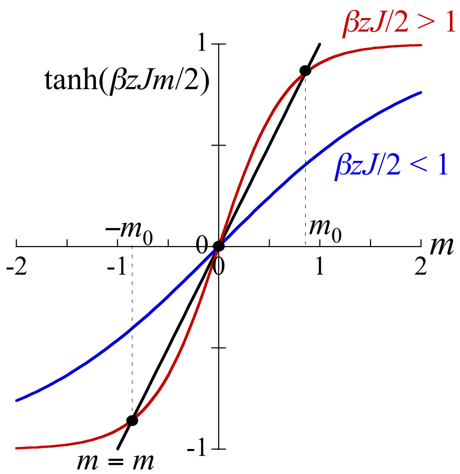
We now need to solve the above equation to determine $m(T,h)$ in the mean-field approximation. Note, from Eq. (4.3.6) we see that the mean-field solution must obey $m(T,h) = -m(T,-h)$, as expected from symmetry.

Zero Magnetic Field, $h = 0$

First we will consider the case where the external magnetic field $h = 0$. Eq. (4.3.6) then becomes,

$$m = \tanh\left[\frac{\beta z J m}{2}\right] \tag{4.3.7}$$

Once can solve this equation graphically, as shown below, by plotting on the same graph the functions $f_1(m) = m$ and $f_2(m) = \tanh(\beta z J m/2)$. The intersections of these two curves locate the desired solutions for m.



For large $x \to \pm\infty$, $\tanh x \to \pm 1$.

For small x we can expand $\tanh x = x - \frac{1}{3}x^3 + O(x^5)$.

The slope of $\tanh(\beta z J m/2)$ at $m = 0$ is therefore $\beta z J/2$.

Therefore, when $\beta z J/2 < 1$, the slope of $f_2(m) = \tanh(\beta z J m/2)$ at $m = 0$ is smaller than the slope of $f_1(m) = m$, and the two curves will intersect only at $m = 0$. The only solution to the mean-field equation (4.3.7) is thus $m = 0$, and one is in the paramagnetic phase.

However, when $\beta z J/2 > 1$, the slope of $f_2(m) = \tanh(\beta z J m/2)$ at $m = 0$ is greater than the slope of $f_1(m) = m$. And since $f_2(m)$ must bend over to saturate at ± 1 as $|m|$ increases, while $f_1(m)$ increases without bound, the two curves must intersect not just at $m = 0$, but also at two new solutions $\pm m_0$. We will soon show that the solution $m = 0$ is unstable, while the solutions at $m = \pm m_0$ are stable. We are thus in the ferromagnetic phase with a net magnetization $\pm m_0$.

The transition between the low temperature ferromagnetic phase, where $m = \pm m_0$, and the high temperature paramagnetic phase, where $m = 0$, takes place when,

$$\boxed{\beta_c z J/2 = 1 \qquad \Rightarrow \qquad k_B T_c = z J/2} \tag{4.3.8}$$

T_c is the critical temperature of the Ising ferromagnetic phase transition.

Free Energy Densities

We now wish to show that, for $T < T_c$, the mean-field solution at $m = 0$ is unstable, while the solutions at $m = \pm m_0$ give the stable equilibrium states. To see this we return to Eq. (4.3.6),

$$m = \tanh\left(\frac{\beta z J m}{2} + \beta h\right) \tag{4.3.9}$$

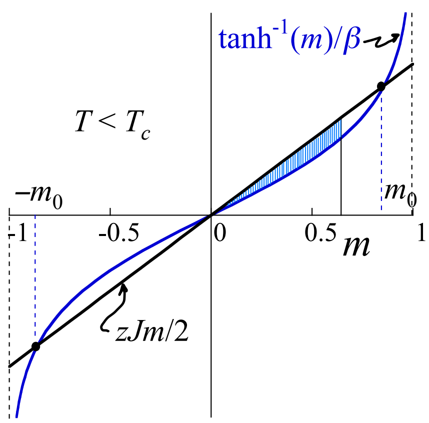
we can invert this to solve for h in terms of m,

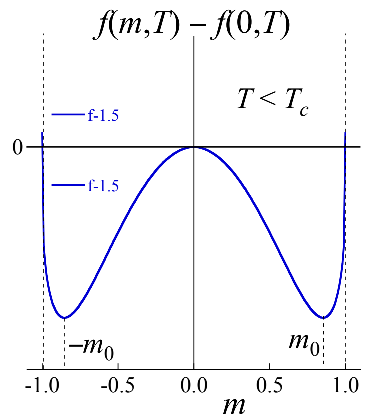
$$h = \frac{1}{\beta}\tanh^{-1}(m) - \frac{zJm}{2} \tag{4.3.10}$$

We can now use the result that h is the conjugate variable to m to integrate and get the Helmholtz free energy density,

$$\left(\frac{\partial f}{\partial m}\right)_T = h \quad \Rightarrow \quad f(m,T) = \int_0^m dm'\, h(m',T) + f(0,T) = \int_0^m dm' \left[\frac{1}{\beta}\tanh^{-1}(m) - \frac{zJm}{2}\right] + f(0,T) \tag{4.3.11}$$

For $T < T_c$, we can represent this integral graphically as shown in the sketch below on the left.





The integral that gives $f(m,T)$ is the area under the curve $\frac{1}{\beta}\tanh^{-1}(m)$ minus the area under the curve $zJm/2$. For $m > 0$, since $\frac{1}{\beta}\tanh^{-1}(m)$ lies below $zJm/2$, this is just the *negative* of the shaded area in the sketch. As m increases, this shaded area increases and so $f(m,T)$ decreases, until we reach $m = m_0$. At $m = m_0$ the curves cross, and so as m increases above m_0 we now start to *subtract* the area between the two curves; thus the signed area between the two curves now decreases, and so $f(m,T)$ increases. Thus $m = m_0$ gives a minimum of $f(m,T)$ at fixed $T < T_c$.

We plot the resulting Helmholtz free energy density $f(m,T) - f(0,T)$ in the sketch above on the right, for both positive and negative m. We see that the values $m = \pm m_0$ give the two minima of the Helmholtz free energy density, and so give the stable equilibrium states. The mean-field solution at $m = 0$ is a local maximum, and so represents an unstable state.

We can see this more formally as follows. Since the above calculation refers to the case where $h = 0$ is fixed, we really should be considering the Gibbs free energy density $g(h,T)$, obtained as the Legendre transform of $f(m,T)$. Using our alternative definition of the Legendre transformation in terms of taking the extremal value, the Gibbs free energy density is given by,

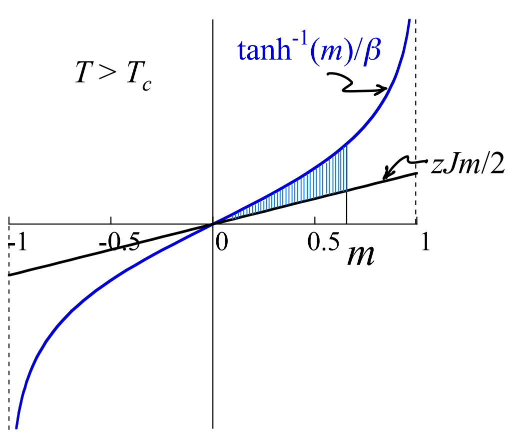
$$g(h,T) = \min_m \left[f(m,T) - mh\right] \tag{4.3.12}$$

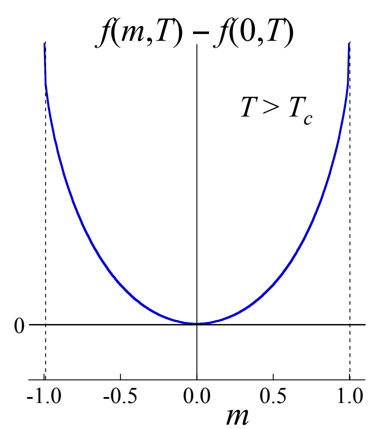
For the case we are interested in above, $h = 0$, and so,

$$g(h=0,T) = \min_m \left[f(m,T)\right] \tag{4.3.13}$$

The minimizing values are just $m = \pm m_0$, and so these are the equilibrium values of the magnetization when $h = 0$.

We can now do the exact same calculation when $T > T_c$. Now the situation looks like in the sketches below.





Again the integral that gives $f(m,T)$ is the area under the curve $\frac{1}{\beta}\tanh^{-1}(m)$ minus the area under the curve $zJm/2$. But when $T > T_c$, and $m > 0$, $\frac{1}{\beta}\tanh^{-1}(m)$ lies above $zJm/2$, and so this integral is just the shaded area in the sketch above on the left. As m increases, this shaded area continues to increase, and so $f(m,T)$ monotonically increases. The resulting $f(m,T) - f(0,T)$ is shown in the sketch above on the right. We see that there is only a single minima at $m = 0$. Constructing $g(h = 0, T) = \min_m[f(m,T)]$, we see that the equilibrium state has magnetization $m = 0$.

The mean-field solution for the Ising model is therefore as follows: For $T > T_c = zJ/2k_B$, the system is paramagnetic with $m = \langle s_i \rangle = 0$. For $T < T_c$, the system is ferromagnetic with $m = \langle s_i \rangle = \pm m_0(T)$, with $m_0(T)$ determined from the solution to $m_0 = \tanh(zJm_0/2k_BT)$. As $T \to T_c$ from below, $m_0 \to 0$ continuously.