

Mean Field $m(h, T)$

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1 Introduction

We begin with the classical Ising Hamiltonian:

$$H = -J \sum_{\langle ij \rangle} S_i S_j - h \sum_i S_i \quad (1)$$

where $J > 0$ is a ferromagnetic exchange interaction and h the external field. The mean field theory assumes very small thermal fluctuation so that the system can be treated as non-interacting spins. Let $\langle S_i \rangle$ be the average of spin over ensemble, hence the thermal fluctuation of site i is $S_i - \langle S_i \rangle$. Since fluctuation is assumed to be small, we ignore the higher order:

$$(S_i - \langle S_i \rangle)(S_j - \langle S_j \rangle) = 0 \quad (2)$$

therefore

$$S_i S_j = S_i \langle S_j \rangle + S_j \langle S_i \rangle - \langle S_i \rangle \langle S_j \rangle \quad (3)$$

The Ising chain is translationally symmetric, so the expectation value of spins, thus local magnetization $m_i \equiv \langle S_i \rangle$, should be independent of position:

$$\langle S_i \rangle = m_i = m \quad (4)$$

We can then rewrite Eq.(3) as:

$$S_i S_j = m(S_i + S_j) - m^2 \quad (5)$$

and the Ising Hamiltonian becomes:

$$H_{\text{mf}} = -J \sum_{\langle ij \rangle} (m(S_i + S_j) - m^2) - h \sum_i S_i \quad (6)$$

We can further simplify this by noting that $\sum_{\langle ij \rangle} S_i = \sum_{\langle ij \rangle} S_j$, since S_i, S_j are single site variables, and that $\sum_{\langle ij \rangle} = \frac{z}{2} \sum_i$ where z is the coordination number. The mean field approximation therefore takes the form:

$$\begin{aligned} H_{\text{mf}} &= -\frac{Jzm}{2} \sum_i (2S_i - m) - h \sum_i S_i \\ &= -(h + Jzm) \sum_i S_i + \frac{NJzm^2}{2} \end{aligned} \quad (7)$$

Now we can calculate the partition function Z :

$$\begin{aligned}
Z &= \text{Tr}\{e^{-\beta H_{\text{mf}}}\} = \sum_{S_1=\pm 1} \dots \sum_{S_N=\pm 1} e^{-\beta H_{\text{mf}}} \\
&= e^{-\beta N J z m^2/2} \sum_{S_1=\pm 1} \dots \sum_{S_N=\pm 1} \prod_j^N e^{\beta(h+Jzm)S_j} \\
&= e^{-\beta N J z m^2/2} \prod_j^N \left(\sum_{S_i=\pm 1} e^{\beta(h+Jzm)S_i} \right) \\
&= e^{-\beta N J z m^2/2} \left(2 \cosh[\beta(h+Jzm)] \right)^N
\end{aligned} \tag{8}$$

Finally, we can calculate the magnetization by evaluating $\langle S_i \rangle$. Note that the thermal average $\langle S_i \rangle$ is homogeneous in the system, hence $m = \langle S_i \rangle$.

$$\begin{aligned}
m &= \frac{\text{Tr}\{S_i e^{-\beta H_{\text{mf}}}\}}{Z} = \frac{1}{Z} \sum_j S_i e^{-\beta H_{\text{mf}}} \\
&= \frac{e^{-\beta N J z m^2/2}}{Z} \sum_j \left(\sum_{S_1=\pm 1} \dots \sum_{S_N=\pm 1} S_i \prod_l^N e^{-\beta(Jzm+h)S_l} \right) \\
&= \frac{e^{-\beta N J z m^2/2}}{Z} \left(\prod_{j \neq i} e^{\beta(Jzm+h)S_j} \right) \left(\sum_{S_i=\pm 1} S_i e^{\beta(Jzm+h)S_i} \right) \\
&= \frac{e^{-\beta N J z m^2/2}}{Z} \left(2 \cosh[\beta(h+Jzm)] \right)^{N-1} \left(2 \sinh[\beta(h+Jzm)] \right) \\
&= \tanh[\beta(h+Jzm)]
\end{aligned} \tag{9}$$

A better way to get m is by taking derivative of $\log Z$ with respect to an effective field $h' \equiv Jzm + h$ (Derivation in A1):

$$m = \frac{1}{N} \frac{\partial \log Z}{\partial h'} \tag{10}$$

where

$$\begin{aligned}
\log Z &= \log \left\{ e^{-\beta N J z m^2/2} \left(2 \cosh[\beta h'] \right)^N \right\} \\
&= \frac{-\beta N J z m^2}{2} + N \log 2 + N \log \{ \cosh[\beta h'] \}
\end{aligned} \tag{11}$$

Plug into Eq.(10), it's straightforward to get:

$$\boxed{m = \tanh(\beta h') = \tanh[\beta(Jzm + h)]} \tag{12}$$

2 Zero field limit

In the zero field limit, we can calculate analytically the magnetization temperature scaling. Setting $h = 0$ gives

$$m(T, 0) = \tanh(\beta J z m) \quad (13)$$

This can be solved graphically. We can see that the phase transition occurs when $\beta J z = 1$ as is showed in Fig.(1,2).

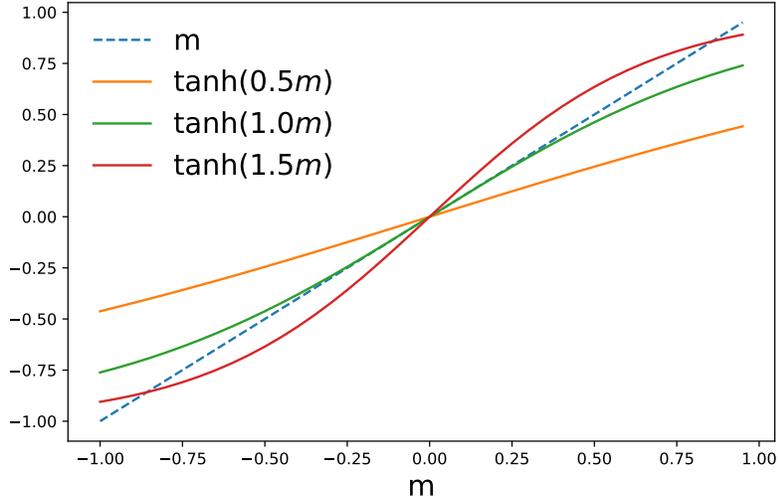


Figure 1: Graphical illustration of phase transition.

Therefore the critical temperature is $T_C = Jz/k_B$, and we can rewrite Eq.(13):

$$m(T, 0) = \tanh \left[\frac{T_C}{T} m \right] \quad (14)$$

At $T = T_C$, $m = 0$. Expanding around $m = 0$ and $T \sim T_C$ gives

$$m \cong \frac{T_C}{T} m - \frac{1}{3} \left(\frac{T_C}{T} \right)^3 m^3 \quad (15)$$

As expected one solution is $m = 0$. The other solution requires some algebra. Factoring m and $\frac{T_C}{T}$ gives

$$\frac{T}{T_C} = 1 - \frac{1}{3} \left(\frac{T_C}{T} \right)^2 m^2 \quad (16)$$

Solving for m yields

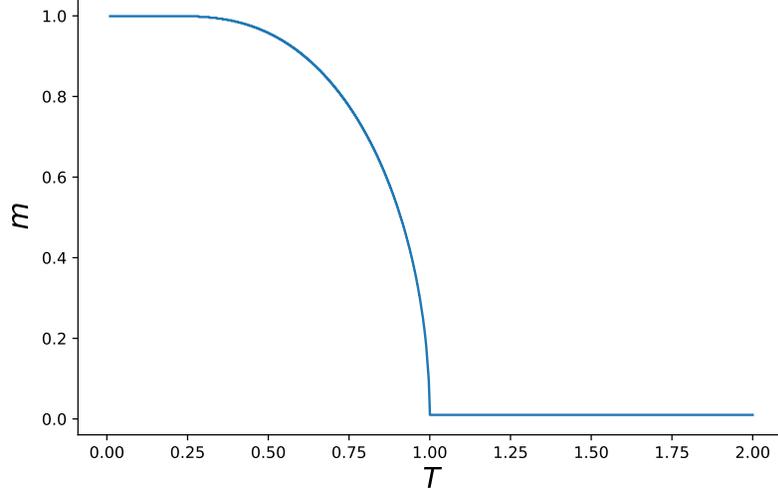


Figure 2: Collected graphical illustration of phase transition as a function of T at zero-field.

$$m(T, 0) = \pm \left[3 \left(\frac{T}{T_C} \right)^2 \left(1 - \frac{T}{T_C} \right) \right]^{1/2} \quad (17)$$

Defining a dimensionless temperature $t \equiv \frac{T_C - T}{T_C}$ gives

$$m(T, 0) = \pm [3t(1+t)^2]^{1/2} \quad (18)$$

As $T \rightarrow T^-$, $t \ll 1$. Therefore

$$m(T, 0) = \pm [3t]^{1/2} \quad (19)$$

and we can conclude that near the critical temperature there is an exponential behavior $m \sim t^\beta$

$$\boxed{m(T, 0) \sim \left(\frac{T_c - T}{T_c} \right)^{1/2}} \quad (20)$$

thus $\beta = 1/2$ for $t \rightarrow 0^-$. At $T > T_c$ there's no magnetization, therefore $\beta = 0$ for $t \rightarrow 0^+$.

3 Graphical solution of $m(h)$

Plotting the intersections of the right and left hand sides of Eq.(12) allows us to show m as a function of the field h . This can be seen in Fig. 3.

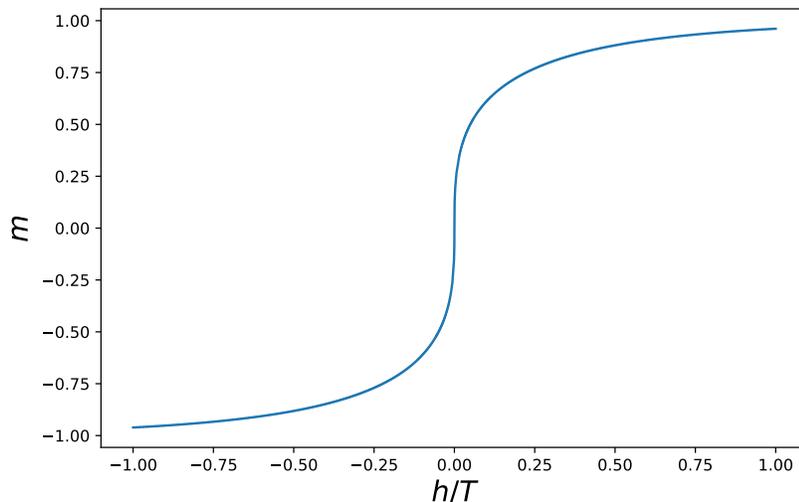


Figure 3: Magnetization as a function of field at $Jz/T = 1$.

4 Free energy

At $h = 0$, the free energy is:

$$F_{mf}(m, 0) = -k_B T \log Z \quad (21)$$

where the partition function Z is defined in Eq.(8). We can expand the $\log[\cosh x]$ term which appears in Eq.(21) by:

$$\log(\cosh x) \simeq \frac{x^2}{2} - \frac{x^4}{12} + O(x^5) \quad (22)$$

Then it is readily apparent that the free energy can be approximated by:

$$\begin{aligned} F_{mf}(m, 0) &\simeq -Nk_B T \log 2 - \frac{N(Jzm)^2}{2k_B T} + \frac{NJzm^2}{2} + \frac{N(Jzm)^4}{12(k_B T)^3} \\ &= -Nk_B T \log 2 + \frac{Nk_B T_c}{2T}(T - T_c)m^2 + \frac{Nk_B T_c^4}{12T^3}m^4 \end{aligned} \quad (23)$$

where we used $Jz = k_B T_c$ in the second line. Note that Eq.(23) has identical form as the Landau-Ginzburg theory, which is:

$$F_{mf}(m, 0) = F_0(T) + a(T)(T - T_c)m^2 + b(T)m^4 + \dots \quad (24)$$

which has Z_2 symmetry, consistent with the Hamiltonian. Now we plot the free energy per site defined by $f \equiv F_{mf}(m, h)/N$ according to our approximation in Eq.(23):

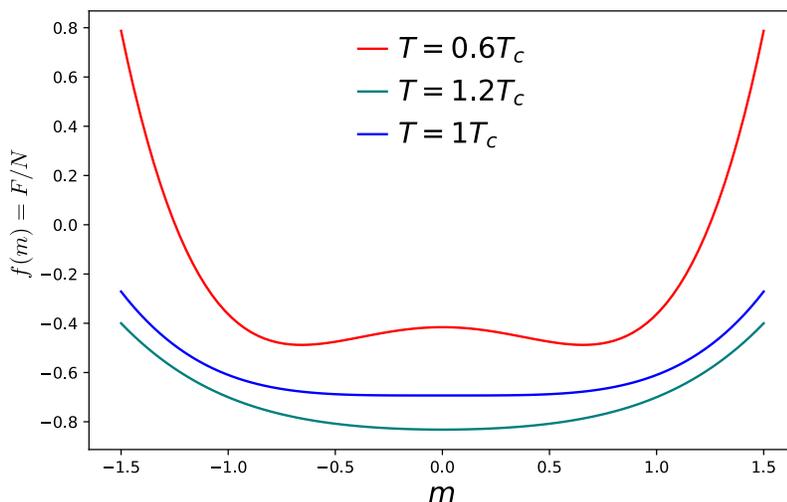


Figure 4: Free energy at different temperature as a function of magnetization m without field. Calculated by approximation in Eq.(23)

As temperature drops below T_c , the profile of $f(m)$ deforms to the "Mexican hat", thus two stable ferromagnetic states emerge. It is worth pointing out that in Fig.(4) the overall shift between different lines are due to the first $F_0(T)$ term which has a temperature dependence.

We can as well remove the $F_0(T)$ term and focus on the the geometric profile of $f(m)$, as showed in Fig.(5). At a lower T , the stable state moves towards maximal magnetization $m = \pm 1$ as expected. Note that the tendency to be polarized at low temperature can only be captured by the exact expression of free energy in Eq.(21), the approximated version in Eq.(23) will give the opposite. It turns out that the higher order does matter a lot in finding the stable state m in free energy profile.

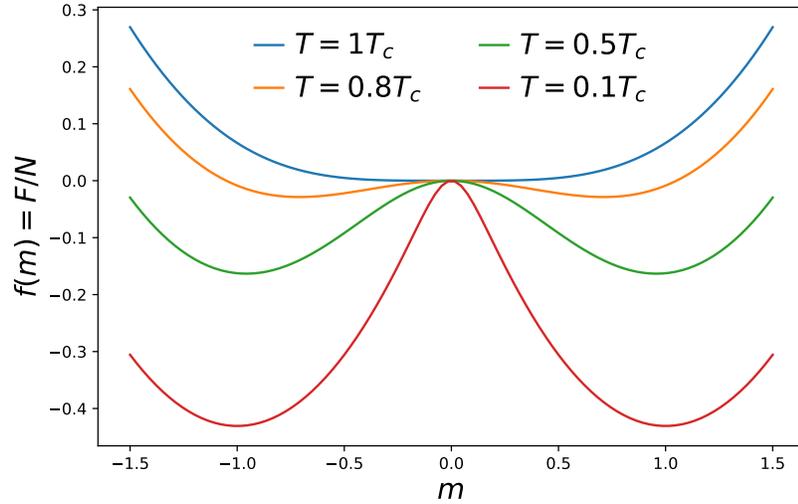


Figure 5: Free energy at different temperature as a function of magnetization m without field. Calculated by exact expression in Eq.(21). The stable state moves towards maximal magnetization $m = \pm 1$ as expected

Now lets calculate the free energy under non-zero field h . It is similarly as Eq.(21). All we have to do is substitute Jzm by $Jzm + h$:

$$F_{mf}(m, h) \simeq -Nk_B T \log 2 - \frac{N(k_B T_c m + h)^2}{2k_B T} + \frac{Nk_B T_c m^2}{2} + \frac{N(k_B T_c m + h)^4}{12(k_B T)^3}$$

It's readily apparent that there must be magnetization m with odd exponent. Therefore the free energy is no longer symmetric about $m = 0$. As showed in Figure.(6):

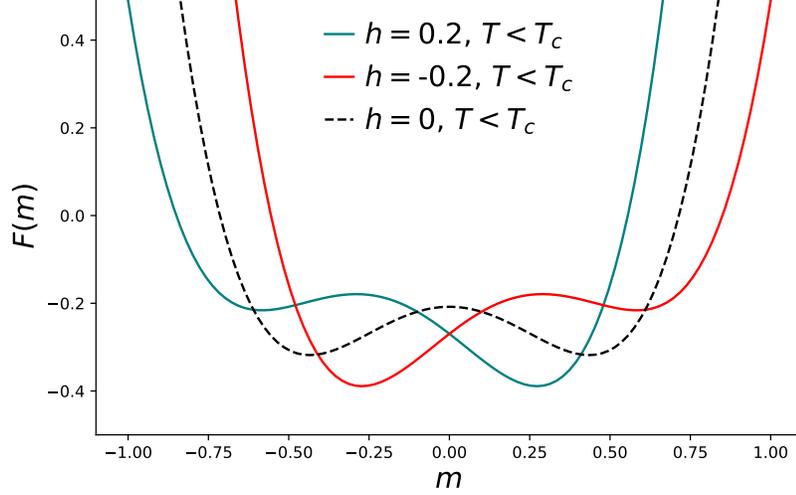


Figure 6: Free energy at $h \neq 0$ as a function of magnetization m . Calculated by approximated result

5 Appendix

Derivation of Eq.(10):

Consider a Hamiltonian with individual spins coupled to a homogeneous field h :

$$H = H_0 - h \sum_i S_i \quad (25)$$

whose partition function is:

$$Z = \text{Tr}\{e^{-\beta H}\} = \text{Tr}\{e^{-\beta H_0 + \beta h \sum_i S_i}\} \quad (26)$$

it is straightforward to see that:

$$\frac{1}{Z} \frac{\partial Z}{\partial h} = \frac{1}{Z} \text{Tr}\left\{ \left(\beta \sum_i S_i \right) e^{-\beta H} \right\} = \beta N m \quad (27)$$

where we used the definition

$$\sum_i S_i = N m \quad (28)$$

N being the number of spins, m the magnetization per site. Therefore

$$m = \frac{1}{N\beta} \frac{1}{Z} \frac{\partial Z}{\partial h} = \frac{1}{N\beta} \frac{\partial \log Z}{\partial h} \quad (29)$$

or written in terms of free energy:

$$m = -\frac{1}{N} \frac{\partial F}{\partial h} \quad (30)$$