Ising Model

At low T, some crystalline solids are magnetized – have non-zero magnetization $\vec{M}$. This arises from individual atomic spins $\vec{S}_i$ ($i = 1, \ldots N$ lattice positions)

$$\vec{M} = \frac{1}{N}\sum_{i=1}^{N} \vec{S}_i \quad , \quad |\vec{M}| = \frac{1}{N}\left|\sum_i \vec{S}_i\right|$$

We can use MC simulations of model spins to study such materials. To get the thermal average at some T, we need

$$\langle \vec{M} \rangle = \frac{1}{N}\left\langle \sum_i \vec{S}_i \right\rangle \quad \text{or} \quad \langle |\vec{M}| \rangle = \frac{1}{N}\left\langle \left|\sum_i \vec{S}_i\right| \right\rangle$$

scalar ≥ 0

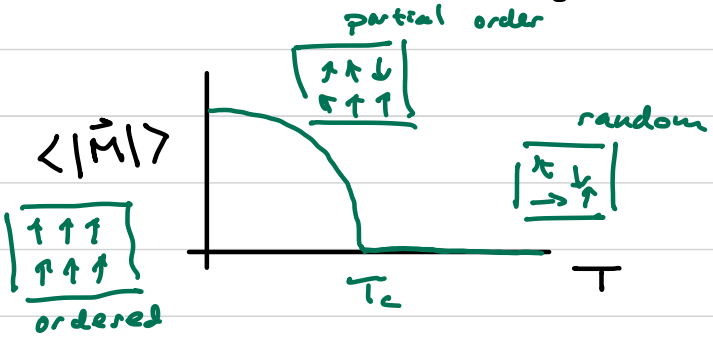
where $\langle \ldots \rangle$ is an average over many MCS.

$$\langle \vec{M} \rangle = \frac{1}{\#MCS}\sum_{\alpha=1}^{\#MCS} \vec{M}_\alpha$$

At low T, interactions tend to align spins $\rightarrow \vec{M} \neq 0$

At high T, $\vec{S}_i$ randomize $\rightarrow \vec{M} = 0$

As T varies, the system undergoes a phase transition at T_c



transition is sharp in limit as $N \rightarrow \infty$ (large N)
"thermodynamic limit"

Heisenberg model: $|\vec{S}_i| = 1$, but can point in any direction (3D)

Ising model: $S_i = \pm 1$ $\quad (\vec{S}_i = \pm \hat{z})$

spins point along $\hat{z}$, either up or down:

$\therefore M = (N_\uparrow - N_\downarrow)/N$ $\quad N_\uparrow$ # of up spins

for $T > T_c$, $N_\uparrow \approx N_\downarrow \rightarrow M \approx 0$

$0 < T < T_c$, $N_\uparrow > N_\downarrow$ (or $N_\downarrow > N_\uparrow$)

$M > 0$ $\quad$ $M < 0$

no preferred direction: $|M| > 0$

$T = 0$ $\quad$ $N_\uparrow = N$ $\quad$ (or $N_\downarrow = N$)

$|M| = 1$

Why do spins align? Exchange interaction

→ QM in origin

→ short-range interaction, usually only between nearest neighbours (NN)

$$E = -\sum_{i,j}^{NN} J_{ij} \vec{S}_i \cdot \vec{S}_j$$

(Heisenberg model)

J_{ij} - exchange constant between spins i and j

sum over NN pairs

$$E = -\sum_{i,j}^{NN} J_{ij} S_i S_j$$

(Ising)

$$E = -J \sum_{\langle ij \rangle} S_i S_j$$

$J_{ij} = J$ if all spins are the same

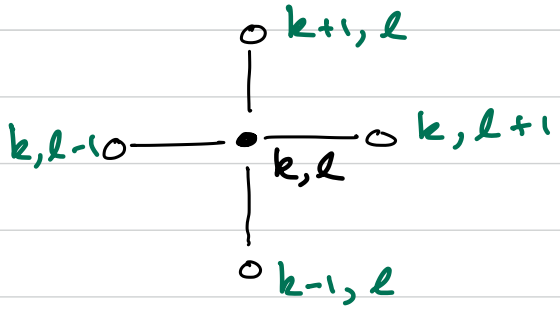
$J > 0$ → low energy for $\uparrow\uparrow$ or $\downarrow\downarrow$

$$= -\frac{J}{2} \sum_{k=1}^{L} \sum_{l=1}^{L} S_{k,l} \left(S_{k,l+1} + S_{k,l-1} + S_{k+1,l} + S_{k-1,l} \right)$$

for a 2D square lattice $L \times L$ spins

k, l - lattice row and column indices

- double counted interactions with double sum
  → hence divide sum by 2



MC allows us to quantify effects of T
energy of interaction → align spins
thermal energy → sample unfavourable spins configurations

→ generate many spin configurations at a particular T and average

Procedure

1) Initialize spins on all lattice sites (randomly up or down, or all up say)

2) Choose a spin at random to flip
   or keeps E the same

3) If flip lowers the energy, accept the new state.
   If flip increases the energy, accept the new state the probability $p = e^{-\beta \Delta E}$.
   If not accepted, retain original configuration.

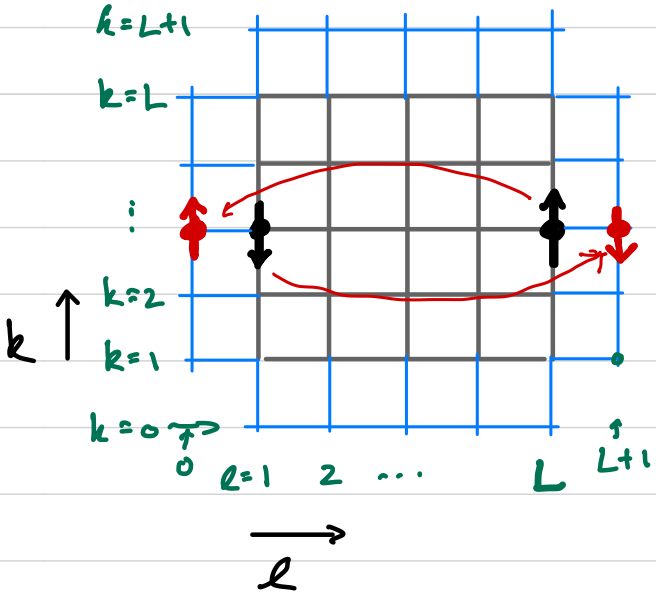
4) update M, E and any other quantities
- accumulate averages

5) go back to step 2 many times until you've run "long enough" - stationary "time" series
- good statistics
report $M(T)$, $E(T)$ etc

6) change T and repeat (from step 2)

Note: surfaces will strongly affect system properties for small systems - and we want bulk properties
→ use periodic boundary conditions

for $L \times L$ square lattice



neighbours for spin $S_{k,\ell}$ on boundary

$$S_{L+1,\ell} = S_{1,\ell}$$

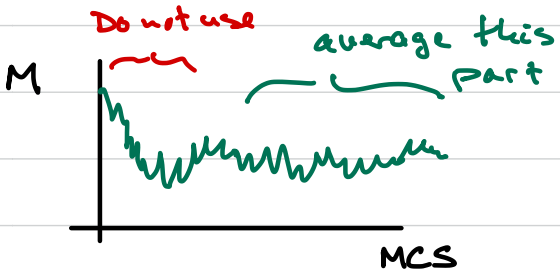
$$S_{k,L+1} = S_{k,1}$$

$$S_{0,\ell} = S_{L,\ell}$$

$$S_{k,0} = S_{k,L}$$

Using the MC procedure will generate a sequence of configurations, values of M, values of E

- do not use first part of sequence while system is



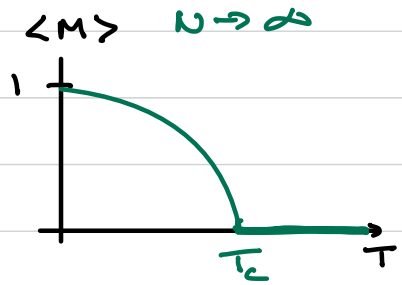
e.g. for N_A MCS,
ignore first $N_A/10$ MCS
then use sweeps $\frac{N_A}{10}+1$ to N_A
to get $\langle \dots \rangle$ (averages)

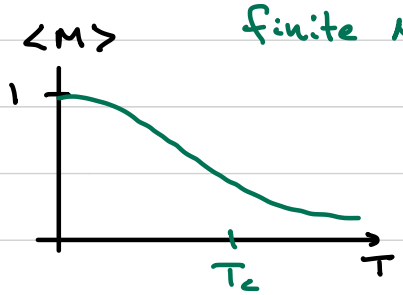
Quantities of interest are

$\langle M \rangle$ vs T

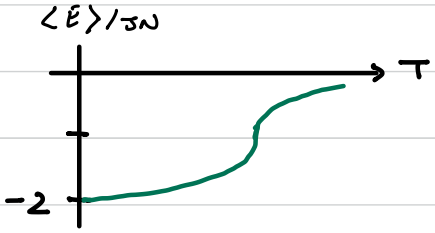
or $\langle |M| \rangle$ vs T

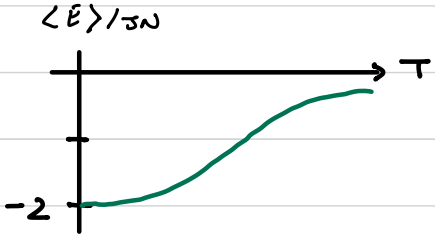
|M| useful for small systems





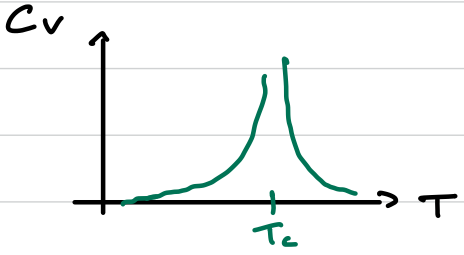
$\frac{\langle E \rangle}{JN}$ vs T

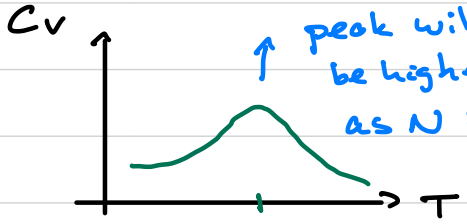




(can set $J = 1$, $k_B = 1$)

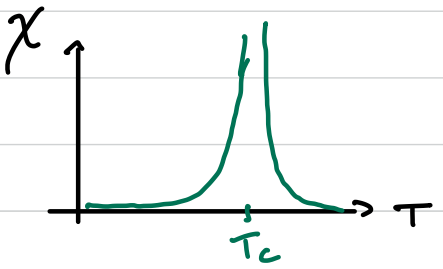
specific heat

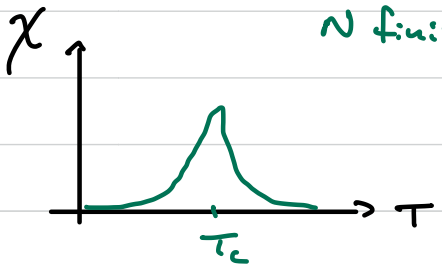




$$C_v = \frac{1}{N}\frac{1}{k_B T^2}\left(\langle E^2 \rangle - \langle E \rangle^2\right) = \frac{1}{N}\frac{d\langle E \rangle}{dT}$$

magnetic susceptibility (per spin)





$$\chi = \frac{N}{k_B T}\left(\langle M^2\rangle - \langle M\rangle^2\right) \quad \text{or, if we call } S = \sum_i S_i$$

$$= \frac{1}{N k_B T}\left(\langle S^2\rangle - \langle S\rangle^2\right) \qquad \left(M = \frac{1}{N} S\right)$$

We expect χ and C_V to diverge at $T = T_c$ in thermodynamic limit ($N \to \infty$).
For finite N, divergence becomes "rounded".

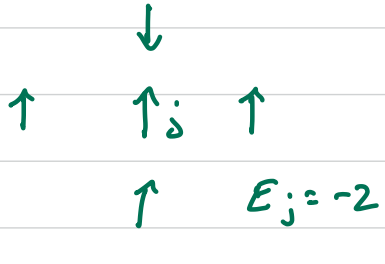
2D Ising model can be solved analytically ($N \to \infty$)

$$T_c = \frac{J}{k_B}\frac{2}{\ln(1+\sqrt{2})} \approx 2.269\,\frac{J}{k_B}$$

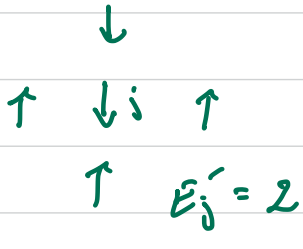
Note on ΔE – for single spin flips, only interactions that include proposed spin contribute to change in system energy

Can define $E_j = -J S_j (S_{up} + S_{down} + S_{right} + S_{left})$

here $S_j = 1$



initial



proposed / final

$S_j' = -1$

$E_j' = -E_j$

$$\Delta E = E_{final} - E_{initial} = E_j' - E_j = -E_j - E_j = -2E_j$$

$\frac{E_j}{J}$ can take on 5 values $-4, -2, 0, 2, 4$

$\therefore$ if $E_j \geq 0$, accept the proposed flip

If $E_j < 0$, $-\Delta E = 2E_j$ and acceptance probability is $e^{-\Delta E/k_BT} = e^{2E_j/k_BT}$

and acceptance probability is ↑ oops

There are only 2 such probabilities:

e^{-8J/k_BT} and e^{-4J/k_BT}

These values can be stored to avoid frequent recalculation.