Ising Model

At low T, some crystalline solids are magnetized - This arises from individual

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

where $\langle \ldots \rangle$ is an average over

At low T,

At high T,

As T varies, the system undergoes

transition is sharp in limit as

Heisenberg model:

Ising model:

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

$\therefore$

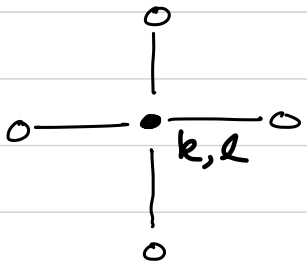
for $T > T_c$,

$0 < T < T_c$,

$T = 0$

Why do spins align?

- double counted interactions with double sum
  → hence



MC allows us to quantify
energy of interaction →
thermal energy →

→ generate many spin configurations at a particular

Procedure

1)

2)

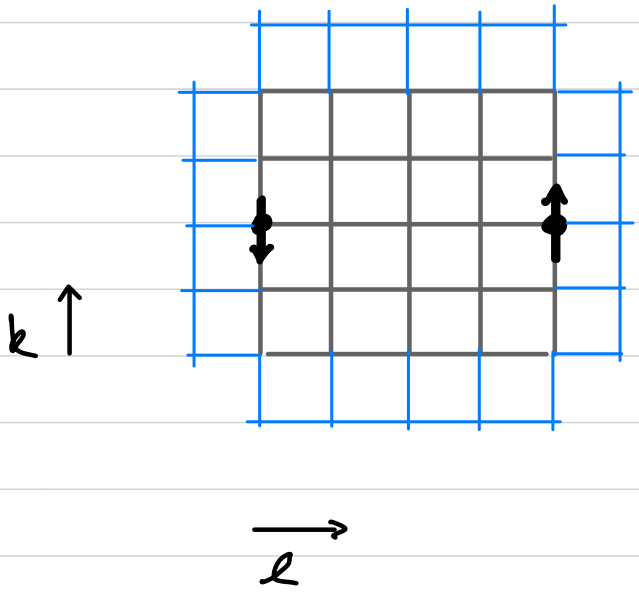
3)

4)

5)

6)

Note: surfaces will strongly affect system properties for small systems



neighbours for spin $S_{k,l}$ on boundary

$S_{L+1,l}$ =

$S_{k,L+1}$ =

$S_{0,l}$ =

$S_{k,0}$ =

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

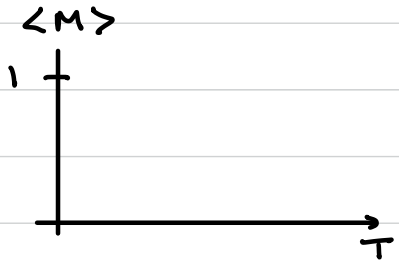
e.g. for N_A MCS, ignore first then use sweeps to get

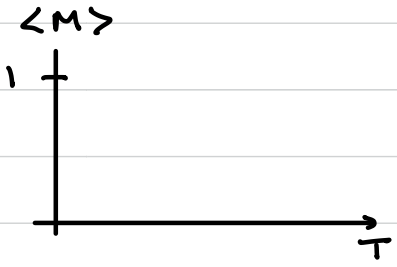
Quantities of interest are

$\langle M \rangle$ vs T

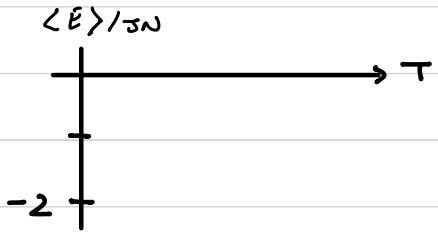
or $\langle |M| \rangle$ vs T

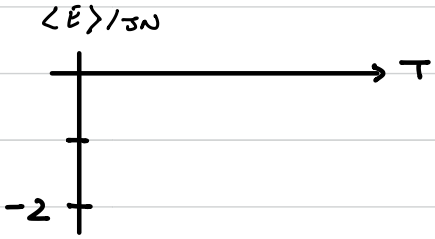
|M| useful for small systems





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





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

specific heat

$C_V =$

magnetic susceptibility

$\chi =$

$=$

or, if we call $S = \sum_i S_i$

$\left(M = \frac{1}{N} S \right)$

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

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

Note on ΔE – for single spin flips, only interactions that include

Can define $E_j =$

here
$S_j =$

$S_j' =$

initial

proposed / final

$\Delta E = E_{final} - E_{initial} =$

$\frac{E_j}{J}$ can take on 5 values

$\therefore$ if $E_j \geq 0$,

if $E_j < 0$,

and acceptance probability is

There are only 2 such probabilities:

These values can be stored to avoid frequent recalculation.