Mean Field Theory Solution of the Ising Model

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Contents

1 Ising model

The (ferromagnetic) Ising model is a simple model of ferromagnetism that provides some insight into how phase transitions and the non-analytic behavior of thermodynamic quantities across phase transitions occur in physics. Consider a lattice containing a spin at each site that can point either up (+1) or down (−1). The (classical) nearest-neighbor Ising Hamiltonian for this system is

$$\boxed{\mathcal{H} = -J\sum_{\langle ij\rangle} s_i s_j - h\sum_{i=1}^{N} s_i}\,, \tag{1}$$

where J is a positive (ferromagnetic) coupling constant, $\langle ij\rangle$ denotes summation over nearest neighbors,[1] s_i (= +1 or −1) is the value of the spin on the ith site, h is an external magnetic field pointing along the z direction,[2] and N is the number of sites on the lattice.

[1] Each pair of sites is only included once in the sum.
[2] $h > 0$ corresponds to the field pointing in the $+z$ direction.

As we will see, in dimensions higher than 1, the Ising model has two distinct phases, namely a *paramagnetic* phase in which its spins are disordered due to thermal fluctuations, and a *ferromagnetic* phase in which its spins start preferentially aligning in one direction. These two phases are separated by a phase transition at some critical temperature $T = T_c$ below which the system becomes ferromagnetic. We can quantitatively distinguish these two phases by defining the *magnetization*[3]

$$\boxed{m \equiv \frac{1}{N} \sum_{i=1}^{N} \langle s_i \rangle}, \tag{2}$$

where

$$\boxed{\langle s_i \rangle = \frac{\mathrm{Tr}(s_i e^{-\beta \mathcal{H}})}{Z}} \tag{3}$$

is the thermal expectation value (or mean value) of s_i, $\beta = 1/(k_{\mathrm{B}}T)$ is the inverse temperature,

$$\boxed{Z = \mathrm{Tr}(e^{-\beta \mathcal{H}})} \tag{4}$$

is the canonical partition function (from which we can extract thermodynamic information about the system), and Tr (trace) denotes a sum over all of the system's possible configurations, which in the case of the Ising model can be written explicitly as

$$\mathrm{Tr} \to \prod_{i=1}^{N} \left(\sum_{s_i = \pm 1} \right) = \sum_{s_1 = \pm 1} \sum_{s_2 = \pm 1} \cdots \sum_{s_N = \pm 1} . \tag{5}$$

The magnetization serves as this system's *order parameter*, meaning we can use it to describe how ordered the system is; for example, in this model, $m = 0$ corresponds to all of the spins being disordered (paramagnetic state) and $m \neq 0$ corresponds to the spins having a preferred direction (ferromagnetic state).

2 Mean field theory solution of the Ising model

The Ising model can only be exactly solved in one and two dimensions, although these solutions are not very simple. It can, however, be approximately solved in any number of dimensions in a relatively simple manner using the mean field theory (MFT) approximation (usually just referred to as mean field theory). This approximation consists of assuming that the system's thermal fluctuations are relatively small and can therefore be neglected to a certain extent. As we will see, from this simple assumption we can then treat a system of interacting particles as a system of non-interacting[4] particles in which each particle only

[3]Some authors define the magnetization without the thermal expectation value, so what we are calling m in these notes, they call $\langle m \rangle$.

[4]That is, not interacting with each other.

interacts with a "mean field" that captures the average behavior of the particles around it. In other words, MFT effectively decouples the Hamiltonian into a simpler Hamiltonian describing a non-interacting system. This makes it a very powerful method that is used often in physics to explore the behavior of complicated many-body systems that cannot be solved exactly.

Remarkably, even though the predictions MFT makes are quantitatively incorrect, it correctly predicts the Ising model's qualitative behavior for two dimensions and higher. This is because fluctuations are more important in lower dimensions, so the MFT approximation is less accurate in lower dimensions.

2.1 Decoupling the Hamiltonian

In order to decouple the Ising Hamiltonian using MFT, we start by writing each spin in the spin interaction terms $s_i s_j$ in the form

$$s_i = \langle s_i \rangle + \delta s_i \,, \tag{6}$$

where

$$\delta s_i \equiv s_i - \langle s_i \rangle \tag{7}$$

denotes fluctuations about the mean value of s_i. The spin interaction terms $s_i s_j$ thus become

$$\begin{aligned} s_i s_j &= (\langle s_i \rangle + \delta s_i)(\langle s_j \rangle + \delta s_j) \\ &= \langle s_i \rangle \langle s_j \rangle + \langle s_j \rangle \delta s_i + \langle s_i \rangle \delta s_j + \delta s_i \delta s_j \,. \end{aligned} \tag{8}$$

We now make the assumption that the fluctuations are very small, so we can ignore the term quadratic in fluctuations:

$$\boxed{\delta s_i \delta s_j = 0} \,. \tag{9}$$

This is the approximation that MFT relies on: *assuming fluctuations are small*. The quantity $s_i s_j$ is then approximately

$$\begin{aligned} s_i s_j &\approx \langle s_i \rangle \langle s_j \rangle + \langle s_j \rangle \delta s_i + \langle s_i \rangle \delta s_j \\ &= \langle s_i \rangle \langle s_j \rangle + \langle s_j \rangle (s_i - \langle s_i \rangle) + \langle s_i \rangle (s_j - \langle s_j \rangle) \\ &= \langle s_j \rangle s_i + \langle s_i \rangle s_j - \langle s_i \rangle \langle s_j \rangle \,. \end{aligned} \tag{10}$$

Since this system is translationally invariant, the expectation value $\langle s_i \rangle$ of any given site i is independent of the site, so we have

$$\langle s_i \rangle = m \,. \tag{11}$$

We can then further simplify $s_i s_j$ to

$$s_i s_j = m(s_i + s_j) - m^2 = m[(s_i + s_j) - m] \tag{12}$$

and approximate the Ising Hamiltonian as

$$\mathcal{H}_{\mathrm{MF}} = -Jm \sum_{\langle ij \rangle} (s_i + s_j - m) - h \sum_{i=1}^{N} s_i \,, \tag{13}$$

where the subscript on the Hamiltonian reminds us that this is only an approximation of the Ising Hamiltonian. Since

$$\sum_{\langle ij \rangle} s_i = \sum_{\langle ij \rangle} s_j \tag{14}$$

due to the symmetry of i and j in the sum over nearest neighbors, we can write

$$\sum_{\langle ij \rangle} (s_i + s_j) = \sum_{\langle ij \rangle} 2 s_i \,, \tag{15}$$

so the Hamiltonian reads

$$\mathcal{H}_{\mathrm{MF}} = -Jm \sum_{\langle ij \rangle} (2 s_i - m) - h \sum_{i=1}^{N} s_i \,. \tag{16}$$

We can write the sum over nearest neighbors as

$$\sum_{\langle ij \rangle} \to \frac{1}{2} \sum_{i=1}^{N} \sum_{j \in \mathrm{nn}(i)} \,, \tag{17}$$

where the factor of 1/2 is to avoid double counting pairs of sites and $\mathrm{nn}(i)$ denotes nearest neighbors of i. Since there is no explicit j dependence inside the summation, this inner sum is simply

$$\sum_{j \in \mathrm{nn}(i)} = q \,, \tag{18}$$

where the coordination number q is equal to the number of neighbors of any given site.[5] We then have

$$\sum_{\langle ij \rangle} \to \frac{q}{2} \sum_{i=1}^{N} , \tag{19}$$

so the Ising Hamiltonian further simplifies to

$$\begin{aligned} \mathcal{H}_{\mathrm{MF}} &= -\frac{qJm}{2} \sum_{i=1}^{N} (2 s_i - m) - h \sum_{i=1}^{N} s_i \\ &= \frac{NqJm^2}{2} - qJm \sum_{i=1}^{N} s_i - h \sum_{i=1}^{N} s_i \\ &= \frac{NqJm^2}{2} - (h + qJm) \sum_{i=1}^{N} s_i \,, \end{aligned} \tag{20}$$

[5]For example, for a 1D lattice, $q = 2$; for a 2D triangular lattice, $q = 3$; for a 2D square lattice, $q = 4$; etc.

or simply

$$\boxed{\mathcal{H}_{\text{MF}} = \frac{NqJm^2}{2} - h_{\text{eff}} \sum_{i=1}^{N} s_i}, \tag{21}$$

where

$$\boxed{h_{\text{eff}} \equiv h + qJm} \tag{22}$$

is the effective magnetic field felt by the spins. We have now effectively decoupled the Hamiltonian into a sum of one-body terms. Again, this conceptually means that particles no longer interact with each other in this approximation, but rather interact only with an effective magnetic field h_{eff} that is comprised of the external field h and the mean field qJm induced by neighboring particles.

2.2 Self-consistency equation

Let's calculate the partition function using the mean field Ising Hamiltonian:

$$\begin{aligned} Z_{\text{MF}} &= \text{Tr}(e^{-\beta\mathcal{H}_{\text{MF}}}) \\ &= \prod_{i=1}^{N} \left(\sum_{s_i=\pm 1} \right) e^{-\beta\mathcal{H}_{\text{MF}}} \\ &= \prod_{i=1}^{N} \left(\sum_{s_i=\pm 1} \right) e^{-\beta NqJm^2/2} e^{\beta h_{\text{eff}} \sum_{j=1}^{N} s_j} \\ &= e^{-\beta NqJm^2/2} \prod_{i=1}^{N} \left(\sum_{s_i=\pm 1} e^{\beta h_{\text{eff}} s_i} \right) \\ &= e^{-\beta NqJm^2/2} \prod_{i=1}^{N} \underbrace{(e^{\beta h_{\text{eff}}} + e^{-\beta h_{\text{eff}}})}_{=2\cosh(\beta h_{\text{eff}})} \\ &= e^{-\beta NqJm^2/2} [2\cosh(\beta h_{\text{eff}})]^N , \end{aligned} \tag{23}$$

so we find

$$\boxed{Z_{\text{MF}} = e^{-\beta NqJm^2/2} [2\cosh(\beta h_{\text{eff}})]^N}. \tag{24}$$

Now, recall from Eq. 2 that the magnetization is given by

$$m \equiv \frac{1}{N} \sum_{i=1}^{N} \langle s_i \rangle \ .$$

Using Eq. 3, we can rewrite this as

$$\begin{aligned}
m &= \frac{1}{N}\sum_{i=1}^{N}\frac{\mathrm{Tr}(s_i e^{-\beta\mathcal{H}_{\mathrm{MF}}})}{Z_{\mathrm{MF}}} \\
&= \frac{1}{N}\frac{1}{Z_{\mathrm{MF}}}\sum_{i=1}^{N} s_i e^{-\beta\mathcal{H}_{\mathrm{MF}}} \\
&= \frac{1}{N\beta}\frac{1}{Z_{\mathrm{MF}}}\frac{\partial Z_{\mathrm{MF}}}{\partial h_{\mathrm{eff}}} \\
&= \frac{1}{N\beta}\frac{\partial(\ln Z_{\mathrm{MF}})}{\partial h_{\mathrm{eff}}}\,, \qquad (25)
\end{aligned}$$

where on the third line we have used the fact that

$$\begin{aligned}
\frac{\partial Z_{\mathrm{MF}}}{\partial h_{\mathrm{eff}}} &= \frac{\partial}{\partial h_{\mathrm{eff}}}\,\mathrm{Tr}(e^{-\beta\mathcal{H}_{\mathrm{MF}}}) \\
&= \mathrm{Tr}\left(\frac{\partial}{\partial h_{\mathrm{eff}}} e^{-\beta\mathcal{H}_{\mathrm{MF}}}\right) \\
&= -\beta\,\mathrm{Tr}\left(\frac{\partial\mathcal{H}_{\mathrm{MF}}}{\partial h_{\mathrm{eff}}} e^{-\beta\mathcal{H}_{\mathrm{MF}}}\right) \\
&= -\beta\,\mathrm{Tr}\left[\left(-\sum_{i=1}^{N} s_i\right) e^{-\beta\mathcal{H}_{\mathrm{MF}}}\right] \\
&= \beta\,\mathrm{Tr}\left[\sum_{i=1}^{N} s_i e^{-\beta\mathcal{H}_{\mathrm{MF}}}\right]\,. \qquad (26)
\end{aligned}$$

Now, from Eq. 24 we can calculate $\ln Z_{\mathrm{MF}}$:

$$\ln Z_{\mathrm{MF}} = -\frac{\beta NqJm^2}{2} + N\ln 2 + N\ln[\cosh(\beta h_{\mathrm{eff}})]\,, \qquad (27)$$

so

$$\frac{\partial(\ln Z_{\mathrm{MF}})}{\partial h_{\mathrm{eff}}} = N\beta\tanh(\beta h_{\mathrm{eff}})\,. \qquad (28)$$

Inserting this back into Eq. 25 gives

$$m = \tanh(\beta h_{\mathrm{eff}})\,. \qquad (29)$$

Inserting the definition of h_{eff} (Eq. 22) back into this equation gives us the *self-consistency equation*

$$\boxed{m = \tanh[\beta(h + qJm)]}\,. \qquad (30)$$

This is a transcendental equation, so we cannot solve for m analytically. However, we can solve for m graphically by plotting m and $\tanh[\beta(h+qJm)]$ (for fixed values of β, h, q, and J).

Let's consider the special case of $h = 0$. In Figure 1 we plot m and $\tanh(\beta qJm)$ on the same plot for various values of βqJ. We can graphically see that the solutions are qualitatively different when $\beta qJ \leq 1$ and $\beta qJ > 1$.[6] These two cases can be understood as follows:

- $\beta qJ \leq 1$ (i.e., $k_\mathrm{B}T \geq qJ$): There is only one solution: $m = 0$. This corresponds to the system being in a *paramagnetic* state.
- $\beta qJ > 1$ (i.e., $k_\mathrm{B}T < qJ$): There are three solutions: $m = 0$ and $m = \pm m_0$, where $m_0 \leq 1$. The $m = \pm m_0$ solutions correspond to the system being in a *ferromagnetic* state (the system is magnetized). As we will discuss later, the $m = 0$ solution turns out to be unstable, so we physically only observe either $m = m_0$ or $m = -m_0$ at these temperatures.

The *critical temperature* T_c below which the system becomes spontaneously magnetized without any external magnetic fields is therefore given by

$$\boxed{k_\mathrm{B}T_c = qJ}\,. \tag{31}$$

It should be noted that for the 1D case, MFT thus predicts a magnetic phase transition at $k_\mathrm{B}T_c = 2J$; however, solving this system exactly we find that there is in fact no phase transition in 1D. Thermal fluctuations turn out to be strong enough to destroy the system's magnetic ordering in 1D, so MFT provides a qualitatively incorrect result in this specific case.

As mentioned earlier, MFT is more accurate in higher dimensions. For example, for the 2D square lattice, MFT predicts $k_\mathrm{B}T_c = 4J$, whereas solving the system exactly we find that $k_\mathrm{B}T_c = 2J/\ln(1+\sqrt{2}) \approx 2.27J$. Also note that since MFT assumes fluctuations are small, it generally overestimates the system's tendency to order and thus overestimates the value of T_c.

2.3 Critical behavior at zero field

In this section we discuss the behavior of the system near the critical temperature T_c. In order to more easily look at the behavior for $T \to T_c$, let's define the reduced temperature t

[6] We can also reach this conclusion a bit more rigorously by noting that there are three solutions when

$$\left[\frac{d}{dm}\tanh(\beta qJm)\right]\Bigg|_{m=0} > 1\,,$$

and one solution otherwise. Evaluating the derivative gives

$$\left[\frac{d}{dm}\tanh(\beta qJm)\right]\Bigg|_{m=0} = \left[\beta qJ\frac{1}{\cosh^2(\beta qJm)}\right]\Bigg|_{m=0} = \beta qJ\,,$$

so we find that we have three solutions solution when $\beta qJ > 1$, and one solution otherwise.

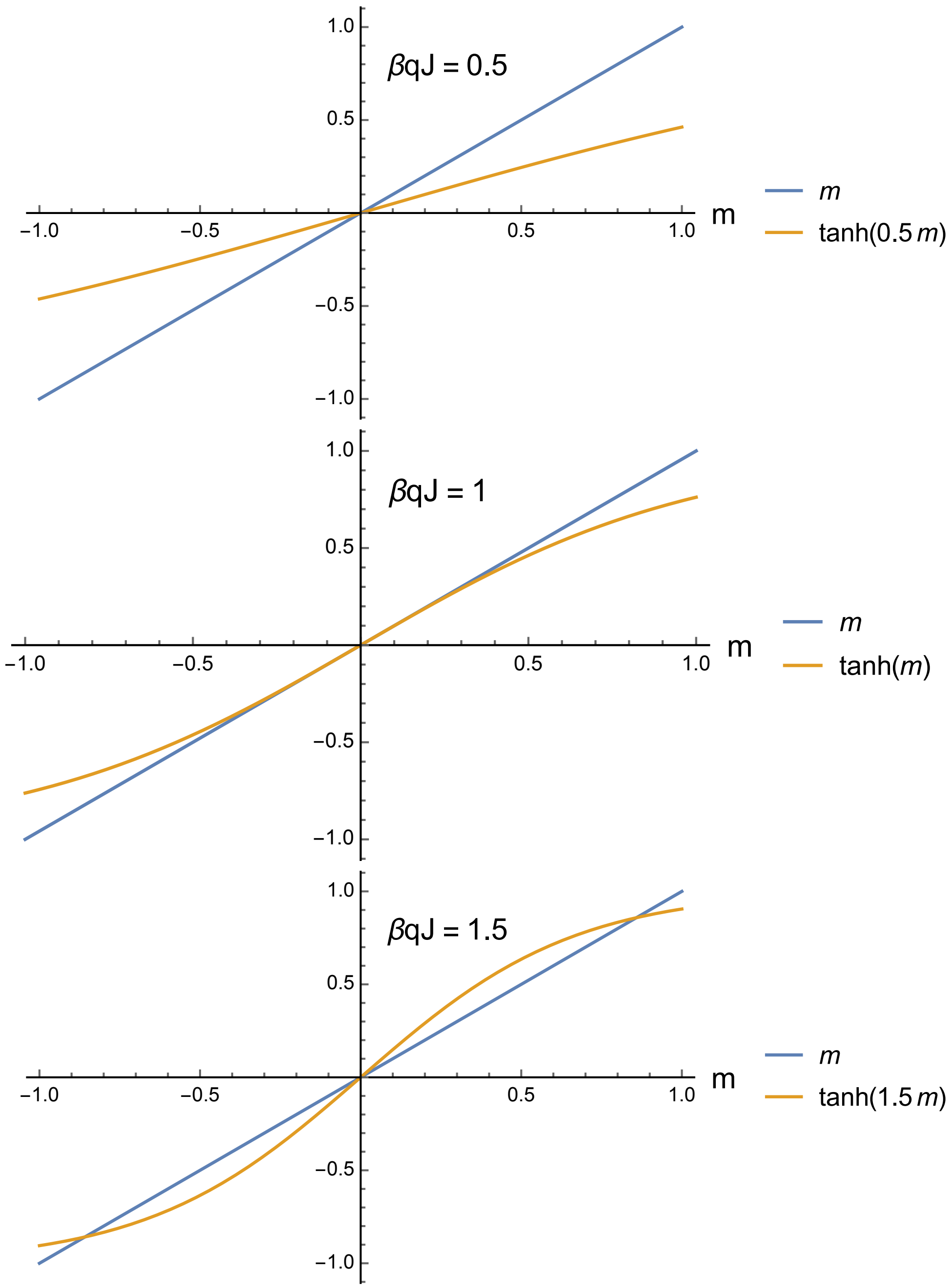

Figure 1: Solving the self-consistent equation graphically for $h = 0$ and various values of βqJ. The top plot is at $T > T_c$, the middle plot is at $T = T_c$, and the bottom plot is at $T < T_c$.

by

$$t \equiv \frac{T - T_c}{T_c} \,. \tag{32}$$

We can then look at the critical behavior by expanding around small t.

2.3.1 Magnetization

We already know that when there is no external magnetic field, we have $m = 0$ when $T \geq T_c$. Let's explore further what happens in the critical regime just below T_c (i.e., $T \to T_c^-$) at zero field ($h = 0$). Using the expansion

$$\tanh(x) = x - \frac{x^3}{3} + \mathcal{O}(x^5) \tag{33}$$

around $x = 0$, we can rewrite the self-consistency equation (Eq. 30) for $h = 0$ around $m = 0$ (near T_c) as

$$\begin{aligned} m &= \beta q J m - \frac{1}{3}(\beta q J m)^3 \\ &= \left(\frac{T_c}{T}\right) m - \frac{1}{3}\left(\frac{T_c}{T}\right)^3 m^3 \,, \qquad T \to T_c^- \,, \end{aligned} \tag{34}$$

or moving everything to the same side,

$$m\left[\left(\frac{T_c}{T} - 1\right) - \frac{1}{3}\left(\frac{T_c}{T}\right)^3 m^2\right] = 0 \,, \qquad T \to T_c^- \,. \tag{35}$$

This gives the solutions $m = 0$ and

$$m = \pm\sqrt{3\left(\frac{T}{T_c}\right)^2\left(\frac{T_c - T}{T_c}\right)} \,, \qquad T \to T_c^- \,. \tag{36}$$

Note that this expression is only sensible for $T \leq T_c$, otherwise m would be imaginary (which is unphysical). However, we have to keep in mind that this expression only applies whenever m is very close to 0, meaning that we are looking only at the region below T_c but very close to T_c. In terms of the reduced temperature t, Eq. 36 reads

$$m = \pm\sqrt{-3(1+t)^2 t} \,, \qquad T \to T_c^- \,. \tag{37}$$

Using the binomial approximation

$$(1 + x)^\alpha \approx 1 + \alpha x \,, \qquad |x| \ll 1 \,, \tag{38}$$

we can simplify this for $t \to 0^-$ (i.e., $T \to T_c^-$) as

$$m \approx \pm\sqrt{-3(1+2t)t} \approx \pm\sqrt{-3t} \,, \qquad T \to T_c^- \,. \tag{39}$$

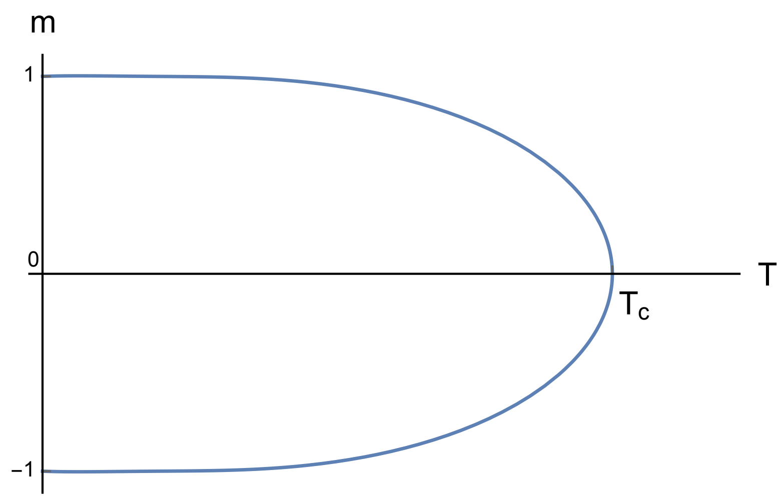

Figure 2: Behavior of the magnetization $m(T,0)$ obtained by solving the Ising model using MFT.

We have thus found that at zero field, the magnetization $m(T,h)$ behaves as

$$\boxed{m(T,0) = \begin{cases} \pm(3|t|)^{1/2}\,, & T \to T_c^- \\ 0\,, & T \to T_c^+ \end{cases}}\,. \tag{40}$$

In the zero-temperature limit ($T \to 0\,,\ \beta \to \infty$), the self-consistency equation gives $m_0 = 1$, so

$$\boxed{m(0,0) = \pm 1}\,. \tag{41}$$

We can use all of this information to sketch the magnetization as a function of temperature in Figure 2. The physical interpretation of this is that above T_c, thermal fluctuations are strong enough to prevent the system from becoming magnetized; this is the paramagnetic phase. However, at T_c a phase transition occurs and the system becomes spontaneously magnetized as you decrease the temperature past T_c; this is the ferromagnetic phase. Even though this behavior is quantitatively wrong (and notably qualitatively wrong in 1D!), it is nevertheless qualitatively correct in 2D and higher dimensions, which is quite remarkable.

2.3.2 Susceptibility

The isothermal (magnetic) susceptibility χ_T is given by

$$\chi_T(T,h) \equiv \left(\frac{\partial m}{\partial h}\right)_T\,. \tag{42}$$

Taking the derivative of both sides of the self-consistency equation (Eq. 30) with respect to h while keeping T constant gives

$$\chi_T = \frac{1}{\cosh^2[\beta(h+qJm)]}\beta(1+qJ\chi_T)\,. \tag{43}$$

Solving for χ_T, we find

$$\chi_T(T,h) = \frac{\beta}{\cosh^2[\beta(h+qJm)] - \beta qJ}\,. \tag{44}$$

Let's now look at the behavior of the at zero field ($h=0$):

$$\chi_T(T,0) = \frac{\beta}{\cosh^2(\beta qJm) - \beta qJ}\,. \tag{45}$$

For $T \to T_c^+$, we have $m=0$, so

$$\chi_T(T,0) = \frac{\beta}{1-\beta qJ} = \frac{1}{k_\mathrm{B}(T-T_c)} = \frac{1}{k_\mathrm{B}T_c}\frac{1}{|t|}\,, \qquad T \to T_c^+\,. \tag{46}$$

For $T \le T_c$ but very close to T_c, we have $m = \pm(3|t|)^{1/2}$ (as found in the previous section), which is very small. We can thus use the expansion

$$\cosh(x) = 1 + \frac{x^2}{2} + \mathcal{O}(x^4) \tag{47}$$

around $x=0$ to write

$$\begin{aligned}\chi_T(T,0) &= \frac{\beta}{[1+\frac{1}{2}(\beta qJ(3|t|)^{1/2})^2]^2 - \beta qJ} \\ &\approx \frac{\beta}{1+3(\beta qJ)^2|t| - \beta qJ} \\ &\approx \frac{1}{2}\frac{1}{k_\mathrm{B}T_c}\frac{1}{|t|}\,, \qquad T \to T_c^-\,.\end{aligned} \tag{48}$$

We have thus found that at zero field, the isothermal susceptibility goes as

$$\boxed{\chi_T(T,0) = \begin{cases} A|t|^{-1}\,, & T \to T_c^- \\ 2A|t|^{-1}\,, & T \to T_c^+ \end{cases}\,, \quad \text{where} \quad A = \frac{1}{2}\frac{1}{k_\mathrm{B}T_c}}\,, \tag{49}$$

and diverges at $T = T_c$. We can use this information to sketch the susceptibility as a function of temperature near T_c in Figure 3.

2.4 Free energy

We can also gain some useful insight into the physics of this system by looking at its (Helmholtz) free energy

$$F \equiv U - TS = -k_\mathrm{B}T\ln Z\,, \tag{50}$$

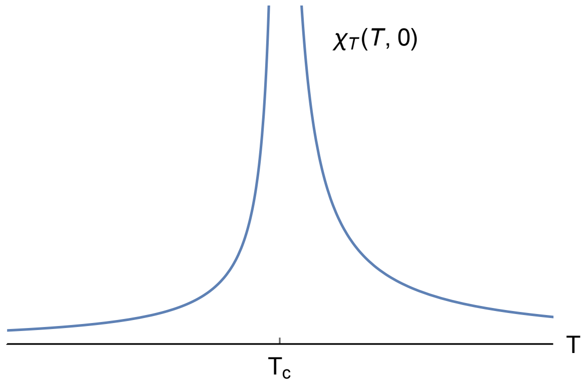

Figure 3: Behavior of the isothermal susceptibility $\chi_T(T,0)$ near T_c obtained by solving the Ising model using MFT.

where S is the system's entropy. Understanding the behavior of the system's free energy is helpful because the equilibrium state of a system at constant temperature and volume minimizes its free energy. Specifically, we are going to be looking at how the system's free energy depends on its magnetization. At zero field, the free energy of this system is

$$\begin{aligned} F_{\mathrm{MF}}|_{h=0} &= -k_{\mathrm{B}}T \ln Z_{\mathrm{MF}} \\ &= \frac{NqJm^2}{2} - Nk_{\mathrm{B}}T\ln 2 - Nk_{\mathrm{B}}T\ln[\cosh(\beta h_{\mathrm{eff}})] \\ &= \frac{NqJm^2}{2} - Nk_{\mathrm{B}}T\ln 2 - Nk_{\mathrm{B}}T\left[\frac{(\beta h_{\mathrm{eff}})^2}{2} - \frac{(\beta h_{\mathrm{eff}})^4}{12} + \mathcal{O}\big((\beta h_{\mathrm{eff}})^6\big)\right] \\ &\approx \frac{NqJm^2}{2} - Nk_{\mathrm{B}}T\ln 2 - Nk_{\mathrm{B}}T\left[\frac{\beta^2(qJm)^2}{2} - \frac{\beta^4(qJm)^4}{12}\right] \\ &= \frac{NqJm^2}{2} - Nk_{\mathrm{B}}T\ln 2 - \frac{N(qJm)^2}{2k_{\mathrm{B}}T} + \frac{N(qJm)^4}{12(k_{\mathrm{B}}T)^3} \\ &= -Nk_{\mathrm{B}}T\ln 2 + \frac{Nk_{\mathrm{B}}T_c}{2T}(T-T_c)\,m^2 + \frac{Nk_{\mathrm{B}}T_c^4}{12T^3}m^4\,, \end{aligned} \tag{51}$$

which, as a function of m, is the form

$$F_{\mathrm{MF}}(m)|_{h=0} = F_0 + a(T-T_c)m^2 + bm^4 \tag{52}$$

up to order m^4. Adding an external magnetic field adds a term linear in h and m:[7]

$$\boxed{F_{\mathrm{MF}}(m) = F_0 - hm + a(T-T_c)m^2 + bm^4}\,. \tag{53}$$

Note that the term constant in m is not relevant to the system's equilibrium state, since it is just an overall energy shift that does not affect the free energy's minima with respect to m. In Figures 4 and 5 we will therefore therefore implicitly ignore the F_0 term.

[7] As well as some higher-order terms that we are going to ignore.

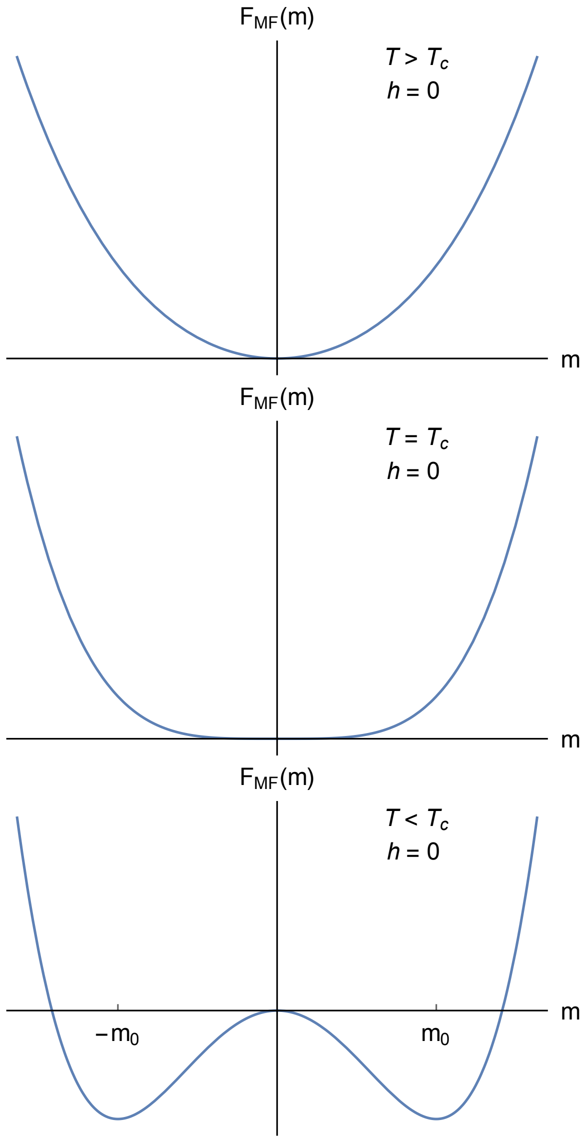

Figure 4: Mean field solution of the free energy as a function of magnetization at zero field at various temperatures. As we cool the system below T_c, the free energy changes smoothly to a "Mexican hat" shape, thereby making the $m = 0$ solution unstable and two new stable solutions at $m = \pm m_0$ appear.

Plots of the free energy at zero field are shown in Figure 4. We can see that as we cool the system below T_c, the $m = 0$ solution becomes metastable and any small perturbation causes the system to spontaneously "roll down" either to $m = m_0$ or $m = -m_0$. When we apply a weak external magnetic field below T_c, the solution magnetized in the direction of the field becomes more energetically favorable and more stable (see Figure 5). If the field is strong enough, the solution magnetized in the direction of the field becomes the only solution.

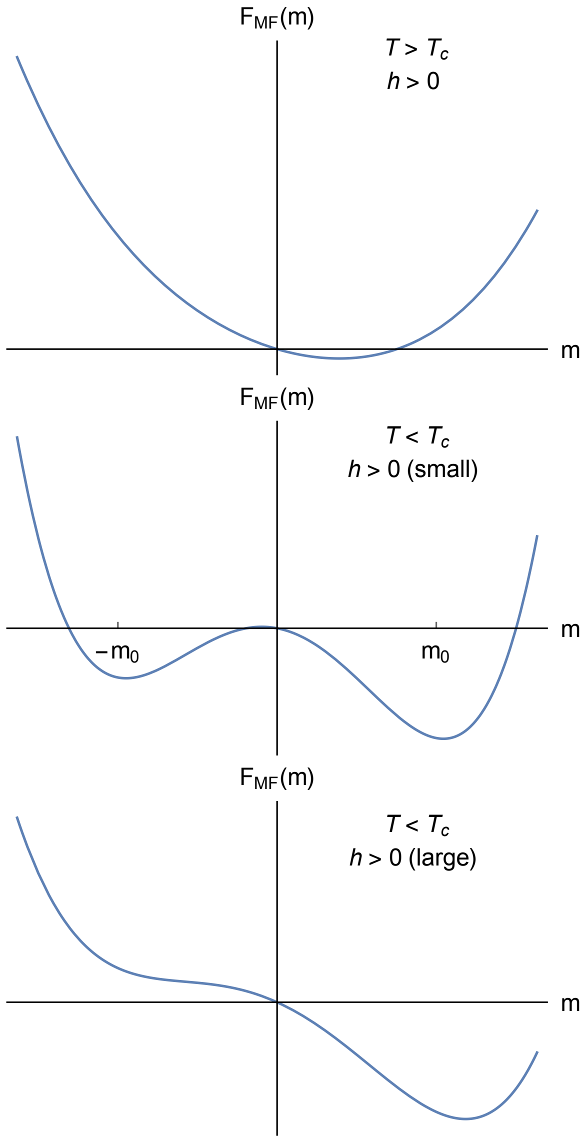

Figure 5: Mean field solution of the free energy as a function of magnetization above and below T_c with an external magnetic field h in the $+z$ direction. Above T_c, the system "rolls" down into a state with positive magnetization, which is what we would expect. Below T_c, the solution $m = m_0$ is now more stable than the $m = -m_0$ solution. For large enough h, $m = -m_0$ stops being a solution and $m = m_0$ becomes the only solution.

3 Mean field theory solution of the Ising model with single-ion anisotropy

Suppose we add a single-ion anisotropy term to the Ising model, so our Hamiltonian is now

$$\mathcal{H} = -J \sum_{\langle ij \rangle} s_i s_j - D \sum_{i=1}^{N} (s_i)^2 - h \sum_{i=1}^{N} s_i \,, \tag{54}$$

where $J > 0$ is a ferromagnetic coupling constant and D is the single-ion anisotropy constant that favors easy-axis magnetization for $D > 0$ and easy-plane magnetization for $D < 0$.

3.1 Decoupling the Hamiltonian

For the interaction term, we will write $s_i s_j$ in the form

$$s_i = \langle s_i \rangle + \delta s_i \,, \tag{55}$$

where

$$\delta s_i \equiv s_i - \langle s_i \rangle \tag{56}$$

denotes fluctuations about the mean value of s_i. The spin interaction terms $s_i s_j$ thus become

$$\begin{aligned} s_i s_j &= (\langle s_i \rangle + \delta s_i)(\langle s_j \rangle + \delta s_j) \\ &= \langle s_i \rangle \langle s_j \rangle + \langle s_j \rangle \delta s_i + \langle s_i \rangle \delta s_j + \delta s_i \delta s_j \,. \end{aligned} \tag{57}$$

We now make the assumption that the fluctuations are very small, so we can ignore the term quadratic in fluctuations:

$$\delta s_i \delta s_j = 0 \,. \tag{58}$$

The quantity $s_i s_j$ is then approximately

$$\begin{aligned} s_i s_j &\approx \langle s_i \rangle \langle s_j \rangle + \langle s_j \rangle \delta s_i + \langle s_i \rangle \delta s_j \\ &= \langle s_i \rangle \langle s_j \rangle + \langle s_j \rangle (s_i - \langle s_i \rangle) + \langle s_i \rangle (s_j - \langle s_j \rangle) \\ &= \langle s_j \rangle s_i + \langle s_i \rangle s_j - \langle s_i \rangle \langle s_j \rangle \,. \end{aligned} \tag{59}$$

Since this system is translationally invariant, the expectation value $\langle s_i \rangle$ of any given site i is independent of the site, so we have

$$\langle s_i \rangle = m \,. \tag{60}$$

We can then further simplify $s_i s_j$ to

$$s_i s_j = m(s_i + s_j) - m^2 = m[(s_i + s_j) - m] \,. \tag{61}$$

Similarly, for the single-ion anisotropy term, we will write $(s_i)^2$ as

$$(s_i)^2 = 2ms_i - m^2 = m(2s_i - m)\,. \tag{62}$$

The mean field Hamiltonian is then

$$\begin{aligned}
\mathcal{H}_{\mathrm{MF}} &= -Jm\sum_{\langle ij\rangle}(s_i + s_j - m) - Dm\sum_{i=1}^{N}(2s_i - m) - h\sum_{i=1}^{N} s_i \\
&= -Jm\sum_{\langle ij\rangle}(2s_i - m) - Dm\sum_{i=1}^{N}(2s_i - m) - h\sum_{i=1}^{N} s_i \\
&= -\frac{qJm}{2}\sum_{i=1}^{N}(2s_i - m) - Dm\sum_{i=1}^{N}(2s_i - m) - h\sum_{i=1}^{N} s_i \\
&= \left(\frac{qJ}{2} + D\right) Nm^2 - [h + (qJ + 2D)m]\sum_{i=1}^{N} s_i\,,
\end{aligned}$$

where q is the coordination number. We thus find

$$\mathcal{H}_{\mathrm{MF}} = \left(\frac{qJ}{2} + D\right) Nm^2 - h_{\mathrm{eff}}\sum_{i=1}^{N} s_i\,, \tag{63}$$

where

$$h_{\mathrm{eff}} \equiv h + (qJ + 2D)m \tag{64}$$

is the effective magnetic field felt by the spins.

3.2 Self-consistency equation

Let's calculate the partition function using the mean field Hamiltonian:

$$\begin{aligned}
Z_{\mathrm{MF}} &= \mathrm{Tr}(e^{-\beta\mathcal{H}_{\mathrm{MF}}}) \\
&= \prod_{i=1}^{N}\left(\sum_{s_i=\pm1}\right) e^{-\beta\mathcal{H}_{\mathrm{MF}}} \\
&= \prod_{i=1}^{N}\left(\sum_{s_i=\pm1}\right) e^{-\beta(\frac{qJ}{2}+D)Nm^2} e^{\beta h_{\mathrm{eff}}\sum_{j=1}^{N} s_j} \\
&= e^{-\beta(\frac{qJ}{2}+D)Nm^2}\prod_{i=1}^{N}\left(\sum_{s_i=\pm1} e^{\beta h_{\mathrm{eff}} s_i}\right) \\
&= e^{-\beta(\frac{qJ}{2}+D)Nm^2}\prod_{i=1}^{N}\underbrace{(e^{\beta h_{\mathrm{eff}}} + e^{-\beta h_{\mathrm{eff}}})}_{=2\cosh(\beta h_{\mathrm{eff}})} \\
&= e^{-\beta(\frac{qJ}{2}+D)Nm^2}[2\cosh(\beta h_{\mathrm{eff}})]^N\,,
\end{aligned} \tag{65}$$

so we find

$$\boxed{Z_{\rm MF} = e^{-\beta(\frac{qJ}{2}+D)Nm^2}[2\cosh(\beta h_{\rm eff})]^N}\,. \tag{66}$$

Now, recall from Eq. 2 that the magnetization is given by

$$m \equiv \frac{1}{N}\sum_{i=1}^{N} \langle s_i \rangle \ .$$

Using Eq. 3, we can rewrite this as

$$\begin{aligned} m &= \frac{1}{N}\sum_{i=1}^{N} \frac{\mathrm{Tr}(s_i e^{-\beta\mathcal{H}_{\rm MF}})}{Z_{\rm MF}} \\ &= \frac{1}{N}\frac{1}{Z_{\rm MF}}\sum_{i=1}^{N} s_i e^{-\beta\mathcal{H}_{\rm MF}} \\ &= \frac{1}{N\beta}\frac{1}{Z_{\rm MF}}\frac{\partial Z_{\rm MF}}{\partial h_{\rm eff}} \\ &= \frac{1}{N\beta}\frac{\partial(\ln Z_{\rm MF})}{\partial h_{\rm eff}}\,, \end{aligned} \tag{67}$$

where on the third line we have used the fact that

$$\begin{aligned} \frac{\partial Z_{\rm MF}}{\partial h_{\rm eff}} &= \frac{\partial}{\partial h_{\rm eff}}\,\mathrm{Tr}(e^{-\beta\mathcal{H}_{\rm MF}}) \\ &= \mathrm{Tr}\left(\frac{\partial}{\partial h_{\rm eff}} e^{-\beta\mathcal{H}_{\rm MF}}\right) \\ &= -\beta\,\mathrm{Tr}\left(\frac{\partial\mathcal{H}_{\rm MF}}{\partial h_{\rm eff}} e^{-\beta\mathcal{H}_{\rm MF}}\right) \\ &= -\beta\,\mathrm{Tr}\left[\left(-\sum_{i=1}^{N} s_i\right) e^{-\beta\mathcal{H}_{\rm MF}}\right] \\ &= \beta\,\mathrm{Tr}\left[\sum_{i=1}^{N} s_i e^{-\beta\mathcal{H}_{\rm MF}}\right]\ . \end{aligned} \tag{68}$$

Now, from Eq. 66 we can calculate $\ln Z_{\rm MF}$:

$$\ln Z_{\rm MF} = -\beta\left(\frac{qJ}{2}+D\right)Nm^2 + N\ln 2 + N\ln[\cosh(\beta h_{\rm eff})]\,, \tag{69}$$

so

$$\frac{\partial(\ln Z_{\rm MF})}{\partial h_{\rm eff}} = N\beta\tanh(\beta h_{\rm eff})\,. \tag{70}$$

Inserting this back into Eq. 67 gives

$$m = \tanh(\beta h_{\rm eff})\,. \tag{71}$$

Inserting the definition of h_{eff} (Eq. 64) back into this equation gives us the self-consistency equation

$$\boxed{m = \tanh\big[\beta\big(h + (qJ + 2D)m\big)\big]}. \tag{72}$$

This corresponds to a system with a phase transition at $k_B T_c = qJ + 2D$. Above this temperature, it is paramagnetic, and below this temperature, it is ferromagnetic. Note that the system will be paramagnetic for all (nonzero) temperatures if $D < -qJ/2$ (remember that $D < 0$ favors easy-plane magnetization).

References

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