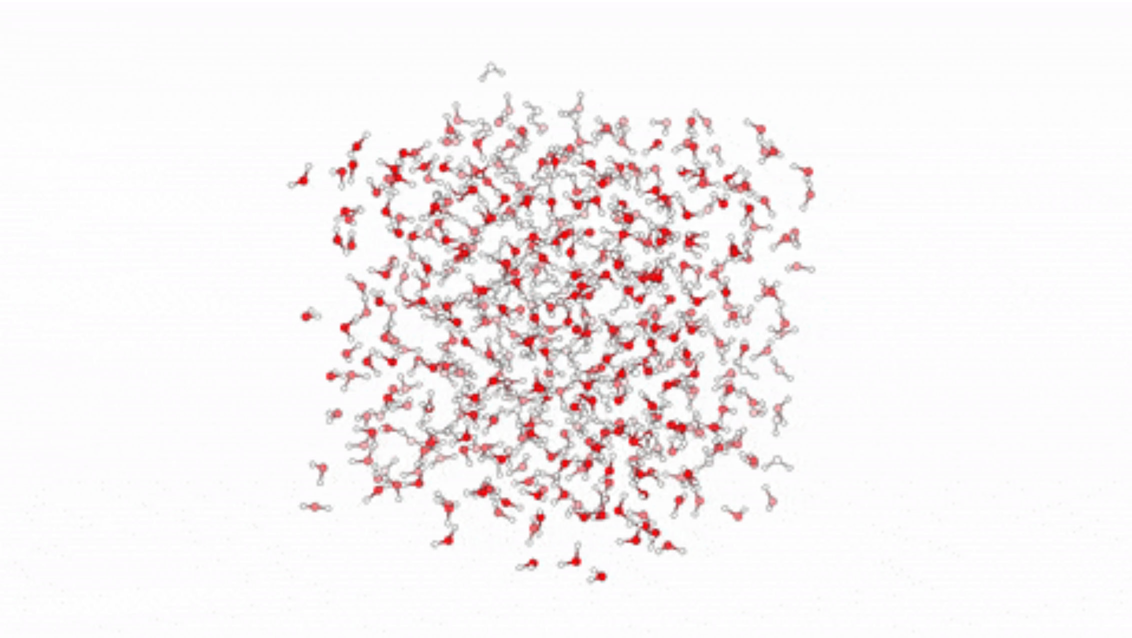
Lesson 7- Ising Model and Computation

Calculation and computation

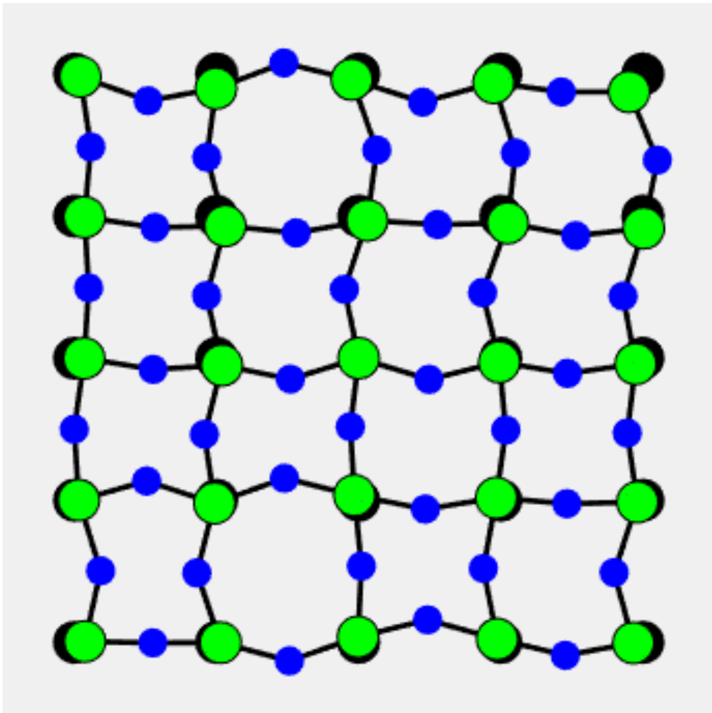
Most statistical mechanical systems cannot be solved explicitly.
Statistical mechanics does provide general relationships and organizing principles (temperature, entropy, free energy, thermodynamic relations) even when a solution is not available.

There are two basic tools for extracting answers out of statistical mechanics for realistic systems. The first is **simulation**. Sometimes one simply mimics the microscopic theory.



Calculation and computation

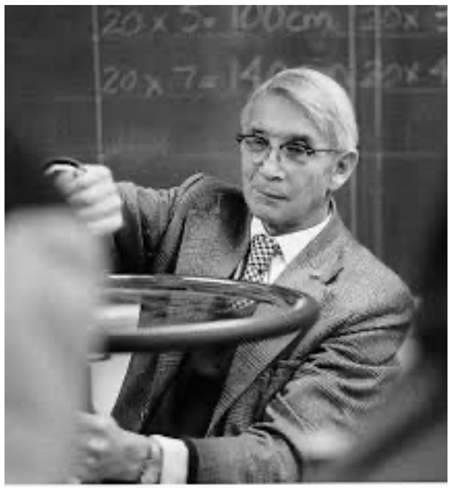
The second tool is to use **perturbation theory**. Starting from a solvable model, one can calculate the effects of small extra terms; for a complex system one can extrapolate from a limit (like zero or infinite temperature) where its properties are known.

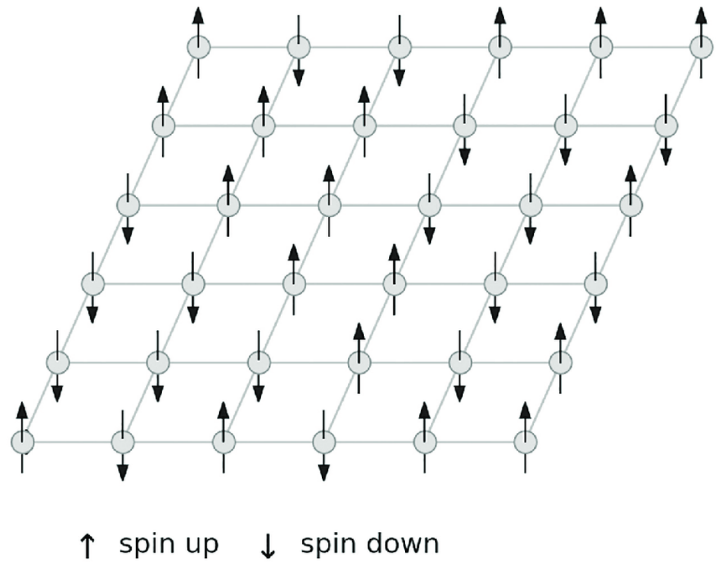


The Ising Model

The Ising Model is a mathematical model of ferromagnetism in statistical mechanics, consisting of discrete variables representing magnetic dipole moments of atomic spins.

Is a lattice model, These models have a variable at each site of a regular grid, and a Hamiltonian or evolution law for these variables.

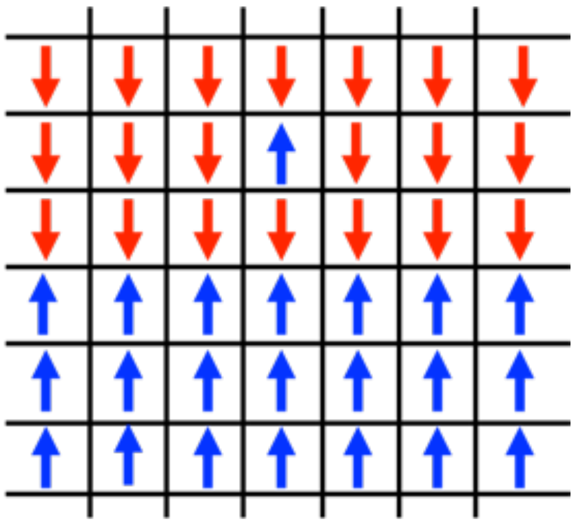




The Ising Model

The Ising model has a lattice of N sites i with a single, two-state degree of freedom si on each site that may take values ± 1. We will be primarily interested in the Ising model on square and cubic lattices (in 2D and 3D). The Hamiltonian for the Ising model is

$$H = -J \sum_{\langle i,j \rangle} s_i s_j - h \sum_i s_i$$



The Ising Model

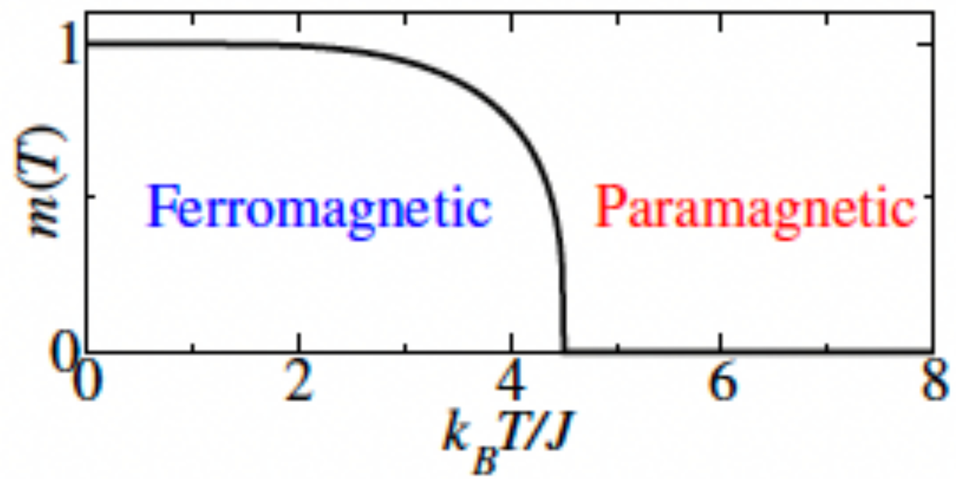
The Ising model was originally used to describe magnets. Hence the degree of freedom s_i on each site is normally called a spin, h is called the external field, and the sum $M = \sum_i s_i$ is termed the magnetization.

The energy of two neighboring spins $-Js_is_j$ is $-J$ if the spins are parallel, and $+J$ if they are antiparallel. Thus if $J > 0$ (the usual case) the model favors **parallel spins**; we say that the interaction is **ferromagnetic**. At low temperatures, the spins will organize themselves to either mostly point up or mostly point down, forming a **ferromagnetic phase**.

The Ising Model

If J < 0 we call the **interaction antiferromagnetic**; the spins will tend to align (for our square lattice) in a checkerboard **antiferromagnetic phase** at low temperatures.

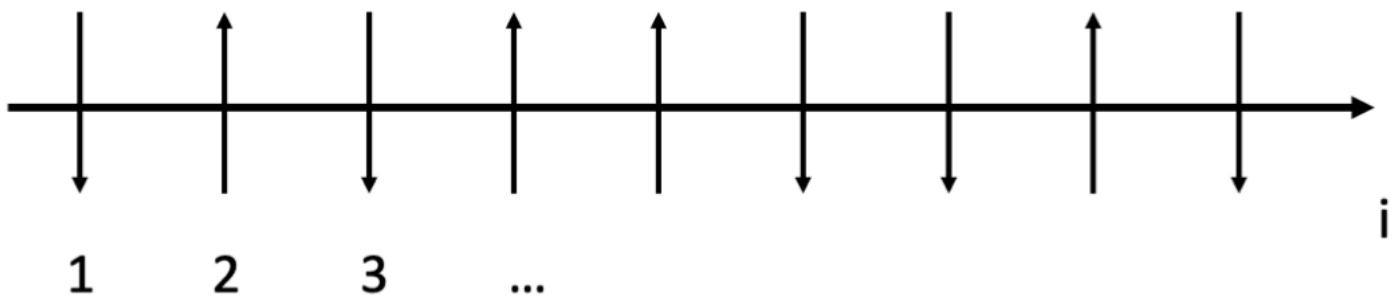
At high temperatures, independent of the sign of J, we expect entropy to dominate; the spins will fluctuate wildly in a **paramagnetic phase** and the magnetization per spin $m(T) = M(T)/N$ is zero.



The Ising Model

The sign convention of h also explains how a spin site j interacts with the external field. Namely, the spin site wants to line up with the external field. If: $h > 0$, the spin site j desires to line up in the positive direction, $h < 0$, the spin site j desires to line up in the negative direction, $h = 0$, there is no external influence on the spin site.

Let us solve the model in 1D, Ising chain, and assuming only neighbouring interactions, in the canonical ensemble.



The Ising Model in 1D

The partition function Z is a sum over all possible spin configurations:

$$Z = \sum_{\{s_i\}} e^{-\beta \mathcal{H}} = \sum_{\{s_i\}} \exp\left(\beta J \sum_{i=1}^{N} s_i s_{i+1} + \beta h \sum_{i=1}^{N} s_i \right)$$

For a system with N_{tot} lattice sites and two possible i -values at each lattice site, a total number of $2^{N_{tot}}$ possible configurations of the arrangement of particles exists.The boundary condition is typically $s_{N+1} = s_1$ (periodic boundary conditions). Note that we can write:

$$Z = \sum_{\{s_i\}} \exp\left(\beta J \sum_{i=1}^{N} s_i s_{i+1} + \beta h \sum_{i=1}^{N} s_i \right) = \sum_{\{s_i\}} \exp\left(\beta J \sum_{i=1}^{N} s_i s_{i+1} + \beta \frac{h}{2} \sum_{i=1}^{N} s_i + \beta \frac{h}{2} \sum_{i=1}^{N} s_{i+1} \right)$$

The Ising Model in 1D

Then the Boltzman factor:

$$\exp(-\beta\mathscr{H}) = \prod_i \exp\left[\frac{\beta h}{2}(s_i + s_{i+1}) + \beta J s_i s_{i+1}\right]$$

Let us call $T(s_i, s_{i+1}) = \exp\left[\frac{\beta h}{2}(s_i + s_{i+1}) + \beta J s_i s_{i+1})\right]$

then we can write $Z = \sum_{\{s_i=\pm 1\}} \prod_i T(s_i, s_{i+1})$ note that $T(s_i, s_{i+1})$ can take four different values with $s_i = \pm 1$,$s_{i+1} = \pm 1$. Let us define a matrix containing these 4 values, first (second) row for $s_i = +1$ ($s_i = -1$) and first (second) column for $s_{i+1=} +1$ ($s_{i+1} = -1$), the so called **transfer matrix** (notation trick):

$$T = \begin{pmatrix} e^{\beta(J+h)} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta(J-h)} \end{pmatrix}$$

The Ising Model in 1D

Then

$$Z = \sum_{s_1=\pm 1} \sum_{s_2=\pm 1} \cdots \sum_{s_N=\pm 1} T(s_1, s_2)T(s_2, s_3)\cdots T(s_{N-1}, s_N)T(s_N, s_1)$$

Remember that matrix multiplication is defined as $(AB)_{ik} = \sum_j A_{ij}B_{jk}$

$$Z = \sum_{s_1=\pm 1} \sum_{s_3=\pm 1} \cdots \sum_{s_N=\pm 1} (T \cdot T)(s_1, s_3)\cdots T(s_{N-1}, s_N)T(s_N, s_1)$$

$$= \sum_{s_1=\pm 1} (T \cdot T \cdots T)_{(s_1, s_1)} = \text{Trace}[T^N] = \lambda_+^N + \lambda_-^N$$

The eigenvalues of T are:

$$\lambda_\pm = (e^{\beta J} \cosh(\beta h)) \pm \sqrt{e^{2\beta J} \sinh^2(\beta h) + e^{-2\beta J}}$$

Exercise: proof the red equalities

The Ising Model in 1D

In the thermodynamic limit ($N \gg 1$)

$$Z = \lambda_+^N + \lambda_-^N = \lim_{N\to\infty} \lambda_+^N (1 + \left(\frac{\lambda_-}{\lambda_+}\right)^N) \approx \lambda_+^N$$

The free energy is:

$$f = -\frac{kT}{N} \ln Z \to -kT \ln \lambda_+$$

We can define the magnetization m of the system is given by the average of the magnetic moments s_i per site as:

$$m = \frac{1}{N}\langle s_1 + s_2 + \cdots + s_N \rangle = \frac{1}{N}\frac{1}{Z}\sum_{\{s_i\}}(s_1 + s_2 + \cdots + s_N)\exp\left(\beta J \sum_{i=1}^{N} s_i s_{i+1} + \beta h \sum_{i=1}^{N} s_i\right)$$

$$= -\frac{\partial}{\partial h} f(h,\beta) = \frac{\partial}{\partial h}(kT \ln \lambda_+) = kT \frac{\partial}{\partial h} \ln\left(e^{\beta J}\cosh(\beta h) + \sqrt{e^{2\beta J}\sinh^2(\beta h) + e^{-2\beta J}}\right)$$

The Ising Model in 1D

$$m = kT \frac{\beta e^{2\beta J} \sinh(\beta h)}{\sqrt{e^{2\beta J} \sinh^2(\beta h) + e^{-2\beta J}}}$$

At high temperature ($\beta \to 0$), the magnetisation is

$$m = kT \frac{\beta e^{2\beta J} \sinh(\beta h)}{\sqrt{e^{2\beta J} \sinh^2(\beta h) + e^{-2\beta J}}} \approx \tanh(\beta h)$$

The Ising Model Mean-Field theory (MFT) approximation

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 (MFT) approximation. The idea is to assume that the system is interacting in a sort of “thermal bath” where fluctuations are negligible. Mathematically, it is equivalent to decouple the Hamiltonian in simpler Hamiltonian describing non-interacting particles.

We start by writing each spin in the spin interaction terms $s_i s_j$ in the form

$$s_i = \langle s_i \rangle + \delta s_i$$

where $\delta s_i \equiv s_i - \langle s_i \rangle$

Then

$$s_i s_j = (\langle s_i \rangle + \delta s_i)(\langle s_j \rangle + \delta s_j) = \langle s_i \rangle \langle s_j \rangle + \langle s_i \rangle \delta s_j + \langle s_j \rangle \delta s_i + \delta s_i \delta s_j$$

The Ising Model Mean-Field theory (MFT) approximation

We now make the assumption that the fluctuations are very small, so we can ignore the term quadratic in fluctuations: $\delta s_i \delta s_j = 0$. Then

$$\begin{aligned} s_i s_j &= \langle s_i \rangle \langle s_j \rangle + \langle s_i \rangle \delta s_j + \langle s_j \rangle \delta s_i \\ &= \langle s_i \rangle \langle s_j \rangle + \langle s_i \rangle (s_i - \langle s_i \rangle) + \langle s_j \rangle (s_j - \langle s_j \rangle) \\ &= \langle s_j \rangle s_i + \langle s_i \rangle s_j - \langle s_i \rangle \langle s_j \rangle \end{aligned}$$

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

$$\langle s_i \rangle = m$$

We can then further simplify $s_i s_j$ to

$$s_i s_j = m(s_i + s_j) - m^2 = m[(s_i + s_j) - m]$$

The Ising Model Mean-Field theory (MFT) approximation

Now we can go back to the Hamiltonian and use our approach:

$$s_i s_j = m[(s_i + s_j) - m]$$

$$H_{MF} = -Jm \sum_{\langle ij \rangle} (s_i + s_j - m) - h \sum_{i=1}^{N} s_i$$

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

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

$$H_{MF} = -Jm \sum_{\langle ij \rangle} (2s_i - m) - h \sum_{i=1}^{N} s_i$$

Moreover (nn = nearest neighbours):

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

The Ising Model Mean-Field theory (MFT) approximation

There is no explicit reference to j in the summation, then:

$$\frac{1}{2}\sum_{i=1}^{N}\sum_{j\in nn(i)} = \frac{1}{2}q\sum_{i=1}^{N}$$

where q is the number of neighbours of each spin i.

The Ising Hamiltonian simplifies to:

$$\begin{aligned}
H_{MF} &= -Jm\sum_{\langle ij\rangle}(2s_i - m) - h\sum_{i=1}^{N} s_i \\
&= -\frac{1}{2}qJm\sum_{i=1}^{N}(2s_i - m) - h\sum_{i=1}^{N} s_i \\
&= \frac{NqJm^2}{2} - (h + qJm)\sum_{i=1}^{N} s_i = \frac{NqJm^2}{2} - h_{eff}\sum_{i=1}^{N} s_i
\end{aligned}$$

The Ising Model Mean-Field theory (MFT) approximation

Note that

$$h_{eff} = h + qJm$$

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.

The Ising Model Mean-Field theory (MFT) approximation

Let us compute the partition function in the MFT

$$Z_{MF} = \mathrm{Tr}(e^{-\beta H_{MF}}) = \prod_{i=1}^{N}\left(\sum_{s_i=\pm 1}\right) e^{-\beta H_{MF}}$$

$$= \prod_{i=1}^{N}\left(\sum_{s_i=\pm 1}\right) e^{-\beta NqJm^2/2} e^{\beta h_{eff}\sum_{j=1}^{N} s_j}$$

$$= e^{-\beta NqJm^2/2}\prod_{i=1}^{N}\left(\sum_{s_i=\pm 1} e^{\beta h_{eff} s_i}\right)$$

$$= e^{-\beta NqJm^2/2}\prod_{i=1}^{N}(e^{\beta h_{eff}} + e^{-\beta h_{eff}})$$

$$= e^{-\beta NqJm^2/2}[2\cosh(\beta h_{eff})]^N$$

The Ising Model Mean-Field theory (MFT) approximation

Let us compute the order parameter m, the magnetization

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

Using the definition of the partition function:

$$m = \frac{1}{N} \sum_{i=1}^{N} \frac{\mathrm{Tr}(s_i e^{-\beta H_{MF}})}{Z_{MF}} = \frac{1}{N Z_{MF}} \sum_{i=1}^{N} (s_i e^{-\beta H_{MF}})$$

$$= \frac{1}{N\beta} \frac{1}{Z_{MF}} \frac{\partial Z_{MF}}{\partial h_{eff}} = \frac{1}{N\beta} \frac{\partial \ln Z_{MF}}{\partial h_{eff}}$$

But

$$\ln Z_{MF} = -\frac{\beta N q J m^2}{2} + N \ln 2 + N \ln[\cosh(\beta h_{eff})]$$

Then

$$\frac{\partial \ln Z_{MF}}{\partial h_{eff}} = N\beta \tanh(\beta h_{eff})$$

The Ising Model Mean-Field theory (MFT) approximation

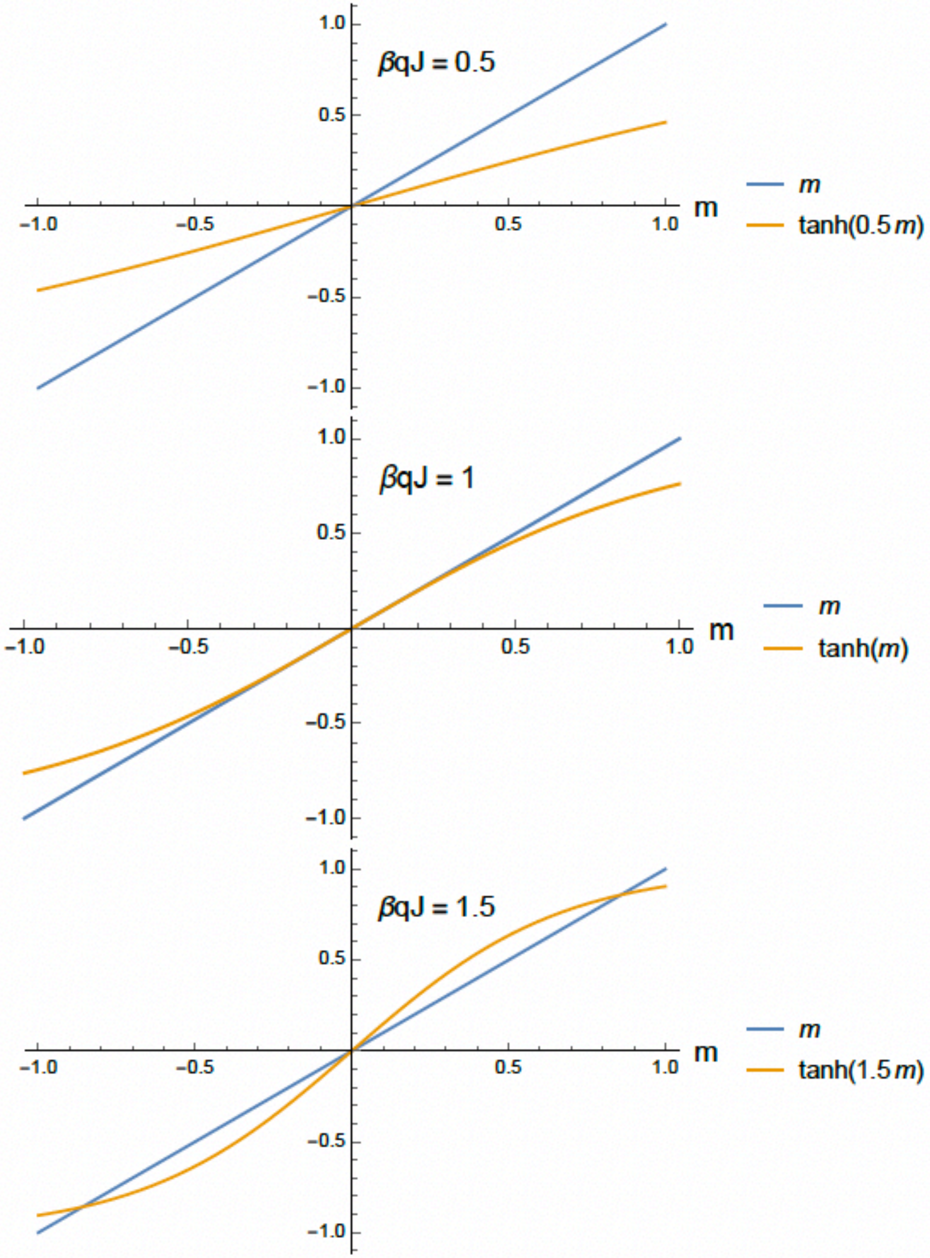
Then the order parameter m, the magnetization

$$m \equiv \frac{1}{N}\sum_{i=1}^{N}\langle s_i\rangle = \tanh(\beta h_{eff}) = \tanh[\beta(h + qJm)]$$

Note that this is a trascendental equation that cannot be solved 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 us do it, consider the case h=0.

The Ising Model Mean-Field theory (MFT) approximation



We can graphically see that the solutions are qualitatively different when $\beta qJ \leq 1$ and $\beta qJ > 1$.

- When $\beta qJ \leq 1$ there is only one solution: $m = 0$, corresponding to the *paramagnetic* state.

- When $\beta qJ > 1$, 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 spontaneously magnetises is

$$k_B T_c = qJ$$

The Ising Model Mean-Field theory (MFT) approximation

Discussion on the previous results: It should be noted that for the 1D case, MFT thus predicts a magnetic phase transition at $k_B T_c = 2J$; however, solving this system exactly we found 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 $k_B T_c = 4J$, whereas solving the system exactly we find that $k_B T_c = 2J/\ln(1+\sqrt{2}) \approx 2.27J$. Also note that **since MFT assumes fluctuations are small, it generally overestimates the system's tendency to order** and thus overestimates the value of Tc.

Computation

How do we solve for the properties of the Ising model?

(1) Solve the one-dimensional Ising model, as Ising did.
(2) Have an enormous brain. Onsager solved the two-dimensional Ising model in a bewilderingly complicated way. Nobody has solved the three-dimensional Ising model.
(3) Perform the **Monte Carlo method** on a computer.

The Monte Carlo method involves doing a kind of random walk through the space of lattice configurations. Let us just outline the heat bath Monte Carlo method:

Computation

The heat bath Monte Carlo method on a square lattice:

1. Generate a random initial spin configuration.
2. Pick a site $i = (x, y)$ at random.
3. Check how many neighbor spins are pointing up:

$$m_i = \sum_{j:\langle ij\rangle} s_j \begin{cases} 4 & \text{(4 neighbors up)}, \\ 2 & \text{(3 neighbors up)}, \\ 0 & \text{(2 neighbors up)}, \\ -2 & \text{(1 neighbor up)}, \\ -4 & \text{(0 neighbors up)}\,. \end{cases}$$

3. Calculate $E_+ = -Jm_i - h,$ and $E_- = +Jm_i + h$, which is the energy for spin i to be +1 or -1 given its current environment.
4. Set spin i up with probability: $e^{-\beta E_+}/(e^{-\beta E_+} + e^{-\beta E_-})$ and down with probability: $e^{-\beta E_-}/(e^{-\beta E_+} + e^{-\beta E_-})$.
5. Repeat.