14 The Ising Model

classical treatment

Chain of spins fixed in space:
↳ each with magnetic moment $\vec{\mu}$

• • • • •

no interactions

external magnetic field: $\vec{B} = B\hat{e}_z$

$\Rightarrow$ Single-particle Hamiltonian $\mathcal{H}_i = -\vec{\mu}_i \cdot \vec{B}$
$= -\mu_{i,z} B$

Hamiltonian for i^{th} spin

Hamiltonian of N magnetic moments:

$$\mathcal{H} = \sum_{i=1}^{N} \mathcal{H}_i = \sum_{i=1}^{N} -B\mu_{i,z}$$

(let the magnitude of magnetic moment be μ: $|\vec{\mu}_i| = \mu$)

Partition fct.: $Q_N = \left(2\cosh(\beta\mu B)\right)^N$

Internal energy: $U = -N\mu B \tanh(\beta\mu B)$

# of spins is fixed: it's natural to work in canonical ensemble.

Magnetization (per unit volume) $\mathcal{M} = kT \frac{\partial}{\partial B}\left(\frac{\log Q_N}{V}\right)$ (in canonical ensemble)

see discussion in Sec. II

$$\mathcal{M} = \frac{1}{V}\left\langle -\frac{\partial \mathcal{H}}{\partial B}\right\rangle$$ (general definition)

Magnetic susceptibility : $\chi = \frac{\partial \mathcal{M}}{\partial B}$

If we're dealing w/ a spin chain, it also makes sense to define magnetization as

$$M = \left\langle \sum_i s_i \right\rangle \quad , \quad \text{where } \mu_{z,i} = s_i\,\mu$$
and $s_i = \pm 1$

note: defined here as dimensionless quantity
⇝ alternatively, μ could be included ...

$$M = M(B, T)$$

Let's make things more interesting and allow for interactions between magnetic moments:

$$\boxed{E\{s_i\} = -J \sum_{\langle ij \rangle} s_i \, s_j - H \sum_{i=1}^{N} s_i}$$

energy for a specific arrangements of the magnetic moments

nearest neighbor terms

$H = \mu B$

(B-field, as before, along positive z-direction)

2D square lattice:

"particle" i has four nearest neighbors

this interaction should only be counted once and not twice

1D spin chain:

i^{th} magnetic moment

"particle" i has two nearest neighbors

the Hamiltonian contains N interaction terms (no double-counting)

J: exchange constant

↳ look at nearest neighbor pair

$\underset{i}{\uparrow} \quad \underset{i+1}{\uparrow} \quad \Rightarrow \quad -J\, s_i\, s_{i+1} = -J$

$\downarrow \quad \downarrow \quad \Rightarrow \quad -J\, s_i\, s_{i+1} = -J$

$\uparrow \quad \downarrow \quad \Rightarrow \quad -J\, s_i\, s_{i+1} = J$

$\downarrow \quad \uparrow \quad \Rightarrow \quad -J\, s_i\, s_{i+1} = J$

Note: the model assumes that the exchange constant is site independent (in general, one might want to start with $J \to J_{ij}$ ⇝ more realistic and more complicated...).

Why only nearest neighbor interactions?

Typically, J depends on distance ⇝ falls off very quickly with increasing distance (effective short-range interactions).

J can be calculated from overlap integrals that involve the Coulomb interaction — and, even though the Coulomb interaction has an infinite range, "screening" turns the long-range Coulomb interaction into an effective short-range interaction.

Importantly: J can be positive or negative.

Very intuitively:

J positive ⇝ ferromagnetism

$$\begin{array}{cccc} \uparrow & \uparrow & \uparrow & \uparrow \\ \uparrow & \uparrow & \uparrow & \uparrow \\ \uparrow & \uparrow & \uparrow & \uparrow \end{array}$$

J negative ⇝ anti-ferromagnetism

$$\begin{array}{cccc} \uparrow & \downarrow & \uparrow & \downarrow \\ \downarrow & \uparrow & \downarrow & \uparrow \\ \uparrow & \downarrow & \uparrow & \downarrow \end{array}$$

typically, this occurs below the Curie or Néel (T_C or T_N) temperature

Examples for ferromagnetic materials: Fe, Ni, EuO

Examples for anti-ferromagnetic materials: MnF_2, $RbMnF_3$

At high T, materials (would) have randomly oriented spins:

note: in general, the magnetic moments have three components → they can point in and out of the plane

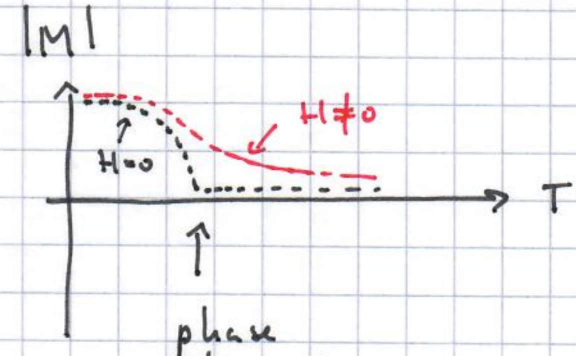
"General" model Hamiltonian:

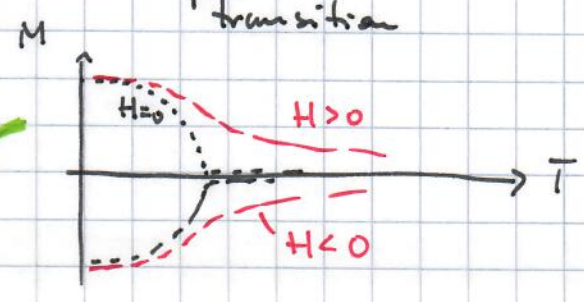
$$\boxed{\mathcal{H} = -J' \sum_{\langle ij \rangle} \underbrace{\vec{\mu}_i \cdot \vec{\mu}_j}_{\mu_{i,x}\mu_{j,x} + \mu_{i,y}\mu_{j,y} + \mu_{i,z}\mu_{j,z}} - B \sum_{i=1}^{N} \mu_{i,z}}$$

"Heisenberg model"

Very roughly: (typical picture for zero T ferromagnet)

↑↑↑↑↑ or ↓↓↓↓↓





For H = 0: spontaneous symmetry-breaking below T_c (either upper or lower branch)

Ising model is simplified version of Heisenberg model:

$$\boxed{\mathcal{H} = -J' \sum_{\langle ij \rangle} \mu_{i,z} \mu_{j,z} - B \sum_{i=1}^{N} \mu_{i,z}}$$

now: $\mu_{i,z} = s_i \mu$

where $s_i = \pm 1$

Since each magnetic moment can take two orientations, the partition fct. has contributions from 2^N configurations.

→ if we use computer, the calculations become big quickly:

Say 3d: $\underbrace{4 \times 4 \times 4 \text{ lattice}}_{\text{quite small}}$

⇝ 64 spins / magnetic moments

⇒ 2^{64} configurations

(a lot of terms to add up)

1D : analytical solution exists

2D : $H=0$ Hamiltonian fully tractable

some results for $H \neq 0$ (special algebraic or graph theoretic approaches)

3D : No exact analytic solution known, not even for $H=0$

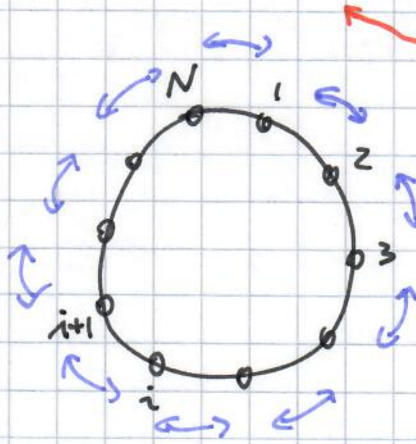
to the best of my knowledge

approximate (e.g., mean-field) approach ...

Let us look at the 1D model more carefully:

$$E = -J \sum_{i=1}^{N} s_i \, s_{i+1} - \frac{1}{2} H \sum_{i=1}^{N} (s_i + s_{i+1})$$

the $\frac{1}{2}$ "symmetizes" the result → we have i and $i+1$ in first and in second sum



toroidal or periodic boundary conditions

⇝ all spins are equal

Let's calculate the partition fct. :

$$Q_N = \sum_{S_1=\pm 1} \dots \sum_{S_N=\pm 1} \exp\left[\beta \sum_{i=1}^{N} \{ J\, s_i s_{i+1} + \tfrac{1}{2} H (s_i + s_{i+1}) \}\right]$$

the analytical result for Q_N is given on page 323a

$$= \sum_{S_1=\pm 1} \dots \sum_{S_N=\pm 1} \langle s_1 | T | s_2 \rangle \langle s_2 | T | s_3 \rangle \cdot \dots \cdot \langle s_{N-1} | T | s_N \rangle$$

$$\langle s_N | T | s_1 \rangle$$

the $\langle s_i | T | s_j \rangle$ notation is "just" a fancy way of rewriting Q_N → but it does have math advantages

def. of short-hand notation

where $\langle s_i | T | s_{i+1} \rangle = \exp\left(\beta \{ J\, s_i s_{i+1} + \tfrac{1}{2} H (s_i + s_{i+1}) \}\right)$

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

Some math details on page 321 ff. (done on 323a)

$$\Rightarrow Q_N = \sum_{S_1=\pm 1} \langle s_1 | \underline{T}^N | s_1 \rangle = \text{Trace}\,(\underline{T}^N)$$

$$= \lambda_+^N + \lambda_-^N$$

where λ_+ and λ_- are the eigenvalues of $\underline{T}$

λ_+ and λ_- are calculated on page 320

Calculating the eigenvalues $\lambda_\pm$: 320

$$\det\begin{pmatrix} e^{\beta(J+H)}-\lambda & e^{-\beta J} \\ e^{-\beta J} & e^{\beta(J-H)}-\lambda \end{pmatrix} = 0$$

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

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

$$\Rightarrow \lambda_\pm = \frac{1}{2}e^{\beta J}\left(e^{\beta H}+e^{-\beta H}\right) \pm \sqrt{\frac{1}{4}e^{2\beta J}\left(e^{\beta H}+e^{-\beta H}\right)^2 - e^{2\beta J} + e^{-2\beta J}}$$

$$= e^{\beta J}\cosh(\beta H) \pm \sqrt{e^{2\beta J}\left(-1+\cosh^2(\beta H)\right) + e^{-2\beta J}}$$

$$\sinh^2(\beta J) = \frac{1}{4}\left(e^{\beta J}-e^{-\beta J}\right)^2$$

$$= \frac{1}{4}\left(e^{2\beta J}+e^{-2\beta J}-2\right)$$

$$\cosh^2(\beta H) - 1 = \frac{1}{4}\left(e^{2\beta H}+e^{-2\beta H}\right) + \frac{1}{2} - 1$$

$$= \sinh^2\beta H$$

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

More math details (will be done on page 323a)

From page 319:

$$Q_N = \sum_{s_1=\pm 1} \sum_{s_2=\pm 1} \cdots \sum_{s_N=\pm 1} \langle s_1|T|s_2\rangle\langle s_2|T|s_3\rangle \ldots \langle s_N|T|s_1\rangle$$

where $\langle s_i|T|s_j\rangle = \exp\left(\beta\left[J s_i s_{i+1} + \frac{1}{2}H(s_i + s_{i+1})\right]\right)$

We have four possibilities:

$\langle +1|T|+1\rangle$

$\langle +1|T|-1\rangle$

$\langle -1|T|+1\rangle$

$\langle -1|T|-1\rangle$

inspired by quantum, we can write

$|+1\rangle$ as $\begin{pmatrix}1\\0\end{pmatrix}$ and $|-1\rangle$ as $\begin{pmatrix}0\\1\end{pmatrix}$

this is the matrix $\underline{T}$ on page 319

We know: $\langle +1|T|+1\rangle = \underbrace{e^{\beta(J+H)}}_{\text{identify as 11 element of } T}$

$\langle +1|T|-1\rangle = e^{-\beta J}$ 12 element of T

$\langle -1|T|+1\rangle = e^{-\beta J}$ 21 element of T

$\langle -1|T|-1\rangle = e^{\beta(J-H)}$ 22 element of T

Now: When we look at $\langle s_i | T | s_{i+1} \rangle$, we can think of this in terms of the matrix $\underline{\underline{T}}$. Depending on s_i and s_{i+1} ($\uparrow$ or $\downarrow$, or $+1$ or -1), the "bra-ket" "filters out" one of the matrix elements of $\underline{\underline{T}}$. Using the $\binom{1}{0}$ and $\binom{0}{1}$ convention, it makes sense to write $\langle s_i | T | s_j \rangle$ in terms of the matrix $\underline{\underline{T}}$:

$$\langle s_i | \underline{\underline{T}} | s_j \rangle$$

these are now $\binom{0}{1}$, $\binom{1}{0}$ or the transpose thereof

Next: We do have a sum $\sum\limits_{s_2=\pm 1} \sum\limits_{s_3=\pm 1} \ldots$

these are sums over a complete set of states (speaking quantum mechanically)

$$\Rightarrow \sum_{s_2=\pm} |s_2\rangle\langle s_2| \rightarrow \text{identity}$$

and the same for $s_3, \ldots$

So: $$\sum_{s_1=\pm 1} \sum_{s_2=\pm 1} \ldots \sum_{s_N=\pm 1} \langle s_1 | T | s_2 \rangle \ldots \langle s_N | T | s_1 \rangle$$

$$= \sum_{s_1 \pm 1} \langle s_1 | \underbrace{\underline{\underline{T}}\,\underline{\underline{T}} \cdot \ldots \cdot \underline{\underline{T}}}_{N\ \underline{\underline{T}}\text{'s}} | s_1 \rangle$$

How to proceed?

We have a product of N matrices that are not diagonal.

Define a matrix $\underline{\underline{U}}$ such that

$$\underline{\underline{U}}^{-1}\,\underline{\underline{T}}\,\underline{\underline{U}} = \underline{\underline{T}}_D = \begin{pmatrix} \lambda_+ & 0 \\ 0 & \lambda_- \end{pmatrix}$$

diagonal matrix

$$\text{Then:}\quad Q_N = \sum_{s_1=\pm1} \langle s_1 | \underbrace{\underline{\underline{U}}\,\underline{\underline{U}}^{-1}}_{\text{identity}}\,\overbrace{\underline{\underline{T}}\,\underbrace{\underline{\underline{U}}\,\underline{\underline{U}}^{-1}}_{}}\,\overbrace{\underline{\underline{T}}\ldots}\,\underbrace{\underline{\underline{U}}\,\underline{\underline{U}}^{-1}}_{}\,\overbrace{\underline{\underline{T}}\,\underline{\underline{U}}}^{\underline{\underline{T}}_D}\,\underline{\underline{U}}^{-1}|s_1\rangle$$

$$= \sum_{s_1=\pm1} \langle s_1 | \underline{\underline{U}}\,\underbrace{\underline{\underline{T}}_D \cdot \ldots \cdot \underline{\underline{T}}_D}_{N \text{ times}}\,\underline{\underline{U}}^{-1}|s_1\rangle$$

$$= \underline{\underline{T}}_D^N$$

How does $\underline{\underline{T}}_D^N$ look like?

$$\begin{pmatrix} \lambda_+ & 0 \\ 0 & \lambda_- \end{pmatrix}\begin{pmatrix} \lambda_+ & 0 \\ 0 & \lambda_{-1} \end{pmatrix} = \begin{pmatrix} \lambda_+^2 & 0 \\ 0 & \lambda_-^2 \end{pmatrix}$$

$$\text{So:}\quad \underline{\underline{T}}_D^N = \begin{pmatrix} \lambda_+^N & 0 \\ 0 & \lambda_-^N \end{pmatrix}$$

We can define $\underbrace{\underline{\underline{U}}^{-1}|s_1\rangle}_{|\tilde{s}_1\rangle}$ as new states.

Just as $|s_1\rangle$ can take two orientations,

$|\tilde{s}_1\rangle$ can take two orientations.

So: $\sum_{s_1=\pm}$ has to be changed to the sum over the two new rotated states. But the result is simple. The $\sum_{s_1=\pm}$ operation is just the trace operation.

Hence: $$Q_N = \sum_{s_1=\pm 1} \langle s_1 | \underline{\underline{U}} \begin{pmatrix} \lambda_+^N & 0 \\ 0 & \lambda_-^N \end{pmatrix} \underline{\underline{U}}^{-1} | s_1 \rangle$$

$$= \mathrm{Tr}\left(\underline{\underline{T}}_D^N \right) = \lambda_+^N + \lambda_-^N$$

End of the math details!

We found $\boxed{Q_N = \lambda_+^N + \lambda_-^N}$ ← λ_+ and λ_- are given on page 320

where $\lambda_\pm = e^{\beta J} \cosh(\beta H) \pm \left[\exp(-2\beta J) + \exp(2\beta J) \sinh^2(\beta H) \right]^{1/2}$

$$\boxed{Q_N = \lambda_+^N \left(1 + \left(\frac{\lambda_-}{\lambda_+} \right)^N \right) \xrightarrow[N \to \infty]{} \lambda_+^N}$$

Since $\lambda_- < \lambda_+$, this term goes to zero as $N \to \infty$

So: $\frac{1}{N} \log Q_N = \log \lambda_+$

Recall: We are interested in magnetization $\mathcal{M}$:

$$\mathcal{M} = \frac{1}{V} \left\langle -\frac{\partial \mathcal{H}}{\partial B} \right\rangle = kT \frac{\partial}{\partial B}\left(\frac{\log Q_N}{V}\right)$$

canonical ensemble

For the spin chain, we don't have a volume but we do have # of particles in spin chain.

So: $$\mathcal{M} = kT \frac{\partial}{\partial B}\underbrace{\left(\frac{\log Q_N}{N}\right)}_{\substack{\log \lambda_+ \\ \| \\ \log\left(e^{\beta J}\cosh(\beta\mu B) + \left[e^{-2\beta J} + e^{2\beta J}\sinh^2(\beta\mu B)\right]^{1/2}\right)}}$$

Doing the derivative in Mathematica yields:

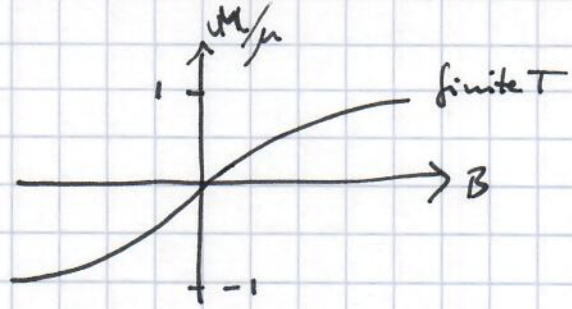
$$\boxed{\mathcal{M} = \mu \frac{\sinh(\beta\mu B)}{\left[e^{-4\beta J} + \sinh(\beta\mu B)\right]^{1/2}}}$$

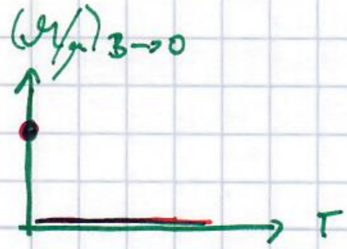
As $B \to 0 \Rightarrow \mathcal{M} \to 0$

provided β is finite

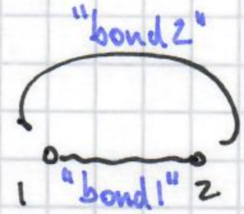
$\Rightarrow$ the model does not support spontaneous magnetization (i.e., no phase transition at finite T)

$\rightsquigarrow$ There is a transition at $T = 0$





Explicit calculation of the two-particle partition fct.:



$$Q_2 = e^{-\beta E_{\uparrow\uparrow}} + e^{-\beta E_{\uparrow\downarrow}} + e^{-\beta E_{\downarrow\uparrow}} + e^{-\beta E_{\downarrow\downarrow}}$$

$$\left.\begin{aligned} E_{\uparrow\uparrow} &= -2J - 2H \\ E_{\downarrow\downarrow} &= -2J + 2H \\ E_{\uparrow\downarrow} &= +2J \\ E_{\downarrow\uparrow} &= +2J \end{aligned}\right\}$$

note: Since we are working with periodic boundary conditions, we need to count the interactions for bond 1 and for bond 2.

$$\Rightarrow Q_2 = e^{2\beta(J+H)} + e^{2\beta(J-H)} + e^{-2\beta J} + e^{-2\beta J}$$

$$= e^{2\beta J}\underbrace{\left(e^{2\beta H} + e^{-2\beta H}\right)}_{(e^{\beta H}+e^{-\beta H})^2 - 2} + 2e^{-2\beta J}$$

$$\Rightarrow Q_2 = e^{2\beta J}\left[\left(e^{\beta H} + e^{-\beta H}\right)^2 - 2\right] + 2e^{-2\beta J}$$

Calculating $\lambda_+^2 + \lambda_-^2$:

$$\lambda_+^2 + \lambda_-^2 = (a+b)^2 + (a-b)^2$$

$$= 2a^2 + 2b^2$$

$$a = e^{\beta J} \cosh(\beta H)$$

$$b = \sqrt{e^{-2\beta J} + e^{2\beta J} \sinh^2(\beta J)}$$

$$= \frac{1}{2} e^{2\beta J} \left(e^{\beta H} + e^{-\beta H}\right)^2$$

$$+ \frac{1}{2} e^{2\beta J} \left(e^{\beta H} + e^{-\beta H}\right)^2 - 2e^{2\beta J} + 2e^{-2\beta J}$$

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

According to our general calculation, we should have

$$Q_2 = \lambda_+^2 + \lambda_-^2$$

Comparison with the explicit calculation of Q_2 shows that this is indeed true.