Ising Model

Ferromagnetism: Below some characteristic temperature, T_c, a finite fraction of spins in some solids get spontaneously polarized in some direction, resulting in a macroscopic magnetic field.
T_c = Curie temperature.

Ising model: Defined on a d-dimensional periodic lattice.
Each site has a spin variable that takes values ± 1.
Can be solved exactly in one and two dimensions.

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

Ground states (T=0):

① $J=0,\ h>0 \Rightarrow s_i = +1 \ \forall i$

Ferromagnet ② $J>0,\ h=0 \Rightarrow s_i = +1 \ \forall i$ or $s_i = -1 \ \forall i$

③ $J>0,\ h\neq 0 \Rightarrow s_i = \text{sign}(h) \ \forall i$

Antiferromagnet ④ $J<0,\ h=0 \Rightarrow$ Neighboring spins are in opposite state. "Neel state"

Excited states (T>0):

Partition function, $$Z = \text{Tr}\, e^{-\beta H} = \sum_{s_1}\sum_{s_2}\cdots\sum_{s_N} e^{-\beta H(\{s_i\})}$$

If we are able to calculate the partition function, then we can calculate some thermodynamic quantities using it.

① Helmholtz free energy, $F = -k_B T \ln Z$

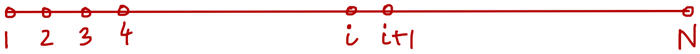
② Internal energy, $U = \langle H \rangle = \dfrac{\text{Tr}\, H e^{-\beta H}}{\text{Tr}\, e^{-\beta H}} = -\dfrac{\partial}{\partial \beta}\ln Z = \dfrac{\partial}{\partial\beta}(\beta F)$

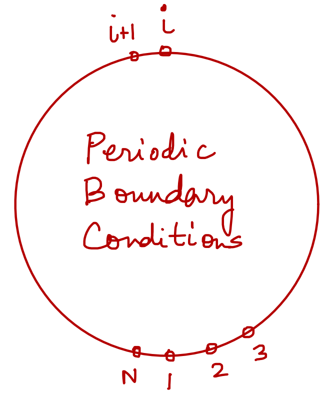
③ Heat capacity, $C = \dfrac{\partial U}{\partial T}$

④ Magnetization, $M = \left\langle \sum_{i=1}^{N} s_i \right\rangle = \dfrac{\text{Tr}\left[\left(\sum_{i=1}^{N} s_i\right) e^{-\beta H}\right]}{Z}$

$$= \frac{1}{\beta}\frac{\partial}{\partial h}\ln Z = -\frac{\partial F}{\partial h}$$

One dimensional Ising model





Periodic boundary conditions: $N+i \equiv i$

$$H = -J\sum_i s_i s_{i+1} - h\sum_i s_i$$

$$= -J\sum_i s_i s_{i+1} - \frac{h}{2}\sum_i (s_i + s_{i+1})$$

$$Z = \mathrm{Tr}\, e^{-\beta H} = \sum_{s_1}\sum_{s_2}\cdots\sum_{s_N} \exp\left[\beta \sum_{i=1}^{N}\left(J s_i s_{i+1} + \frac{h}{2}(s_i + s_{i+1})\right)\right]$$

$$= \sum_{s_1}\sum_{s_2}\cdots\sum_{s_N}\prod_{i=1}^{N} \exp\left[\beta\left(J s_i s_{i+1} + \frac{h}{2}(s_i+s_{i+1})\right)\right]$$

$$= \sum_{s_1}\sum_{s_2}\cdots\sum_{s_N}\prod_{i=1}^{N} \langle s_i | T | s_{i+1}\rangle$$

T is known as the transfer matrix

$$\langle s|T|s'\rangle = \exp\left[\beta\left(J s s' + \frac{h}{2}(s+s')\right)\right]$$

$$Z = \sum_{s_1}\sum_{s_2}\cdots\sum_{s_N} \langle s_1|T|s_2\rangle\langle s_2|T|s_3\rangle\langle s_3|T|s_4\rangle\cdots\langle s_N|T|s_1\rangle$$

$$\because \sum_s |s\rangle\langle s| = \mathbb{1}, \qquad Z = \sum_{s_1}\langle s_1|T^N|s_1\rangle = \mathrm{Tr}\, T^N$$

Matrix elements of T:

$$\left.\begin{aligned} \langle +|T|+\rangle &= e^{\beta(J+h)} \\ \langle -|T|-\rangle &= e^{\beta(J-h)} \\ \langle +|T|-\rangle &= \langle -|T|+\rangle = e^{-\beta J} \end{aligned}\right\} \quad T = \begin{pmatrix} e^{\beta(J+h)} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta(J-h)} \end{pmatrix}$$

Eigenvalues of T:

$$\begin{vmatrix} e^{\beta(J+h)} - \lambda & e^{-\beta J} \\ e^{-\beta J} & e^{\beta(J-h)} - \lambda \end{vmatrix} = 0$$

$$\Rightarrow e^{2\beta J} - \lambda e^{\beta(J+h)} - \lambda e^{\beta(J-h)} + \lambda^2 + e^{-2\beta J} = 0$$

$$\Rightarrow \quad \lambda^2 - 2e^{\beta J}\cosh\beta h\,\lambda + e^{2\beta J} - e^{-2\beta J} = 0$$

$$\Rightarrow \quad \lambda = e^{\beta J}\cosh\beta h \pm \sqrt{e^{2\beta J}\cosh^2\beta h - e^{2\beta J} + e^{-2\beta J}}$$

$$= e^{\beta J}\left[\cosh\beta h \pm \sqrt{\sinh^2\beta h + e^{-4\beta J}}\right] \equiv \lambda_\pm$$

$$\Rightarrow \quad Z = \mathrm{Tr}\, T^N = \lambda_+^N + \lambda_-^N \sim \lambda_+^N \quad \text{as } N \to \infty$$

The Helmholtz free energy per site is,

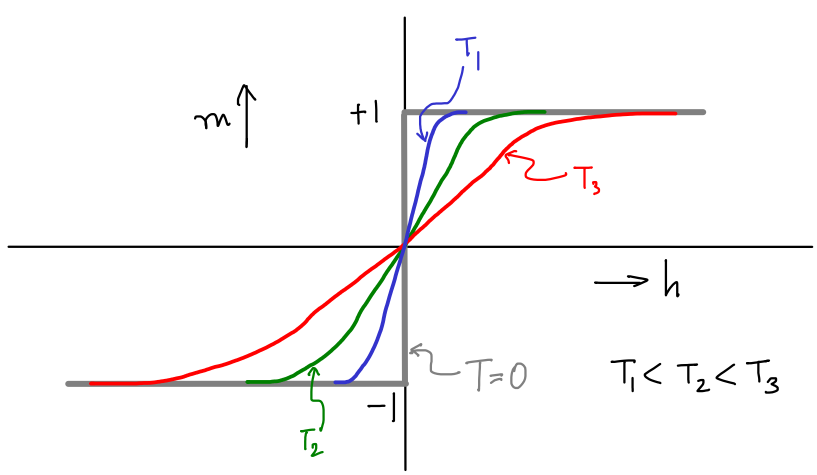
$$f = -\frac{1}{N}k_BT\ln Z \sim -k_BT\ln\lambda_+$$

$$= -J - k_BT\ln\left[\cosh\beta h + \sqrt{\sinh^2\beta h + e^{-4\beta J}}\right].$$

$\Rightarrow$ Magnetization per site,

$$m = -\frac{\partial f}{\partial h} = k_BT\,\frac{\beta\sinh\beta h + \dfrac{2\beta\sinh\beta h\cosh\beta h}{2\sqrt{\sinh^2\beta h + e^{-4\beta J}}}}{\cosh\beta h + \sqrt{\sinh^2\beta h + e^{-4\beta J}}}$$

$$= \frac{\sin\beta h}{\sqrt{\sinh^2\beta h + e^{-4\beta J}}}$$



Magnetization calculation using the transfer matrix

Let us focus on the $h=0$ case.

$$H = -J\sum_i s_i s_{i+1}\ ,\quad T = \begin{pmatrix} e^{\beta J} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta J} \end{pmatrix} \quad \text{and} \quad \lambda_+ = 2\cosh\beta J\ ,\ \lambda_- = 2\sinh\beta J$$

Eigenvectors of T:

$$T\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \lambda_\pm \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$$

For λ_+,

$$\left.\begin{aligned} & e^{\beta J}x_1 + e^{-\beta J}x_2 = 2\cosh\beta J\, x_1 \\ \Rightarrow\quad & e^{-\beta J}x_2 = e^{-\beta J}x_1 \\ \Rightarrow\quad & x_1 = x_2 \end{aligned}\right\} \text{eigenvector} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

For λ_-,

$$\left.\begin{aligned} & e^{\beta J}x_1 + e^{-\beta J}x_2 = 2\sinh\beta J\, x_1 \\ \Rightarrow\quad & e^{-\beta J}x_2 = -e^{-\beta J}x_1 \\ \Rightarrow\quad & x_1 = -x_2 \end{aligned}\right\} \text{eigenvector} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

$\Rightarrow$ If $S = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$, then $S^{-1}TS = \Lambda = \begin{pmatrix} \lambda_+ & 0 \\ 0 & \lambda_- \end{pmatrix}$

The magnetization per site,

$$m = \langle s_i \rangle = \frac{1}{Z}\sum_{s_1}\cdots\sum_{s_N} s_i\, e^{\beta\sum_{i=1}^{N}\left(Js_is_{i+1} + \frac{h}{2}(s_i + s_{i+1})\right)}$$

$$\Rightarrow\quad m = \frac{1}{Z}\sum_{s_1}\sum_{s_2}\cdots\sum_{s_N}\langle s_1|T|s_2\rangle\langle s_2|T|s_3\rangle\cdots\langle s_{i-1}|T|s_i\rangle s_i\langle s_i|T|s_{i+1}\rangle\cdots$$
$$\cdots\langle s_N|T|s_1\rangle$$

$$= \frac{1}{Z}\sum_{s_1}\sum_{s_i}\langle s_1|T^{i-1}|s_i\rangle s_i\langle s_i|T^{N-i+1}|s_1\rangle$$

Now,

$$\sum_{s_i}|s_i\rangle s_i\langle s_i| = |+\rangle\langle +| - |-\rangle\langle -| = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \sigma_z \quad \text{(the third Pauli matrix)}$$

$$\Rightarrow\quad m = \frac{1}{Z}\operatorname{Tr} T^{i-1}\sigma_z T^{N-i+1} = \frac{1}{Z}\operatorname{Tr} T^N\sigma_z$$
$$= \frac{1}{Z}\operatorname{Tr}\left(SS^{-1}TSS^{-1}TSS^{-1}\cdots S^{-1}TSS^{-1}\sigma_z\right)$$

$$= \frac{1}{Z} \mathrm{Tr}\left(S \Lambda^N S^{-1} \sigma_z \right) \quad , \quad \text{where } \Lambda = \begin{pmatrix} \lambda_+ & 0 \\ 0 & \lambda_- \end{pmatrix}$$

$$= \frac{1}{Z} \mathrm{Tr}\left(\Lambda^N S^{-1} \sigma_z S \right)$$

$$S^{-1} \sigma_z S = \frac{1}{2} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$\Rightarrow \quad m = \frac{1}{Z} \mathrm{Tr}\left(\begin{pmatrix} \lambda_+^N & 0 \\ 0 & \lambda_-^N \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \right) = \frac{1}{Z} \mathrm{Tr} \begin{pmatrix} 0 & \lambda_+^N \\ \lambda_-^N & 0 \end{pmatrix} = 0 \quad \text{(as expected)}$$