BHARATHIDASAN UNIVERSITY

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Programme: M.Sc., Physics

Course Title : Thermodynamics and Statistical Physics
Course Code : 22PH202

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UNIT - V

PHASE TRANSITIONS

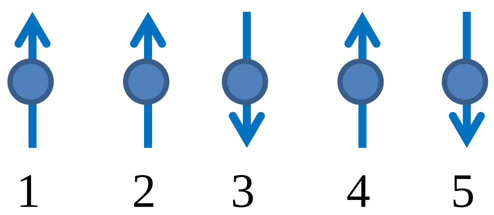
One dimensional Ising Model

Aim:

To obtain exact solution of the one-dimensional Ising Model.

Hamiltonian of the Ising Model:

- The Ising model is a discrete mathematical description of particles, where the particle's magnetic moment is independent and fixed to lattice configuration of a finite number of sites.
- Let us restrict the magnetic moment for all particles to the same direction and allow they be parallel or antiparallel.



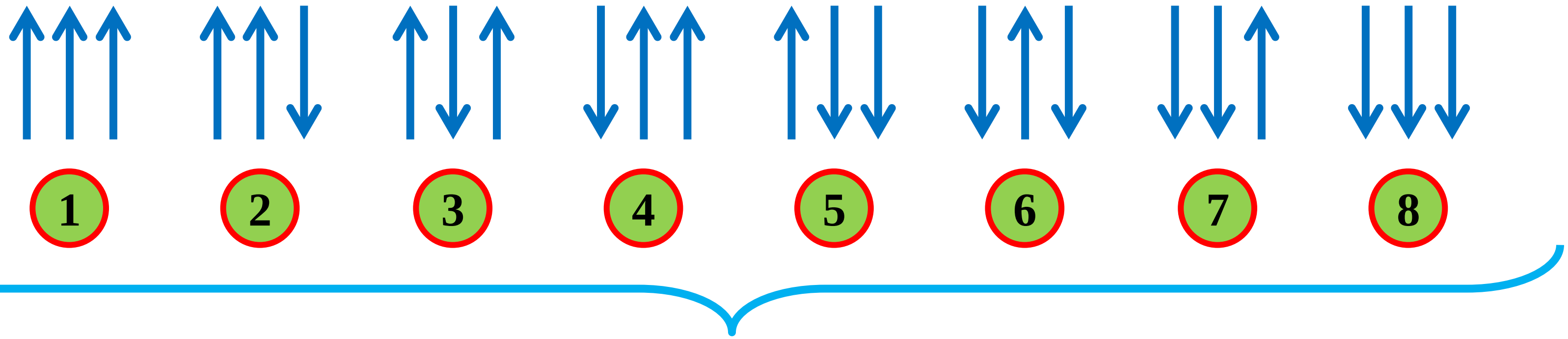
- Let the total number of sites to be N, labelled $i = \{1, 2, 3, \dots\}$ and to each site assign a spin variable $\sigma_i = \pm 1$ indicating "upwards" $(+1)$ or "downwards" (-1) magnetic moment.
- Each spin configuration corresponds to one microstate where then the Hamiltonian of the system depends on the total spin configuration.
- The spin configuration σ is the set of the direction for the spins for all sites

$$\sigma = \{\sigma_1, \sigma_2, \dots \sigma_N\} \qquad (1)$$

Then we have in total 2^N number of possible spin configurations.

Demo : N = 3

We have $2^3 = 8$ configurations (microstates)



No. of microstates or No. of configurations

The Hamiltonian is assumed to be

Energy contribution from intermolecular interaction between sites

Energy contribution from spin interaction with the external field (in the presence of magnetic field)

$$E(\sigma) = E_0(\sigma) + E_1(\sigma) \qquad (2)$$

Symmetry:

Flipping the direction of all magnetic moments should not affect intermolecular energy, that is $E_0(\sigma) = E_0(-\sigma)$ (3)

- In the Ising model the spin at every site is either up $(+1)$ or down (-1). We assume the interaction is between nearest neighbours only.

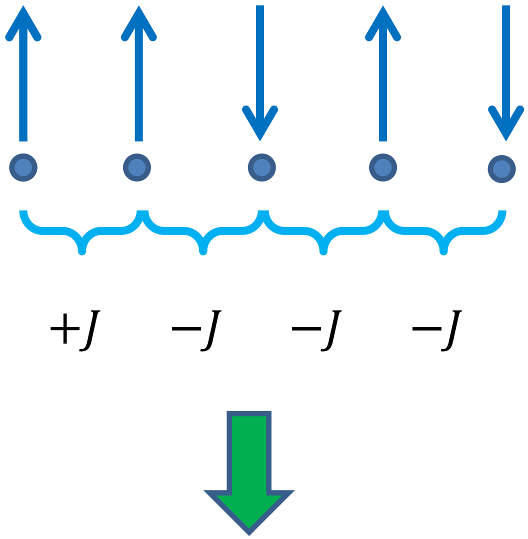
- If the spins are parallel let us assign an interaction energy $+J$ and if they are antiparallel let us assign an interaction energy $-J$.

Then

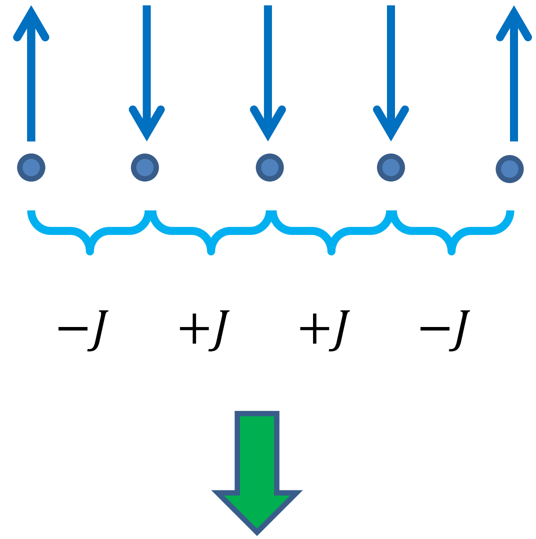
Interactions constant ($J > 0$)

$$E_0(\sigma) = -J \sum_{j=1}^{N} \sigma_i \sigma_{j+1} \qquad (4)$$

Nearest Neighbour Ising model



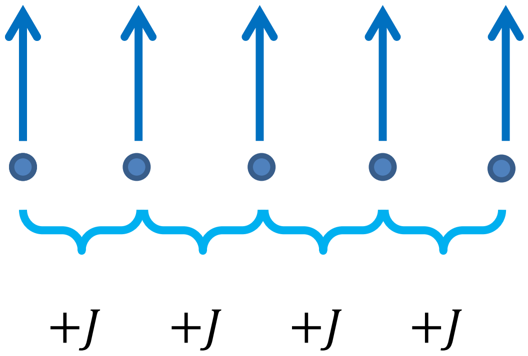
Net Energy contribution



No Energy contribution

Lowest Energy State:

- All spins are aligned in the same direction.
- In that case it is a ferromagnetic model.



Particle interaction with the field is

$$E_1(\sigma) = -H\sum_{j=1}^{N}\sigma_j$$

Relation between the direction of field and the magnetic moment

∴ The total energy is

Energy comes out from nearest neighbouring spins

Energy comes out due to external field

$$E(\sigma) = E_0(\sigma) + E_1(\sigma) = -J\sum_{j=1}^{N}\sigma_i\sigma_{j+1} - H\sum_{j=1}^{N}\sigma_j$$

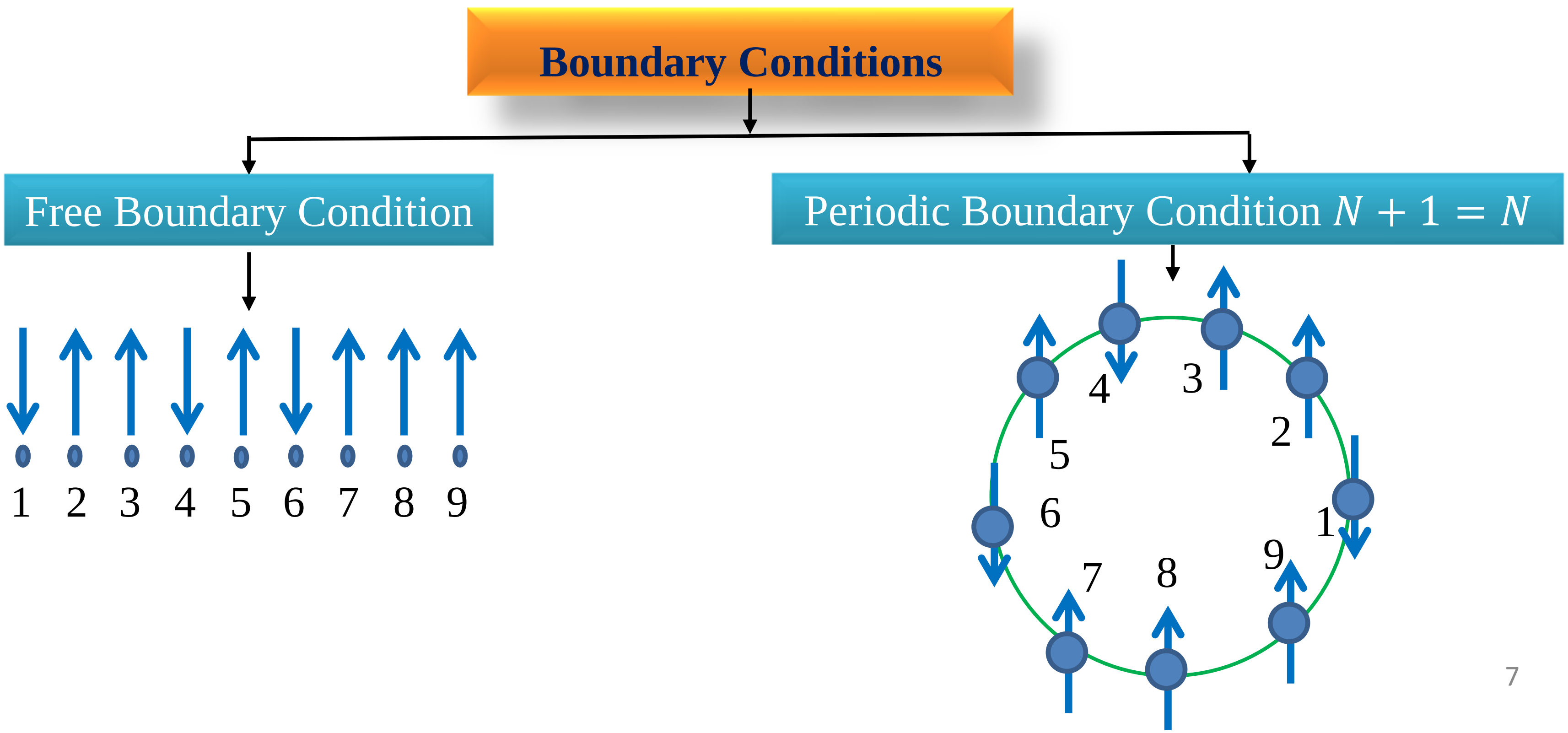
The Partition function

- The number of spins is fixed.
- We will choose *canonical ensemble* and evaluate the partition function.
- The spins are interacting. So the relation

Total partition function ← $Z_N \neq Z_1^N$ → Single partition function

Enumeration of microstates:

- We have 2^N possible number of microstates.
- Let us calculate Z_N for small N and generalize our result.
- For a finite chain, we need to specify the boundary conditions.



We know

$$Z_N = \sum_{\sigma} e^{-\beta E(\sigma)} \quad = \sum_{\sigma} e^{-\beta\left[-J\sum_{j=1}^{N}\sigma_i\sigma_{j+1} - H\sum_{j=1}^{N}\sigma_j\right]}$$

$$= \sum_{\sigma} e^{l\sum_{j=1}^{N}\sigma_i\sigma_{j+1} + h\sum_{j=1}^{N}\sigma_j}$$

$$l = \beta J$$

h= βH

Technique :

Let us evaluate the partition function Z_N.

$$Z_N = \sum_{\sigma} e^{l(\sigma_1\sigma_2+\sigma_2\sigma_3+\sigma_3\sigma_4+\cdots)+h(\sigma_1+\sigma_2+\sigma_3+\sigma_4+\cdots)}$$

Let us split the second expression as

$$Z_N = \sum_{\sigma} e^{l(\sigma_1\sigma_2+\sigma_2\sigma_3+\sigma_3\sigma_4+\cdots)+\frac{h}{2}\sigma_1+\frac{h}{2}\sigma_1+\frac{h}{2}\sigma_2+\frac{h}{2}\sigma_2+\cdots}$$

$$Z_N = \sum_{\sigma} e^{\left[l\sigma_1\sigma_2+\frac{h}{2}(\sigma_1+\sigma_2)\right]+\left[l\sigma_2\sigma_3+\frac{h}{2}(\sigma_2+\sigma_3)\right]+\cdots+\left[l\sigma_N\sigma_1+\frac{h}{2}(\sigma_N+\sigma_1)\right]}$$

Demo with five terms:

Periodic Boundary Condition

$$Z_N = \sum_{\sigma} e^{l\sum_{j=1}^{5}\sigma_i\sigma_{j+1} + h\sum_{j=1}^{5}\sigma_j}$$

$$= \sum_{\sigma} e^{l(\sigma_1\sigma_2+\sigma_2\sigma_3+\sigma_3\sigma_4+\sigma_4\sigma_5+\sigma_5\sigma_1)+h(\sigma_1+\sigma_2+\sigma_3+\sigma_4+\sigma_5)}$$

1 5 1 2 2 3 3 4 4 5

$$= \sum_{\sigma} e^{l(\sigma_1\sigma_2+\sigma_2\sigma_3+\sigma_3\sigma_4+\sigma_4\sigma_5+\sigma_5\sigma_1)+\frac{h}{2}\sigma_1+\frac{h}{2}\sigma_1+\frac{h}{2}\sigma_2+\frac{h}{2}\sigma_2+\frac{h}{2}\sigma_3+\frac{h}{2}\sigma_3+\frac{h}{2}\sigma_4+\frac{h}{2}\sigma_4+\frac{h}{2}\sigma_5+\frac{h}{2}\sigma_5}$$

$$= \sum_{\sigma} e^{\left[l\sigma_1\sigma_2+\frac{h}{2}(\sigma_1+\sigma_2)\right]+\left[l\sigma_2\sigma_3+\frac{h}{2}(\sigma_2+\sigma_3)\right]+\left[l\sigma_3\sigma_4+\frac{h}{2}(\sigma_3+\sigma_4)\right]+\left[l\sigma_4\sigma_5+\frac{h}{2}(\sigma_4+\sigma_5)\right]+\left[l\sigma_5\sigma_1+\frac{h}{2}(\sigma_5+\sigma_1)\right]}$$

$$= \sum_{\sigma} e^{l\sigma_1\sigma_2+\frac{h}{2}(\sigma_1+\sigma_2)} \times e^{l\sigma_2\sigma_3+\frac{h}{2}(\sigma_2+\sigma_3)} \times e^{l\sigma_3\sigma_4+\frac{h}{2}(\sigma_3+\sigma_4)} \times e^{l\sigma_4\sigma_5+\frac{h}{2}(\sigma_4+\sigma_5)} \times e^{l\sigma_5\sigma_1+\frac{h}{2}(\sigma_5+\sigma_1)}$$

Note : The periodic boundary condition implies that each spin is equivalent.

$$Z_N = \sum_{\sigma_1}\sum_{\sigma_2}\sum_{\sigma_3}\sum_{\sigma_4}\sum_{\sigma_5} T(\sigma_1,\sigma_2)T(\sigma_2,\sigma_3)T(\sigma_3,\sigma_4)T(\sigma_4,\sigma_5)T(\sigma_5,\sigma_1)$$

with $T(\sigma_i,\sigma_{i+1}) = e^{l\sigma_i\sigma_{i+1}+\frac{h}{2}(\sigma_i+\sigma_{i+1})}$

Possible spin state of each spin variable

$\sigma_1 = +1, \sigma_1 = -1$

Determination of $T(\sigma_i, \sigma_{i+1})$:

Let us have a look on $T(\sigma_i, \sigma_{i+1})$

$$T(\sigma_i, \sigma_{i+1}) = e^{l\sigma_i\sigma_{i+1}+\frac{h}{2}(\sigma_i+\sigma_{i+1})}$$

- σ_i can take two values $(+,-)$
- σ_{i+1} can take two values $(+,-)$

Hence to sum over we have to consider all microstates. That is

$$\mathrm{T}(+,+), \mathrm{T}(+,-), \mathrm{T}(-,+) \; and \; \mathrm{T}(-,-)$$

Let us write in matrix form

$$T(\sigma_i, \sigma_{i+1}) = \begin{pmatrix} \mathrm{T}(+,+) & \mathrm{T}(+,-) \\ \mathrm{T}(-,+) & \mathrm{T}(-,-) \end{pmatrix} = \begin{pmatrix} e^{l+h} & e^{-l} \\ e^{-l} & e^{l-h} \end{pmatrix}$$

Evaluation of Products : $T(\sigma_1, \sigma_2) \times T(\sigma_2, \sigma_3)$

Hence

$$T(\sigma_1, \sigma_2)T(\sigma_2, \sigma_3) = \begin{pmatrix} T_{++} & T_{+-} \\ T_{-+} & T_{--} \end{pmatrix} \times \begin{pmatrix} T_{++} & T_{+-} \\ T_{-+} & T_{--} \end{pmatrix}$$

$$= \begin{pmatrix} T_{++}T_{++} + T_{+-}T_{-+} & T_{++}T_{+-} + T_{+-}T_{--} \\ T_{-+}T_{++} + T_{--}T_{-+} & T_{-+}T_{+-} + T_{--}T_{--} \end{pmatrix} \qquad (A)$$

In matrix multiplication, we already know

$$(AB)_{ik} = \sum_j A_{ij}B_{jk}$$

$$T(\sigma_1,\sigma_2)T(\sigma_2,\sigma_3) = \begin{pmatrix} T_{++}T_{++} + T_{+-}T_{-+} & T_{++}T_{+-} + T_{+-}T_{--} \\ T_{-+}T_{++} + T_{--}T_{-+} & T_{-+}T_{+-} + T_{--}T_{--} \end{pmatrix} \qquad (A)$$

***Demo:* $i, j, k = 1, 2$:**

Then

$$(AB)_{ik} = \sum_{j=1}^{2} A_{ij}B_{jk} = A_{i1}B_{1k} + A_{i2}B_{2k}$$

$i = 1, k = 1 \rightarrow \quad (AB)_{11} = A_{11}B_{11} + A_{12}B_{21}$

$i = 1, k = 2 \rightarrow \quad (AB)_{12} = A_{11}B_{12} + A_{12}B_{22}$

$i = 2, k = 1 \rightarrow \quad (AB)_{21} = A_{21}B_{11} + A_{22}B_{21}$

$i = 2, k = 2 \rightarrow \quad (AB)_{22} = A_{21}B_{12} + A_{22}B_{22}$

$$\begin{pmatrix} (AB)_{11} & (AB)_{12} \\ (AB)_{21} & (AB)_{22} \end{pmatrix} = \begin{pmatrix} A_{11}B_{11} + A_{12}B_{21} & A_{11}B_{12} + A_{12}B_{22} \\ A_{21}B_{11} + A_{22}B_{21} & A_{21}B_{12} + A_{22}B_{22} \end{pmatrix} \qquad (B)$$

By considering $1 = +ve$ and $2 = -ve$, we identify $(A) = (B)$.

∴ Using matrix multiplication property,

$$(AB)_{ik} = \sum_{j} A_{ij}B_{jk}$$

$A = T, B = T$ ⬇ $i = \sigma_1, j = \sigma_2, k = \sigma_3$

$$(T^2)_{\sigma_1\sigma_3} = \sum_{\sigma_2} T_{\sigma_1\sigma_2}T_{\sigma_2\sigma_3}$$

$$(T^2)_{\sigma_1\sigma_3} = \sum_{\sigma_2} T_{\sigma_1\sigma_2} T_{\sigma_2\sigma_3}$$

Recall **:** We are evaluating

$$\sum_{\sigma_1}\sum_{\sigma_2}\sum_{\sigma_3}\sum_{\sigma_4}\sum_{\sigma_5} T_{\sigma_1,\sigma_2} T_{\sigma_2,\sigma_3} T_{\sigma_3,\sigma_4} T_{\sigma_4,\sigma_5} T_{\sigma_5,\sigma_1}$$

2×2 matrix

$$\sum_{\sigma_1}\sum_{\sigma_3}\sum_{\sigma_4}\sum_{\sigma_5} (T^2)_{\sigma_1,\sigma_3} T_{\sigma_3,\sigma_4} T_{\sigma_4,\sigma_5} T_{\sigma_5,\sigma_1}$$

2×2 matrix

$$\sum_{\sigma_1}\sum_{\sigma_4}\sum_{\sigma_5} (T^3)_{\sigma_1,\sigma_4} T_{\sigma_4,\sigma_5} T_{\sigma_5,\sigma_1}$$

2×2 matrix

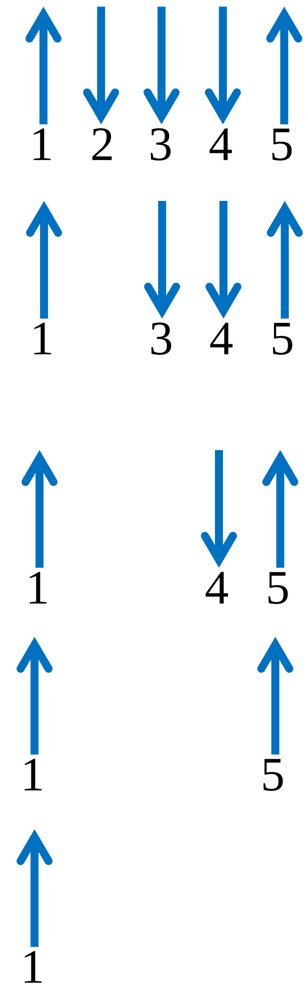
$$\sum_{\sigma_1}\sum_{\sigma_5} (T^4)_{\sigma_1,\sigma_5} T_{\sigma_5,\sigma_1} \Rightarrow \sum_{\sigma} (T^5)_{\sigma_1,\sigma_1}$$

2×2 matrix

Diagonal elements

We are summing diagonal elements

Equivalent to Trace of the matrix



- Recall T is a real symmetric matrix. Hence it can be diagonalized as

$$T = PDP^{-1} \Rightarrow D = P^{-1}TP = \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix}$$

- D is a diagonal matrix with its eigenvalues λ_1 and λ_2.

$$T^2 = PDP^{-1} \times PDP^{-1} = PD^2P^{-1} \qquad T^3 = PD^2P^{-1} \times PDP^{-1} = PD^3P^{-1}$$

$$T^N = PD^NP^{-1}$$

$$Tr(T^N) = Tr(PD^NP^{-1}) = Tr(D^N) = Tr\begin{pmatrix} \lambda_1^N & 0 \\ 0 & \lambda_2^N \end{pmatrix} = \lambda_1^N + \lambda_2^N$$

Determination of eigenvalues :

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

- The eigenvalues $(\lambda_{\pm})$ are given by the solution of the determinant equation

$$\begin{vmatrix} e^{l+h} - \lambda & e^{-l} \\ e^{-l} & e^{l-h} - \lambda \end{vmatrix} = 0$$

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

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

$$\lambda_{+,-} = e^{\beta J}\left[\cosh(\beta H) \pm \sqrt{\sinh^2(\beta H) + e^{-4\beta J}}\right]$$

- It can easily be verified that $\lambda_+ > \lambda_-$ for all β and H.

$$\therefore \left(\frac{\lambda_-}{\lambda_+}\right)^N \to 0 \text{ as } N \to \infty$$

We know,

$$F = -kT\log Z \qquad \lambda_{+,-} = e^{\beta J}\left[\cosh(\beta H) \pm \sqrt{\sinh^2(\beta H) + e^{-4\beta J}}\right]$$

Let us calculate H. F. E per spin

?

$$\frac{1}{N}F = \frac{1}{N}(-kT\log Z) = -kT\left(\frac{\log Z}{N}\right)$$

Recall

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

$$\log Z = \log\left[(\lambda_+)^N\left(1 + \left(\frac{\lambda_-}{\lambda_+}\right)^N\right)\right] = \log\left((\lambda_+)^N\right) + \log\left[1 + \left(\frac{\lambda_-}{\lambda_+}\right)^N\right]$$

$$= N\log\lambda_+ + \log\left[1 + \left(\frac{\lambda_-}{\lambda_+}\right)^N\right]$$

$$\frac{\log Z}{N} = \log\lambda_+ + \frac{1}{N}\log\left[1 + \left(\frac{\lambda_-}{\lambda_+}\right)^N\right]$$

When N is very large the second term can be dropped.

$$\therefore \ \frac{\log Z}{N} = \log\lambda_+$$

$$\therefore \ \frac{1}{N}F = -kT\log\lambda_+ = -kT\log\left\{e^{\beta J}\left[\cosh(\beta H) + \sqrt{\sinh^2(\beta H) + e^{-4\beta J}}\right]\right\}$$

$$= -J - kT\log\left[\cosh(\beta H) + \sqrt{\sinh^2(\beta H) + e^{-4\beta J}}\right]$$

Magnetization per spin M at non-zero T and H

$$M = -\frac{\partial f}{\partial H} = \frac{\sinh \beta H}{(\sinh^2(\beta H) + e^{-4\beta J})^{\frac{1}{2}}}$$

An analytical function for real H $and\ +ve\ T$

No phase transition

Recall

Magnetic system

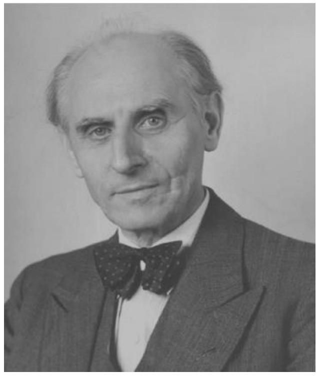
Paramagnet if $M \neq 0$ only when $H \neq 0$

Ferromagnet if $M \neq 0$ only when $H = 0$

$H = 0$ & $M = 0$ It becomes ferromagnet at $T = 0$, $e^{-4\beta J} \to 0$

Ising Model (A brief history)

Ph.D. advisor



Wilhelm Lenz

- Inventor (1920)

Ernst Ising

- Ph.D. Thesis 1924 (solved one dimensional problem)
- 1936 – Name has been given as Ising model

Lars Onsager

- Solved two dimensional problem (1968).
- Noble prize winner

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