Lecture 22

05.04.2019

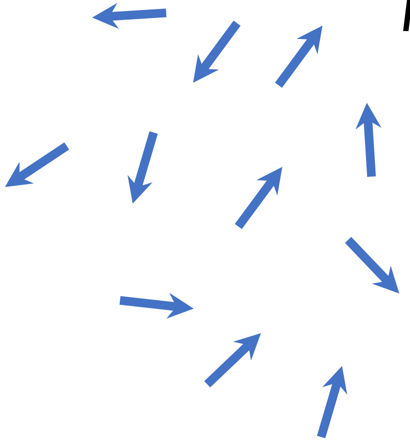
Ferromagnetic system
Ising model
1D solution

Magnetic materials

- Have a magnetic dipole moment associated with the net spin of atoms
- Spins interact with an external magnetic field or with each other
- Susceptible to change their magnetization in the presence of a magnetic field
  - ❑Paramagnetism – retain magnetization only in the presence of a magnetic field
  - ❑Ferromagnetism – have a permanent magnetization even in the absence of an applied magnetic field

Paramagnetic materials

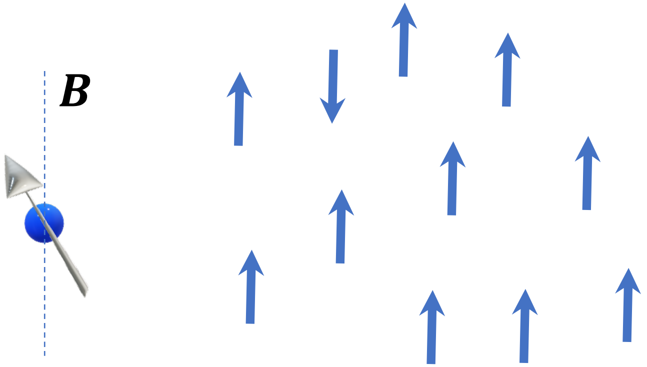
No applied magnetic field



No mean magnetization

$\langle m \rangle = 0, \forall\, T \text{ at } B = 0$

With applied magnetic field



Mean magnetization dependent On B and temperature

$$\langle m \rangle(T, B) = N\mu_B \tanh(\beta \mu_B B)$$

Susceptibility

$$\chi(B,T) = \left(\frac{\partial \langle m \rangle}{\partial B}\right)_T = \frac{1}{kT}\frac{N\mu_B^2}{\cosh^2(\beta \mu_B B)}$$

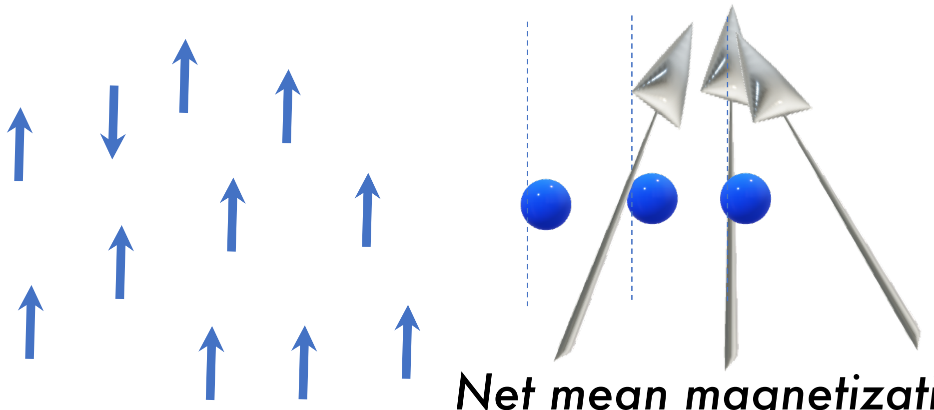
Example:

Aluminum, copper, gold

Iron bearing minerals at sufficiently big temperatures

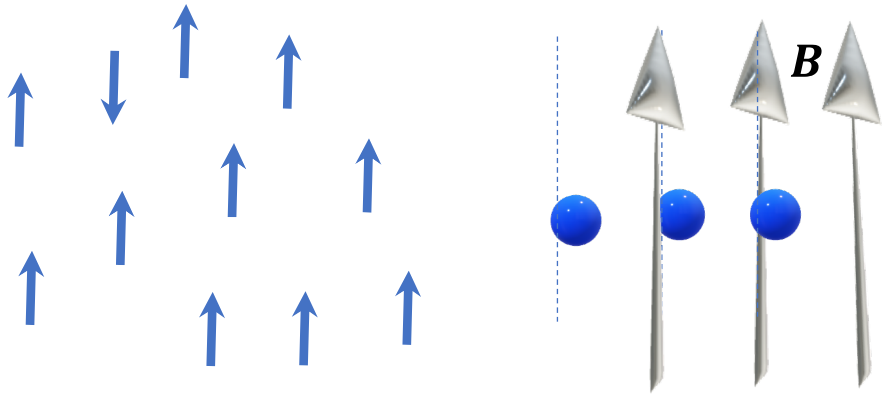
Ferromagnetic materials

No applied magnetic field



Net mean magnetization
Due to spin-spin interactions
$\langle m \rangle \neq 0, at\ B = 0\ and\ T < T_c$

With applied magnetic field



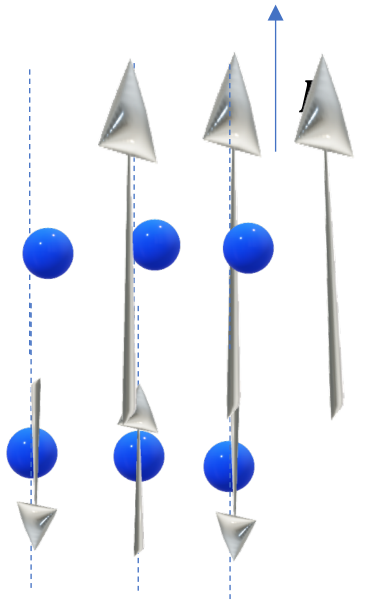
Net mean magnetization
Due to spin-spin interactions
And applied magnetic field
$\langle m \rangle \neq 0$

Example:

Iron bearing minerals at low temperatures
Nickel, magnetite, cobalt and their alloys

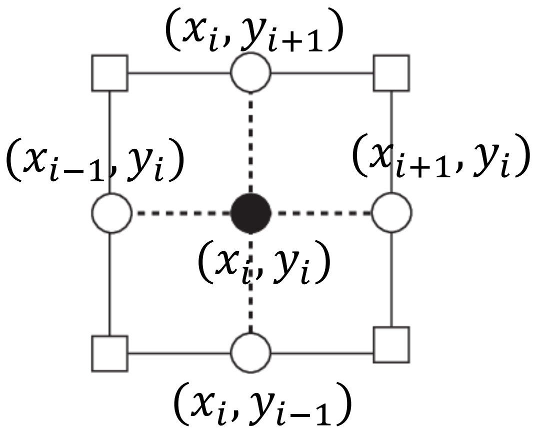
Ising model for ferromagnets

A system of N spins $s_i = \pm 1$ *on a periodic lattice and in a uniform magnetic field* B. *Spins interact with their nearest neighbor on the lattice*

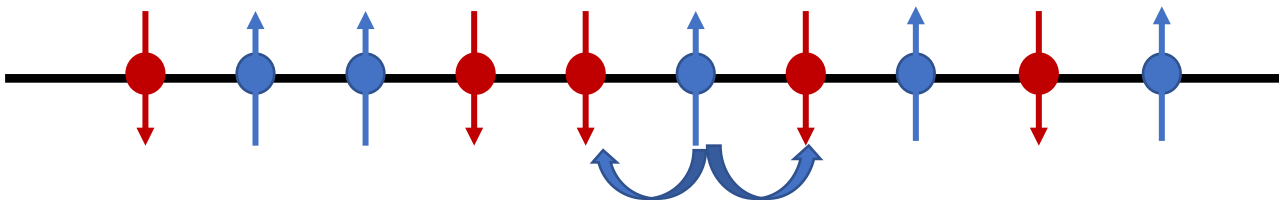


$$H_N = -J \sum_{i} \sum_{\substack{j= \\ n.n.\, of\, i}} s_i s_j - \sum_{i} s_i B \,, \qquad (\mu_B = 1)$$

- $\text{J} > 0$ is the coupling constant, such that the energy is minimized when neighboring spins point in the same direction
- Summation over the nearest neighbors (n.n.) j atoms that are coupled to the ith atom on a crystal lattice (short hand notation used sometime $\equiv \langle \text{ij} \rangle$)
- The form of the spin-spin interaction as $-J s_i s_j$ originates the Coulomb interactions between the electrons (spin carriers); magnetic dipole interactions are too weak.



Ising model in 1D



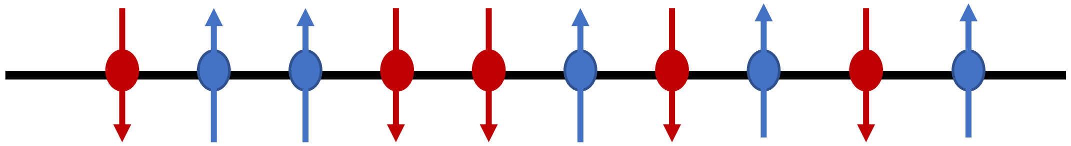
$$H_N = -J \sum_{i=0}^{N-1} s_i s_{i+1} - \sum_i s_i B \,, s_i = \pm 1$$

Periodic boundary conditions $s_N \equiv s_0$

Partition function for N spins: weighted sum over all spin configurations $\{s_i\}$

$$Z_N = \sum_{\{s_i\}} e^{-\beta H_N(\{s_i\})}$$

Ising model in 1D



$$H_N = -J\sum_{i=0}^{N-1} s_i s_{i+1} - \sum_i s_i B\,, s_i = \pm 1$$

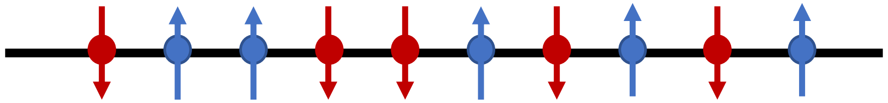
Periodic boundary conditions $s_N \equiv s_0$

Partition function for N spins

$$Z_N = \sum_{\{s_i\}} e^{-\beta H_N(\{s_i\})}$$

$$= \sum_{\{s_i\}} e^{\beta J(s_0 s_1 + s_1 s_2 \cdots + s_{N-1} s_0) + \beta B(s_0 + s_1 + \cdots + s_{N-1})}$$

Transfer matrix $T_{i,j}$



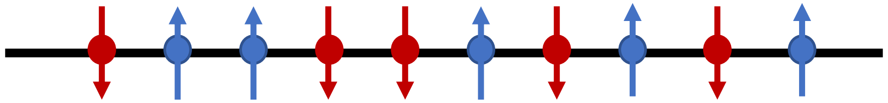
Z_N can be represented as a product of (2×2) transfer matrices $T_{i,i+1}$

Partition function for N spins

$$Z_N = \sum_{\{s_i\}} e^{\beta J(s_0 s_1 + s_1 s_2 \cdots + s_{N-1} s_0) + \beta B(s_0 + s_1 + \cdots + s_N)}$$

$$= \sum_{\{s_i\}} e^{\beta J s_0 s_1 + \beta B \frac{s_0 + s_1}{2}} \cdot e^{\beta J s_1 s_2 + \beta B \frac{s_1 + s_2}{2}} \cdots e^{\beta J s_N s_0 + \beta B \frac{s_{N-1} + s_0}{2}}$$

Transfer matrix



Partition function for N spins

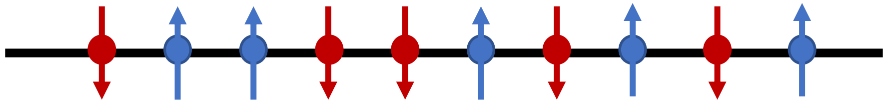
$$Z_N = \sum_{\{s_i\}} e^{\beta J s_0 s_1 + \beta B \frac{s_0 + s_1}{2}} \cdot e^{\beta J s_1 s_2 + \beta B \frac{s_1 + s_2}{2}} \cdots e^{\beta J s_{N-1} s_0 + \beta B \frac{s_{N-1} + s_0}{2}} = \sum_{\{s_i\}} T_{s_0}^{s_1} \cdot T_{s_1}^{s_2} \cdots T_{s_N}^{s_0}$$

$$T_{s_i}^{s_{i+1}} = \exp\left(\beta J s_i s_{i+1} + \beta B \frac{s_i + s_{i+1}}{2}\right), \qquad s_i = \pm 1$$

Identical transfer matrices for all spin pairs

$$\begin{array}{r c c} & s_{i+1} = 1 & s_i = -1 \\ \begin{array}{r} s_i = 1 \\ s_i = -1 \end{array} & \multicolumn{2}{c}{\begin{pmatrix} e^{\beta(J+B)} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta(J-B)} \end{pmatrix}} \end{array}$$

Trace of Transfer matrix



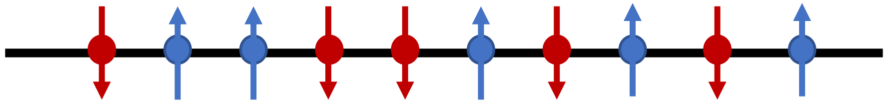
Partition function for N spins

$$Z_N = \sum_{\{s_i\}} T_{s_0}^{s_1} \cdot T_{s_1}^{s_2} \cdots T_{s_N}^{s_0} = Tr(T^N) = \lambda_1^N + \lambda_2^N,$$

Where $\lambda_{1,2}$ are the eigenvalues of the transfer matrix

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

Transfer matrix: eigenvalues



Partition function for N spins

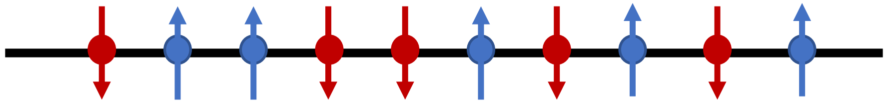
$$Z_N = \sum_{\{s_i\}} T_{s_0}^{s_1} \cdot T_{s_1}^{s_2} \cdots T_{s_N}^{s_0} = Tr(T^N) = \lambda_1^N + \lambda_2^N,$$

$\lambda_{1,2}$ *are determined as the solution of the characteristic equation*

$$\begin{Vmatrix} e^{\beta(J+B)} - \lambda & e^{-\beta J} \\ e^{-\beta J} & e^{\beta(J-B)} - \lambda \end{Vmatrix} = 0 \rightarrow$$

$$\left(e^{\beta(J+B)} - \lambda\right)\left(e^{\beta(J-B)} - \lambda\right) - e^{-2\beta J} = 0$$

Transfer matrix: eigenvalues



$\lambda_{1,2}$ are determined as the solution of the characteristic equation

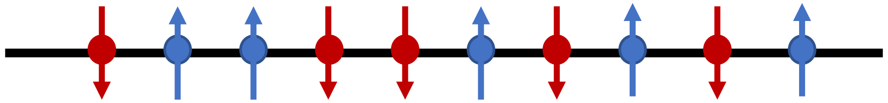
$$\lambda^2 - 2\lambda e^{\beta J}\cosh(\beta B) + 2\sinh(2\beta J) = 0$$

With the solution

$$\lambda_{1,2} = e^{\beta J}\cosh(\beta B) \pm \sqrt{e^{2\beta J}\cosh^2(\beta B) - 2\, sinh(2\beta J)}$$

$$\lambda_{1,2} = e^{\beta J}\cosh(\beta B) \pm \sqrt{e^{2\beta J}\sinh^2(\beta B) + e^{-2\beta J}}$$

Solution for $J = 0$ *and* $B \neq 0$ *(Paramagnetic limit)*



$$Z_N = Tr(T^N) = \lambda_1^N + \lambda_2^N,$$

- $\lambda_1 = 2\cosh(\beta B), \;\; \lambda_2 = 0$

$$Z_N = 2^N \cosh^N(\beta B) \rightarrow G_N(T, B) = -NkT \ln[2\cosh(\beta B)]$$

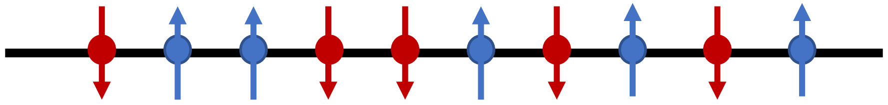
Paramagnetic mean magnetization

$$M = -\left(\frac{\partial G}{\partial B}\right)_T = N \tanh(\beta B)$$

Paramagnetic susceptibility

$$\chi = \left(\frac{\partial M}{\partial B}\right)_T = N\beta \frac{1}{\cosh^2(\beta B)} \sim \frac{1}{T}$$

Solution for $J \neq 0$ and $B = 0$



$$Z_N = Tr(T^N) = \lambda_1^N + \lambda_2^N,$$

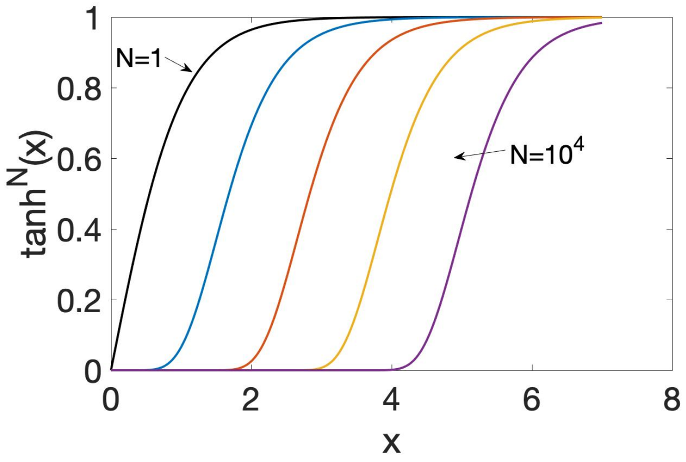
$$\lambda_{1,2} = e^{\beta J}\cosh(\beta B) \pm \sqrt{e^{2\beta J}\sinh^2(\beta B) + e^{-2\beta J}}$$

- $B = 0 \rightarrow$ $\quad \lambda_1 = 2\cosh(\beta J),\ \ \lambda_2 = 2\sinh(\beta J)$

$$Z_N = 2^N \cosh^N(\beta J)(1 + \tanh^N(\beta J))$$

$$\lim_{N\rightarrow\infty} \tanh^N(x) = 0$$

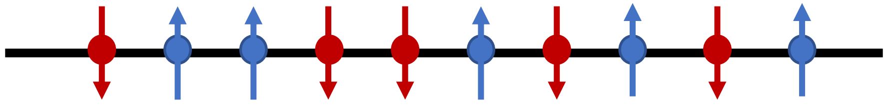
Z_N *is dominated by the largest eigenvalue* $\lambda_{1,2}^N$



$$Z_N \approx 2^N \cosh^N(\beta J)$$

$$G_N(T) = -NkT\ln[2\cosh(\beta J)]$$

Solution for $J \neq 0$ *and* $B = 0$



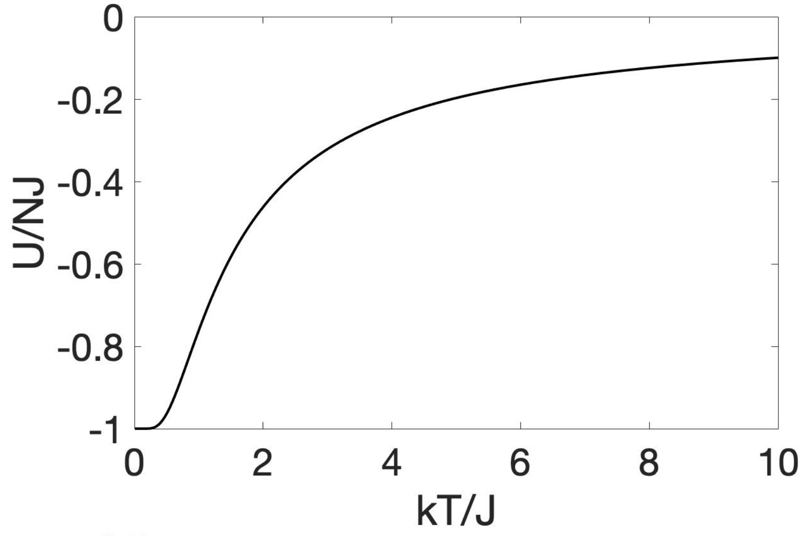
$$Z_N \approx 2^N \cosh^N(\beta J)$$

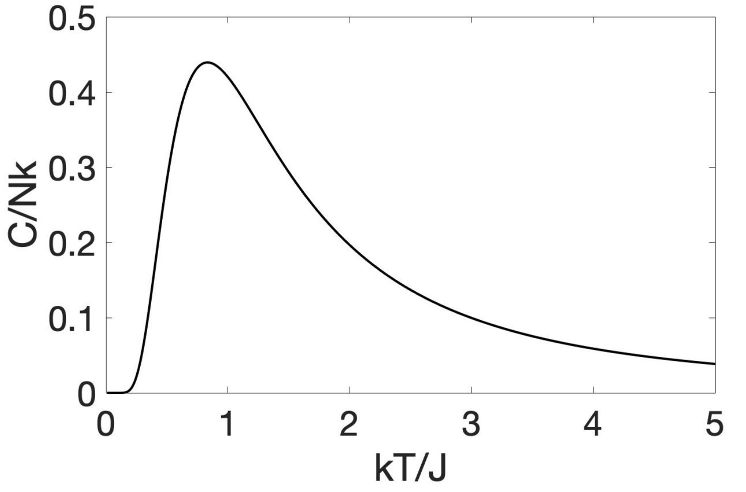
Internal energy

$$U(T,N) = -\frac{\partial \ln(Z_N)}{\partial \beta} = -JN\tanh(\beta J)$$

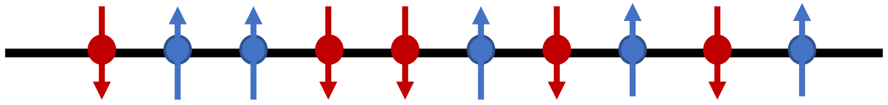
Heat capacity

$$C(T) = \left(\frac{\partial U}{\partial T}\right)_N = Nk\left(\frac{J\beta}{\cosh(\beta J)}\right)^2$$





Solution for $B \neq 0$



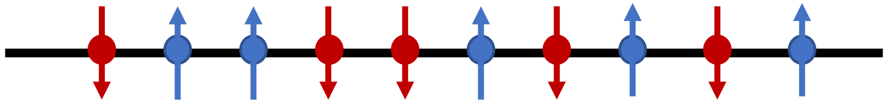
Z_N is determined by the largest eigenvalue, i.e. λ_1^N

$$Z_N = \lambda_1^N \left[1 + \left(\frac{\lambda_2}{\lambda_1}\right)^N\right] = \left[e^{\beta J}\cosh(\beta B) + \sqrt{e^{2\beta J}\sinh^2(\beta B) + e^{-2\beta J}}\right]^N$$

Gibbs free energy

$$G_N(T,B) = -NkT\ln\left[e^{\beta J}\cosh(\beta B) + \sqrt{e^{2\beta J}\sinh^2(\beta B) + e^{-2\beta J}}\right]$$

Mean magnetization $B \neq 0$

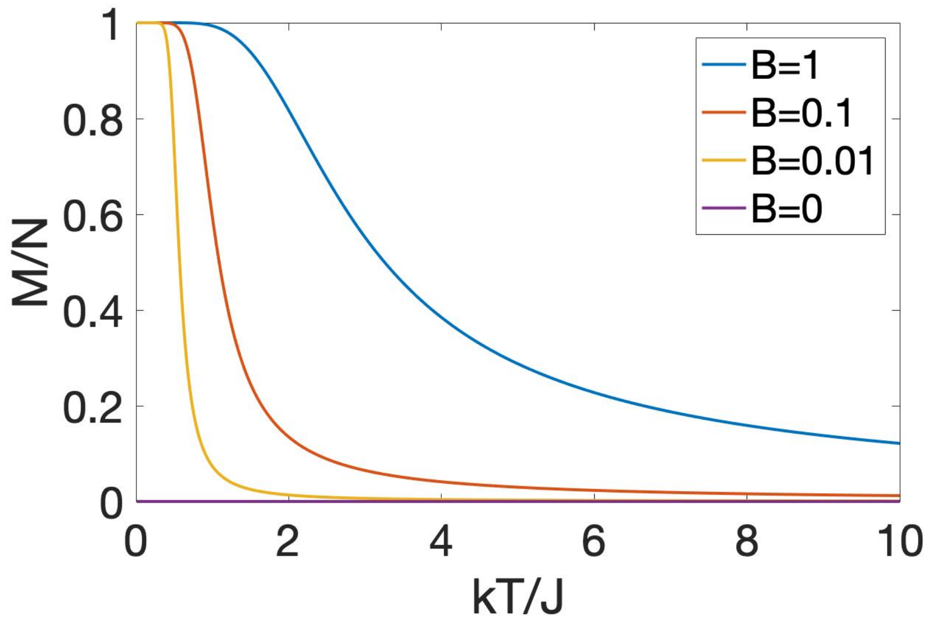


$$G_N(T,B) = -NkT\, ln\left[e^{\beta J}\cosh(\beta B) + \sqrt{e^{2\beta J}\sinh^2(\beta B) + e^{-2\beta J}}\right]$$

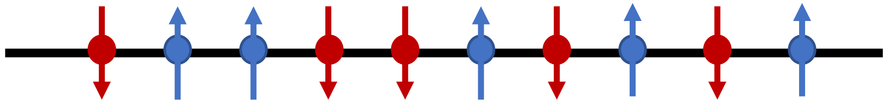
Mean magnetization

$$M(T,B) = -\left(\frac{\partial G_N(T,B)}{\partial B}\right)_T$$

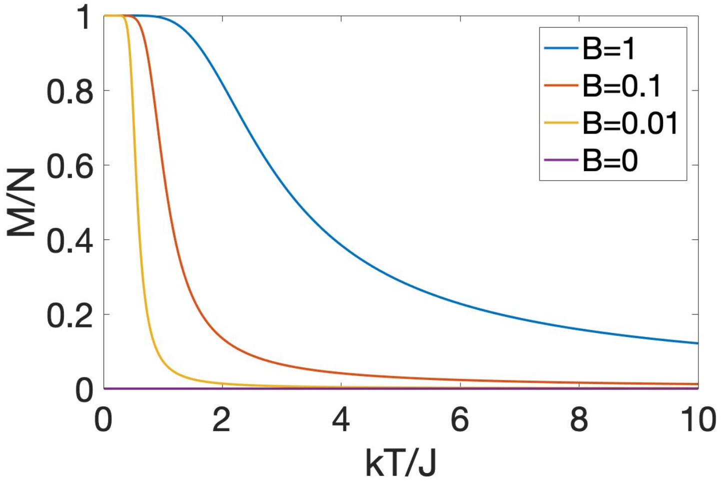
$$M = N\frac{\sinh(\beta B)}{\sqrt{\sinh^2(\beta B) + \exp(-4\beta J)}}$$



Mean magnetization $B \to 0$



$$\frac{M}{N} = \frac{\sinh(\beta B)}{\sqrt{\sinh^2(\beta B) + \exp(-4\beta J)}}$$

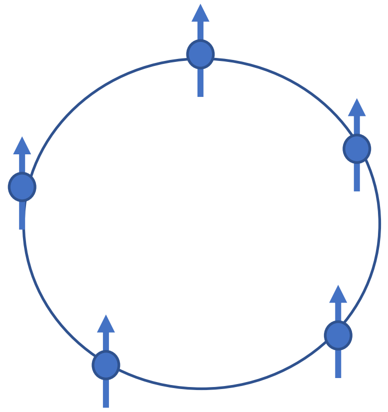


In the limit of B $\to 0$, $\langle s \rangle \to 0$ at every temperature:

- Nearest neighbor spin-spin interaction in 1D can not create spin order at any finite temperature

- Any themal fluctuation destroys the net magnetization

1D Ising model: No phase transition



At any nonzero temperature, it is energetically favorable to create defects (kinks) due to thermal fluctuations

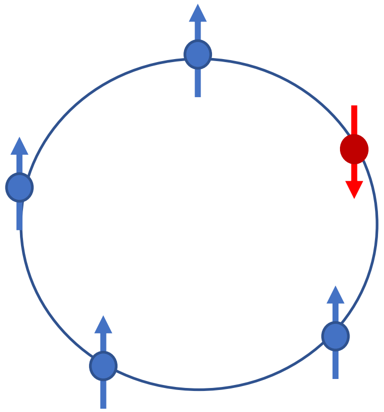
Change in energy for flipping a spin (kink in the ordered state)

$$U_0 = -NJ\ (order), \qquad U_1 = -(N-2)J + 2J\ (with\ a\ kink) \rightarrow \Delta U = 4J$$

Change in entropy for flipping a spin anywhere in the 1D chain (N sites)

$$\Delta S = k \log N$$

The spin flipping due to thermal fluctuations is favored when it lowers the **Helmholtz free energy**



$$\Delta F = \Delta U - T\Delta S < 0 \rightarrow J - kT \log N < 0$$

This is always satisfied at any $\mathrm{T} > 0$, hence the spin order is spontaneously broken by kinks due thermal fluctuations.