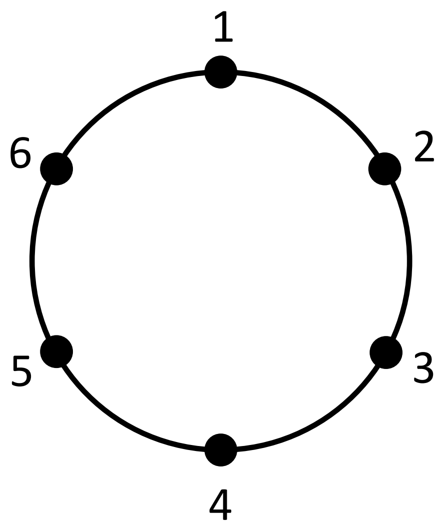
Modelling of Complex Systems

Phase transitions

Ising model with all-to-all interaction

Ising model on a ring

$$N = 6, \sigma_i = \pm 1$$

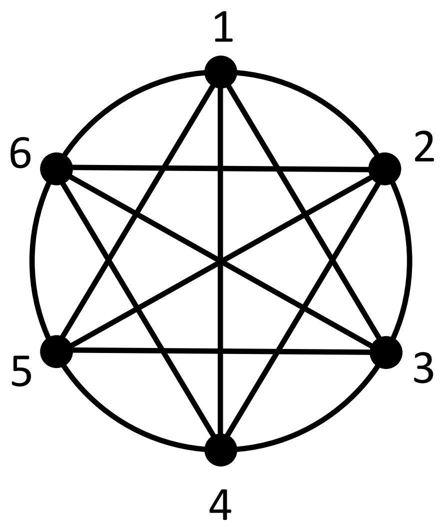


$$E = -J(\sigma_1\sigma_2 + \sigma_2\sigma_3 + \ldots + \sigma_6\sigma_1) - H(\sigma_1 + \sigma_2 + \ldots + \sigma_6)$$

Result was in the 1D Ising model there is no phase transition at $T > 0$.

Ising model with long range interaction (all-to-all interaction)

$$N = 6, \sigma_i = \pm 1$$



$$E = -\frac{J}{N}\sum_{i=1}^{N}\sum_{j=i+1}^{N}\sigma_i\sigma_j - H\sum_{i=1}^{N}\sigma_i$$

The coupling J should be inversely proportional to N in order to keep the system's energy proportional to the system size.

Ising model with long range interaction (all-to-all interaction)

Recall the definition of the partition function,

$$Z = \sum_{\sigma_1=\pm 1} \sum_{\sigma_2=\pm 1} \dots \sum_{\sigma_N=\pm 1} e^{-\beta E(\vec{\sigma})}$$

where $\beta = 1/T$. The usefulness of the partition function is to make it easier to calculate the free energy

$$F(T, H) = -T \ln Z$$

and the (total) magnetization

$$M(T, H) = -\frac{dF}{dH}$$

Let us find Z.

Ising model with long range interaction (all-to-all interaction)

Let's start by noticing the equality:

$$\sum_{i=1}^{N}\sum_{j=i+1}^{N}\sigma_i\sigma_j = \frac{1}{2}\left[\sum_{i=1}^{N}\sum_{j=1}^{N}\sigma_i\sigma_j - \sum_{i=1}^{N}{\sigma_i}^2\right]$$

$$= \frac{1}{2}\left[\left(\sum_{i=1}^{N}\sigma_i\right)^2 - N\right]$$

So, we can rewrite the energy as:

$$E = -\frac{J}{N}\sum_{i=1}^{N}\sum_{j=i+1}^{N}\sigma_i\sigma_j - H\sum_{i=1}^{N}\sigma_i$$

$$= -\frac{J}{2N}\left(\sum_{i=1}^{N}\sigma_i\right)^2 + \cancel{\frac{J}{2}} - H\sum_{i=1}^{N}\sigma_i$$

This constant term is just an energy shift and can be omitted.

Ising model with long range interaction (all-to-all interaction)

$$E = -\frac{J}{2N}\left(\sum_{i=1}^{N}\sigma_i\right)^2 - H\sum_{i=1}^{N}\sigma_i$$

Then, the partition function is

$$Z = \sum_{\{\vec{\sigma}\}} \exp\left[\beta\frac{J}{2N}\left(\sum_{i=1}^{N}\sigma_i\right)^2 + \beta H\sum_{i=1}^{N}\sigma_i\right]$$

Let us define $\frac{\beta J}{2N}\left(\sum_{i=1}^{N}\sigma_i\right)^2 \equiv \frac{1}{2}A^2$, that is $A = \sqrt{\frac{\beta J}{N}}\sum_{i=1}^{N}\sigma_i$ and write:

$$Z = \sum_{\{\vec{\sigma}\}} \exp\left(\frac{A^2}{2}\right)\exp\left(\beta H\sum_{i=1}^{N}\sigma_i\right)$$

Ising model with long range interaction (all-to-all interaction)

The Hubbard-Stratonovich transformation

The Gauss integral can be used to write the equality

$$1 = \int_{-\infty}^{+\infty} dx \frac{e^{-\frac{x^2}{2}}}{\sqrt{2\pi}} \underset{x \to x' - A}{=} \int_{-\infty}^{+\infty} dx' \frac{e^{-\frac{(x'-A)^2}{2}}}{\sqrt{2\pi}}$$

$$= e^{-\frac{A^2}{2}} \int_{-\infty}^{+\infty} dx \frac{e^{-\frac{x^2}{2}+Ax}}{\sqrt{2\pi}}$$

Therefore, we arrive at the transformation

$$e^{\frac{A^2}{2}} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} dx e^{-\frac{x^2}{2}+Ax}$$

with which we replace the spin-spin interaction term in Z.

Ising model with long range interaction (all-to-all interaction)

$$Z = \sum_{\{\vec{\sigma}\}} \exp\left(\frac{A^2}{2}\right) \exp\left(\beta H \sum_{i=1}^{N} \sigma_i\right)$$

$$= \frac{1}{\sqrt{2\pi}} \sum_{\{\vec{\sigma}\}} \int_{-\infty}^{+\infty} dx \exp\left(-\frac{x^2}{2} + Ax + \beta H \sum_{i=1}^{N} \sigma_i\right)$$

where $A = \sqrt{\beta J/N} \sum_i \sigma_i$.

Now let us change the integration variable $x = m\sqrt{\beta J N}$ and rearrange terms:

$$Z = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} dx \exp\left(-\frac{x^2}{2}\right) \sum_{\{\vec{\sigma}\}} \exp\left[\left(\sqrt{\frac{\beta J}{N}} x + \beta H\right) \sum_{i=1}^{N} \sigma_i\right]$$

$$= \sqrt{\frac{\beta J N}{2\pi}} \int_{-\infty}^{+\infty} dm \exp\left(-\frac{\beta J N}{2} m^2\right) \sum_{\{\vec{\sigma}\}} \exp\left[\beta \left(Jm + H\right) \sum_{i=1}^{N} \sigma_i\right]$$

Ising model with long range interaction (all-to-all interaction)

$$Z = \sqrt{\frac{\beta J N}{2\pi}} \int_{-\infty}^{+\infty} dm \exp\left(-\frac{\beta J N}{2} m^2\right) \sum_{\{\vec{\sigma}\}} \exp\left[\beta\left(Jm + H\right) \sum_{i=1}^{N} \sigma_i\right]$$

It is now apparent that the H-S transformation can be interpreted as the average of the partition function of a system of non-interacting spins in a field $Jm + H$, where the Jm component of the field fluctuates according to a Gaussian distribution. The advantage of this approach is that **non-interacting spins are independent**, so we can express the sum over microstates $\vec{\sigma}$ as

$$\sum_{\{\vec{\sigma}\}} \exp\left[\beta\left(Jm + H\right) \sum_{i=1}^{N} \sigma_i\right] = \prod_{i=1}^{N} \sum_{\sigma_i = \pm 1} \exp\left[\beta\left(Jm + H\right)\sigma_i\right]$$

$$= \prod_{i=1}^{N} 2\cosh\left[\beta\left(Jm + H\right)\right] = \left\{2\cosh\left[\beta\left(Jm + H\right)\right]\right\}^N$$

Recall that $\cosh x = (e^x + e^{-x})/2$.

Ising model with long range interaction (all-to-all interaction)

Finally, having got rid of the summations we get the partition function in the form of an integral

$$
\begin{aligned}
Z &= \sqrt{\frac{\beta J N}{2\pi}} \int_{-\infty}^{+\infty} dm \exp\left(-\frac{\beta J N}{2} m^2\right) \left\{2\cosh\left[\beta\left(Jm + H\right)\right]\right\}^N \\
&= \sqrt{\frac{\beta J N}{2\pi}} \int_{-\infty}^{+\infty} dm \exp\left[-\frac{\beta J N}{2} m^2 + N \ln\left\{2\cosh\left[\beta\left(Jm + H\right)\right]\right\}\right] \\
&= \sqrt{\frac{\beta J N}{2\pi}} \int_{-\infty}^{+\infty} dm e^{-\beta N f(m)}
\end{aligned}
$$

where

$$
f(m) = \frac{J}{2} m^2 - \beta^{-1} \ln\left\{2\cosh\left[\beta\left(Jm + H\right)\right]\right\}
$$

Ising model with long range interaction (all-to-all interaction)

$$Z = \sqrt{\frac{\beta J N}{2\pi}} \int_{-\infty}^{+\infty} dm e^{-\beta N f(m)}$$

$$f(m) = \frac{J}{2} m^2 - \beta^{-1} \ln\left\{2\cosh\left[\beta\left(Jm + H\right)\right]\right\}$$

$f(m)$ has a global minimum at some $m = m_0$, so we can evaluate the integral above using Lapalce's method:

When N is large, the integral is dominated by the contribution of a narrow region around the minimum of $f(m)$. This means that we can replace $f(m)$ by $f(m_0) + f''(m_0)(m - m_0)^2/2$ (if m_0 is a minimum then $f'(m_0) = 0$):

$$Z = \sqrt{\frac{\beta J N}{2\pi}} \int_{-\infty}^{+\infty} dm e^{-\beta N\left[f(m_0) + \frac{f''(m_0)}{2}(m - m_0)^2\right]}$$

$$= \sqrt{\frac{\beta J N}{2\pi}} e^{-\beta N f(m_0)} \int_{-\infty}^{+\infty} dm e^{-\beta N \frac{f''(m_0)}{2}(m - m_0)^2} = \sqrt{\frac{J}{f''(m_0)}} e^{-\beta N f(m_0)}$$

Ising model with long range interaction (all-to-all interaction)

All that is left is to find m_0, the minimum of $f(m)$, which is given by the condition $\frac{df}{dm} = 0$:

$$\frac{df}{dm} = \frac{d}{dm}\left(\frac{J}{2}m^2 - \beta^{-1}\ln\left\{2\cosh\left[\beta\left(Jm + H\right)\right]\right\}\right)$$
$$= Jm - J\tanh\left[\beta\left(Jm + H\right)\right] = 0$$

$$\Longrightarrow m_0 = \tanh\left[\beta\left(Jm_0 + H\right)\right]$$

Ising model with long range interaction (all-to-all interaction)

Now we can get the free energy

$$F = -T \ln Z = -T \ln \left[\sqrt{\frac{J}{f''(m_0)}} e^{-\beta N f(m_0)} \right]$$

$$= N f(m_0) - T \ln \sqrt{\frac{J}{f''(m_0)}}$$

In the thermodynamic limit $N \to \infty$ the free energy per spin is

$$\frac{F}{N} = f(m_0)$$

where m_0 is the solution of the equation $m_0 = \tanh\left[\beta\left(J m_0 + H\right)\right]$.

The physical meaning of function f is now clear, it's the free energy per spin!

Ising model with long range interaction (all-to-all interaction)

And what is the meaning of $m_0 = \tanh\left[\beta\left(Jm_0 + H\right)\right]$?

Let us calculate the mean magnetic moment:

$$\begin{aligned}\frac{M}{N} &= -\frac{1}{N}\frac{dF}{dH} = -\frac{df(m_0)}{dH} = -\cancelto{0}{\frac{\partial f(m_0)}{\partial m_0}}\frac{dm_0}{dH} - \frac{\partial f(m_0)}{\partial H} \\ &= -\frac{\partial}{\partial H}\left(\frac{J}{2}m_0^2 - \beta^{-1}\ln\left\{2\cosh\left[\beta\left(Jm_0 + H\right)\right]\right\}\right) \\ &= \tanh\left[\beta\left(Jm_0 + H\right)\right] = m_0\end{aligned}$$

(The term $\frac{\partial f(m_0)}{\partial m_0} = 0$ simply because m_0 was defined as the minimum of f.)

Then, $\boldsymbol{m_0}$ **is the magnetization per spin**, which is determined by minimizing the free energy, in complete consistency with the laws of thermodynamics!

Ising model with long range interaction (all-to-all interaction)

Let us find the magnetization at $H = 0$, that is the solution to the equation

$$m = \tanh\left(\beta J m\right)$$

by the graphical method.

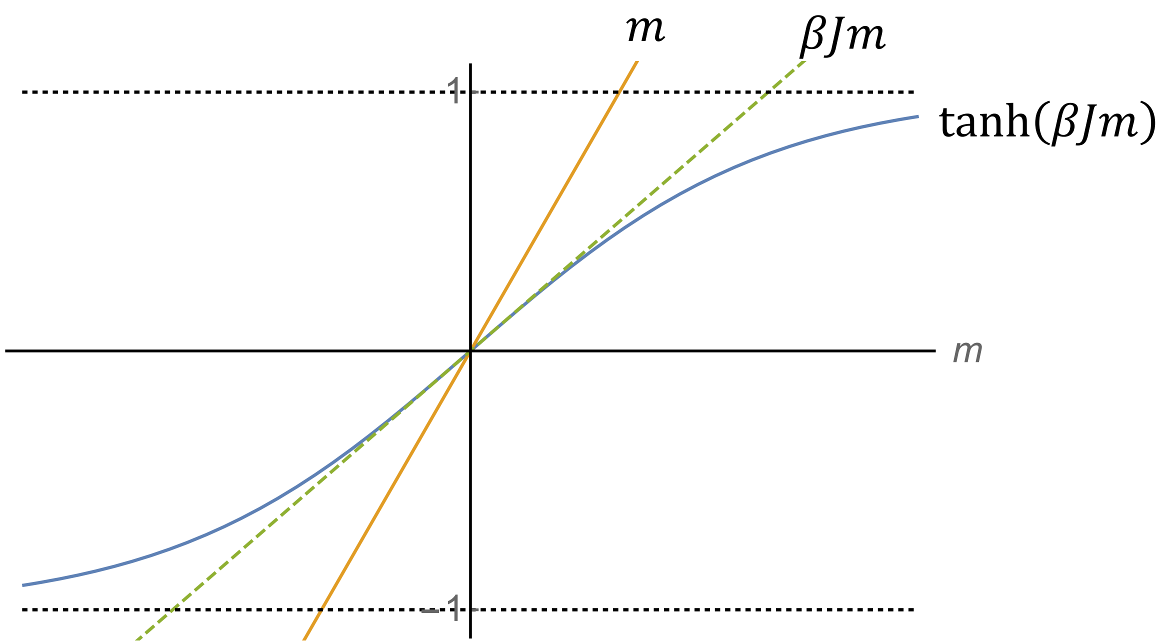
In this method we draw in the same plot the two sides of the equation we want to solve, and look for points of intersection of the two curves. Those points are the solutions to the equation.

Notice that expanding the right-hand side of the equation for small m we get $\tanh(\beta J m) \approx \beta J m + O(m^3)$, so

- for high temperatures, we have that the slope of the RHS near the origin is $\beta J < 1$,
- while for low temperatures, the slope is $\beta J > 1$.

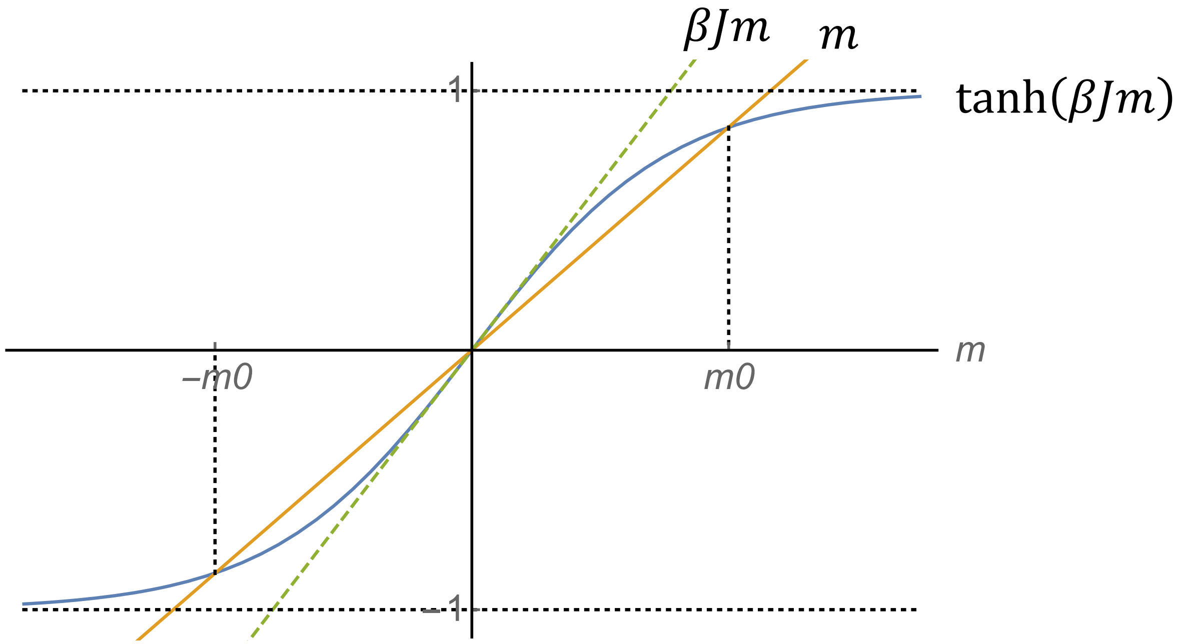
Ising model with long range interaction (all-to-all interaction)

High temperature



There is only one solution at $m = 0$.

Low temperature



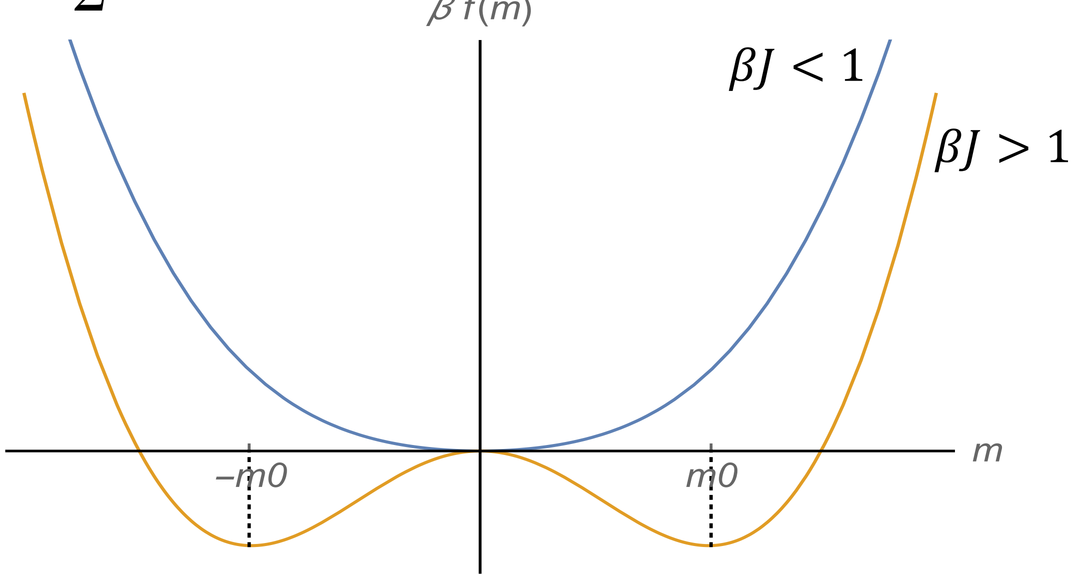
There are three solutions at $m = 0$ and $m = \pm m_0$.

The non-trivial solutions appear when the slope of the RHS $\beta J = 1$.

Ising model with long range interaction (all-to-all interaction)

The free energy $f(m) = \frac{J}{2}m^2 - \beta^{-1}\ln\left[2\cosh\left(\beta J m\right)\right]$:

Recall $\beta = 1/\mathrm{T}$.

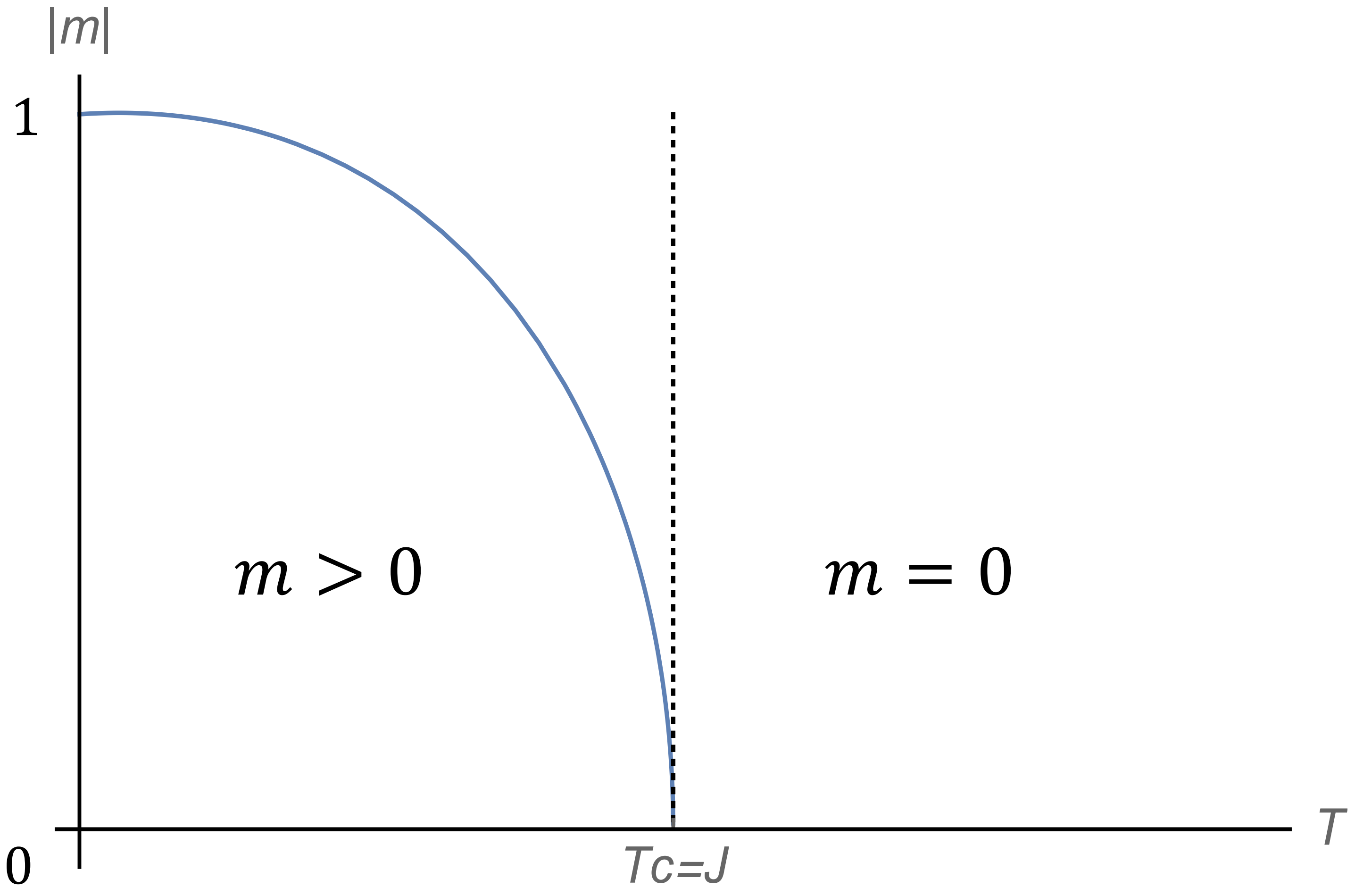


At $T > J$ the trivial solution $m = 0$ is a minimum of the free energy, and the system has no spontaneous magnetization.

At $T < J$ the trivial solution $m = 0$ is a maximum of the free energy, while the non-trivial solutions $m = \pm m_0$ are minima of the free energy, this means that for these temperatures there is a spontaneous magnetization $m \neq 0$.

The Ising model undergoes a phase transition at $T_c = J$.

Ising model with long range interaction (all-to-all interaction)



Which orientation the system choose $+|m|$ or $-|m|$?
It depends on the history and on the (random) fluctuations.

Ising model with long range interaction (all-to-all interaction)

Critical region

Let us find the magnetization a a function of T in the region near the critical point T_c. At $H = 0$ the magnetization is given by the solution of

$$m = \tanh\left(\beta J m\right)$$

Since the transition is continuous, m is small at T near T_c. So we expand

$$\tanh x = x - \frac{x^3}{3} + \ldots$$

and get

$$m \approx \beta J m - \frac{1}{3}(\beta J m)^3$$

Which has a trivial solution $m = 0$ and non-trivial solutions given by

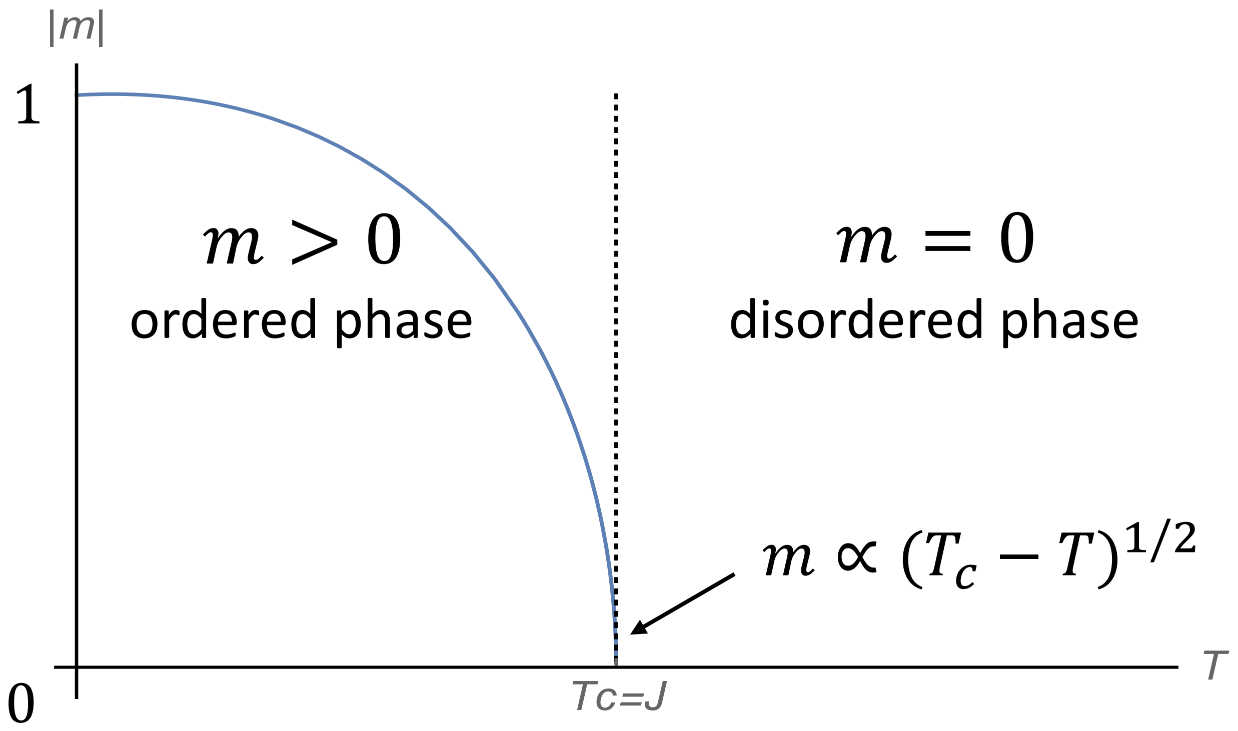
$$1 = \beta J - \frac{1}{3}(\beta J)^3 m^2 \Rightarrow m^2 = 3\frac{J - \beta^{-1}}{\beta^2 J^3} \Rightarrow m = \pm a(J - T)^{1/2}$$

where $T_c \equiv J$ and $a \equiv \sqrt{3\,T^2/{T_c}^3}$.

Ising model with long range interaction (all-to-all interaction)

Critical region

For $T > T_c$ only the solution $m = 0$ exists.
The solution $m = a(T_c - T)^{1/2}$ is valid for $T < T_c$ and $T_c - T \ll T_c$.
Furthermore, when $T \to 0$ the equation $m = \tanh(Jm/T)$ gives $m = \pm 1$.



$$\left.\frac{dm}{dT}\right|_{T=T_c} \propto \left.(T_c - T)^{-\frac{1}{2}}\right|_{T=T_c} \to \infty$$

Ising model with long range interaction (all-to-all interaction)

Critical region

Suppose we are in the disordered phase, and gradually decrease the temperature. How can we tell that we are approaching the critical point?

- We can measure the susceptibility $\chi = \frac{dm}{dH}$:

Differentiate both sides of

$$m = \tanh(\beta J m + \beta H)$$

$$\frac{dm}{dH} = \frac{d}{dH}\tanh(\beta J m + \beta H) = \frac{1}{\cosh^2(\beta J m + \beta H)}\left(\beta J \frac{dm}{dH} + \beta\right)$$

$$\chi = \frac{1}{\cosh^2(\beta J m + \beta H)}(\beta J \chi + \beta)$$

$$\chi = \frac{\beta}{\cosh^2(\beta J m + \beta H) - \beta J}$$

Ising model with long range interaction (all-to-all interaction)

Critical region

Then, the zero field susceptibility is

$$\chi = \frac{1}{T\cosh^2(Jm/T) - J}$$

At $T > T_c = J$ (disordered phase) we have $m = 0$, and therefore

$$\chi = \frac{1}{T - T_c}$$

The susceptibility diverges as $T \to {T_c}^+$.

This is a sign of a continuous phase transition.

Ising model with long range interaction (all-to-all interaction)

Critical region

$$\chi = \frac{1}{T\cosh^2(Jm/T) - J} \qquad m = \tanh(Jm/T)$$

In the ordered phase ($T < T_c$) we have $m \neq 0$.

Let us use the identity $\frac{1}{\cosh^2 x} = \frac{\cosh^2 x - \sinh^2 x}{\cosh^2 x} = 1 - \tanh^2 x$:

$$\frac{1}{\cosh^2(Jm/T)} = 1 - \tanh^2(Jm/T) = 1 - m^2$$

Then

$$\chi = \frac{1}{\frac{T}{1-m^2} - J} = \frac{1 - m^2}{T - J + Jm^2}$$

Ising model with long range interaction (all-to-all interaction)

Critical region

Recalling that, near $T_c = J$, in the ordered phase ($T < T_c$) we have a magnetization $m \approx \sqrt{3}\left(1 - {}^{T}/_{T_c}\right)^{1/2}$:

$$\chi = \frac{1 - m^2}{T - J + Jm^2}$$

$$\approx \frac{1 - 3(1 - T/T_c)}{T - T_c + T_c 3(1 - T/T_c)}$$

$$\Rightarrow \chi \approx \frac{1}{2(T_c - T)}$$