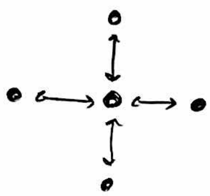
The Ising model

- Ising-Lenz (Ernest Ising, Wilhelm Lenz, 1920s)
- Originally model for ferromagnetism in statistical mechanics, have been used to describe <u>many</u> phenomena (e.g. neuroscience)
- Grid/lattice of spins (variables) that can take ~~two~~ on of two values: +1, −1
- Each spin interacts with its neighbours



2D

$$\begin{array}{ccccc} & \vdots & \vdots & \vdots & \\ \cdots & +1 & +1 & -1 & \cdots \\ \cdots & +1 & -1 & -1 & \cdots \\ \cdots & -1 & -1 & +1 & \cdots \\ & \vdots & \vdots & \vdots & \end{array}$$

- $\uparrow\uparrow$ and $\downarrow\downarrow$ pairs have lower energy than $\uparrow\downarrow$ and $\downarrow\uparrow$ pairs

1D

$$\begin{array}{cccc} \ldots +1 & -1 & -1 & +1 \ldots \\ \uparrow & \downarrow & \downarrow & \uparrow \end{array}$$

- System can exchange heat with environment (A thermal bath at temp. T)

- Change in system energy due to heat $\longleftrightarrow$ flip spins
  "Thermal fluctuations"

- Main topics for Project 4:
  - Study properties of system (at equilibrium) as function of the temperature T and for different lattice sizes
    - Mean energy
    - Mean magnetization
    - Heat capacity
    - Magn. susceptibility

  Compare to analytical solution for T_c by Lars Onsager, 1944

  - Determine <u>critical temperature</u> (T_c), the transition temperature where system goes from ordered, magnetized state to disordered, non-magnetized state

$\boxed{\text{Phase transition}}$

- Many types of quantities to keep track of here! Important to distinguish them!

- Spin value for a single spin : $s_i \in \{-1, +1\}$

- "Spin configuration" : The spin state of the entire system (lattice) : $\bar{s} = [s_1, s_2, \dots, s_N] = [\pm 1, \pm 1, \dots, \pm 1]$

    - Number of spins : N
    - Lattice length : $L \Rightarrow N = L^2$
    - The domain for $\bar{s}$ consists of 2^N possible values for $\bar{s}$ (There are 2^N possible system states (microstates))

- System energy for a particular spin config. $\bar{s}$:

$$E(\bar{s}) = -J \sum_{\langle kl \rangle} s_k s_l \qquad \left(\text{no external magnetic field}\right)$$

$\sum_{\langle kl \rangle}$: Sum over all neighbouring spin pairs (no double counting)

J : Coupling constant, here $J > 0$

8 End lecture

- System magnetization for a particular spin config $\bar{s}$:

$$M(\bar{s}) = \sum_{i}^{N} s_i \qquad \left(\text{sum over all spins in lattice}\right)$$

$\uparrow \uparrow \uparrow \uparrow \qquad M(\bar{s}) = +4$

$\uparrow \downarrow \downarrow \uparrow \qquad M(\bar{s}) = 0$

- State degeneracy : The number of different states $\bar{s}$ that have the same value of some quantity, e.g. $E(\bar{s})$ or $M(\bar{s})$

$\uparrow \uparrow \uparrow$	$M=3$
$\uparrow \uparrow \downarrow$	$M=1$
$\uparrow \downarrow \uparrow$	$M=1$
$\uparrow \downarrow \downarrow$	$M=-1$
$\downarrow \uparrow \uparrow$	$M=1$
$\downarrow \uparrow \downarrow$	$M=-1$
$\downarrow \downarrow \uparrow$	$M=-1$
$\downarrow \downarrow \downarrow$	$M=-3$

$M=3$, degen.: 1
$M=1$, degen.: 3
$M=-1$, degen.: 3
$M=-3$, degen.: 1

- Prob. distribution for $\bar{s}$: Boltzmann distribution

$$\boxed{p(\bar{s};T) = \frac{1}{Z} e^{-\beta E(\bar{s})}}$$

- $\beta \equiv \frac{1}{k_B T}$

  Boltzmann constant

- Z : partition function (see below)

Note: $p(\bar{s};T)$ is the pdf for states $\bar{s}$, not the pdf for energy E, or something else...

$$p(\bar{s};T) = p(s_1, s_2, \dots ; T)$$

(so a joint pdf for the individual spin states $s_1, s_2, \dots$)

$$= \frac{1}{Z} e^{-\beta E(\bar{s})}$$

$$= \frac{1}{Z} e^{\beta J \sum_{\langle kl \rangle} s_k s_l}$$

$$= \frac{1}{Z} e^{\beta J [s_1 s_2 + s_2 s_3 + \dots]}$$

[Assumed 1D model here for simplicity]

$$= \frac{1}{Z} e^{\beta J s_1 s_2} e^{\beta J s_2 s_3} \dots$$

- So the prob. $p(\bar{s};T)$ for a state $\bar{s}$ only depends on $\bar{s}$ through the energy $E(\bar{s})$ of that state — no other details of $\bar{s}$ matter.

- Consequence of the fundamental postulate of stat. mechanics: Assign equal prob. to all microstates (here $\bar{s}$) that have the exact same composition (can't change here) and exact same energy

[Different ways to argue for this, e.g. through E.T. Jaynes information theoretic approach, "max entropy"]

- Partition function:

$$\boxed{Z = \sum_{\substack{\text{all possible} \\ \text{states } \bar{s}}} e^{-\beta E(\bar{s})}}$$

- For a fixed T, serves as the normalization constant in the pdf $p(\bar{s};T)$
- Basically describes how the distr. of prob. across state space changes as we vary T

$\Rightarrow$ Can be used to derive how thermodyn. quantities dep. on T.

- Other prob. distributions:

$$P_E(E;T) = ? \qquad \text{Domain}: E \in ?$$
$$P_M(M;T) = ? \qquad \text{Domain}: M \in ?$$

- Expectation values:

$$\langle E \rangle, \langle E^2 \rangle, \langle |M| \rangle, \langle M^2 \rangle$$

- Heat capacity and magnetic susceptibility

const. volume

$$C_v = \frac{\partial \langle E \rangle}{\partial T} \qquad C_v(T) = \frac{1}{k_B T^2} \mathrm{Var}(E) = \frac{1}{k_B T^2}\left[\langle E^2 \rangle - \langle E \rangle^2\right]$$

$$\chi = \frac{\partial \langle M \rangle}{\partial H} \qquad \chi(T) = \frac{1}{k_B T} \mathrm{Var}(M) = \frac{1}{k_B T}\left[\langle M^2 \rangle - \langle M \rangle^2\right]$$

field intensity

- Actually, we will rather take energy and magnetization densities (per spin) as our starting point. (To easily compare for different lattice sizes)

$$\boxed{\varepsilon \equiv \frac{E}{N}} \qquad \boxed{m \equiv \frac{M}{N}}$$

$$\Rightarrow \quad P_\varepsilon(\varepsilon;T), \quad P_m(m;T)$$
$$\Rightarrow \quad \langle \varepsilon \rangle, \langle \varepsilon^2 \rangle, \langle |m| \rangle, \langle m^2 \rangle$$
$$\Rightarrow \quad C_v(T) = \frac{1}{k_B T^2}\left[\langle \varepsilon^2 \rangle - \langle \varepsilon \rangle^2\right]$$
$$\Rightarrow \quad \chi(T) = \frac{1}{k_B T}\left[\langle m^2 \rangle - \langle m \rangle^2\right]$$

- Basic idea for Proj. 4:

  - Choose lattice size (L, $N = L^2$) and temperature (T)
  - Use (Markov Chain) Monte Carlo to sample system states $\bar{s}$ according to $p(\bar{s}; T)$
  - Use $\bar{s}$ samples to compute any derived quantity of interest, e.g. state energies ($E(\bar{s})$) expectation values $\langle E \rangle$, ... etc.
  - Repeat for different choices of L and T
  - Study T- and L-dependence of results, in particular how system behaves around T_c.

- Warning: Know your type of sum!

$$\sum_{\substack{\text{all spins} \\ \text{in lattice}}}, \quad \sum_{\substack{\text{all neighbouring} \\ \text{spin pairs}}}, \quad \sum_{\substack{\text{all possible} \\ \text{states } \bar{s}}}, \quad \sum_{\substack{\text{all } \bar{s} \\ \underline{\text{samples}}}}$$

$$\sum_{\substack{\text{all possible} \\ \text{values for } E(\bar{s})}}, \quad \sum_{\substack{\text{all } \underline{\text{samples}} \\ E(\bar{s})}}, \quad \ldots$$