Lecture 8: The Ising model

Introduction

- ▶ Up to now: Toy systems with interesting properties (random walkers, cluster growth, percolation)
- ▶ Common to them: No interactions
- ▶ Add interactions now, with significant role
- ▶ Immediate consequence: much richer structure in model, in particular: phase transitions
- ▶ Simulate interactions with RNG (Monte Carlo method)
- ▶ Include the impact of temperature: ideas from thermodynamics and statistical mechanics important
- ▶ Simple system as example: coupled spins (see below), will use the canonical ensemble for its description

The Ising model

- A very interesting model for understanding some properties of magnetic materials, especially the phase transition ferromagnetic ⟷ paramagnetic
- Intrinsically, magnetism is a quantum effect, triggered by the spins of particles aligning with each other
- Ising model a superb toy model to understand this dynamics
- Has been invented in the 1920's by E.Ising
- Ever since treated as a first, paradigmatic model

The model (in 2 dimensions)

- ▶ Consider a square lattice with spins at each lattice site
- ▶ Spins can have two values: $s_i = \pm 1$
- ▶ Take into account only nearest neighbour interactions (good approximation, dipole strength falls off as $1/r^3$)
- ▶ Energy of the system:

$$E = -J \sum_{\langle ij \rangle} s_i s_j$$

- ▶ Here: exchange constant $J > 0$ (for ferromagnets), and $\langle ij \rangle$ denotes pairs of nearest neighbours.
- ▶ (Micro-)states α characterised by the configuration of each spin, the more aligned the spins in a state α, the smaller the respective energy E_α.
- ▶ Emergence of spontaneous magnetisation (without external field): sufficiently many spins parallel

Adding temperature

- Without temperature T: Story over.
- With temperature: disordering effects, spins flip randomly.
- In the following assume system to be in contact with external heat bath - can use canonical ensemble (look it up, if you're interested).
- Effect: System will again "explore" all possibilities (like in the case of milk in tea, lecture 6)
- In contrast here: No uniform probability, but
$$\mathcal{P}_\alpha \sim \exp\left[-\frac{E_\alpha}{k_B T}\right] \text{ (Boltzmann factor)}$$
  for the system to be in a micro-state α.
- Consequence: Increasing temperatures open micro-states with larger energies $\longleftrightarrow$ less alignment

Observables

▶ How to calculate macroscopic observables?
Example: the magnetisation of the system M.

▶ First step: calculate the observable for a micro-state:
$$M_\alpha = \sum_i s_i$$

▶ Sample over all micro-states:
$$M = \sum_\alpha M_\alpha \mathcal{P}_\alpha$$

▶ Therefore, name of the game:
How to calculate the $\mathcal{P}_\alpha$/sample over the micro-states.

▶ Will present two solutions in the following

Analytic solution: Mean field theory (MFA)

- Mean field theory an extremely powerful approximation
- Will introduce it with the specific example of the Ising model at hand.
- However nice: It is not precise!
- Basic idea: Replace the individual spins $s_i = \pm 1$ with an average value $\langle s \rangle \in [-1, 1]$. Then
$$M = \sum_i s_i \longrightarrow \sum_i \langle s \rangle = N \langle s \rangle \equiv N \langle s_i \rangle$$
- In other words: Deduce an average alignment (works for an infinitely large system - all spins equivalent).
- With the equation above we used that we can pick every spin as average spin. But how can we calculate without the micro-states?
- Answer: A trick (see below)

The trick for the solution

- Add a magnetic field (seems a detour, but wait & see!):
$$E = -J \sum_{\langle ij \rangle} s_i s_j - \mu H \sum_i s_i$$

  (Magnetic field H interacts with spins through their magnetic moment μ.)

- Consider a system made of one single spin: $E_{\pm} = \mp \mu H$.

- Two micro-states with $\mathcal{P}_{\pm} = C \exp\left[\pm \frac{\mu H}{k_B T}\right]$

- Normalisation C from $\mathcal{P}_+ + \mathcal{P}_- = 1$
$$\implies C = \frac{1}{\exp\left(\frac{\mu H}{k_B T}\right) + \exp\left(-\frac{\mu H}{k_B T}\right)} = \frac{1}{2 \cosh\left(\frac{\mu H}{k_B T}\right)}$$

- Therefore thermal average of the single spin:
$$\langle s_i \rangle = \mathcal{P}_+ - \mathcal{P}_- = \tanh \frac{\mu H}{k_B T}$$

Rounding it off

- Having the solution for a single spin in a background field, we replace the background field with the average spins!

$$E = -\sum_i \left(\sum_{\langle ij \rangle} s_j + \mu H \right) s_i = -\mu H_{\text{eff}} \sum_i s_i$$

- The effective magnetic field is thus

$$H_{\text{eff}} = \frac{J}{\mu} \sum_{\langle ij \rangle} s_j + H$$

- Mean field approximation then sets $H = 0$ and replaces the actual s_j with the average value:

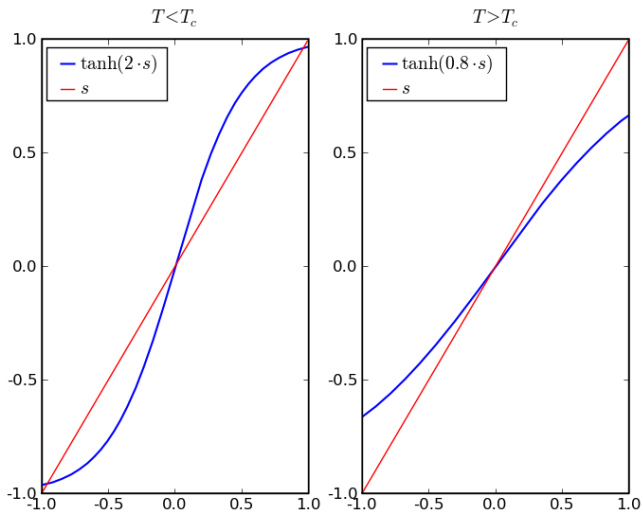$$H_{\text{mfa}} = \frac{jJ}{\mu} \langle s \rangle$$

(Here $j = 4$ is number of nearest neighbours)

- This implies the following implicit equation:

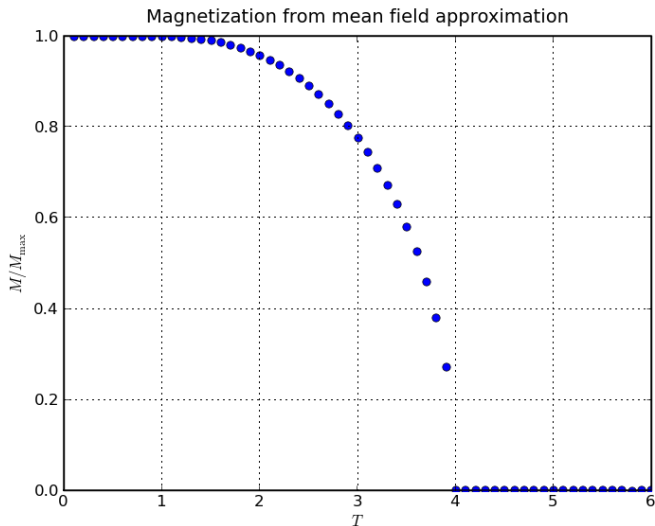$$\langle s \rangle = \tanh \frac{jJ\langle s \rangle}{k_B T}$$

Results: Schematic

- Notice two different regimes: either 1 or 3 solutions

True results

- Obtained from solving $f(\langle s \rangle) = \langle s \rangle - \tanh \dfrac{4\langle s \rangle}{T} = 0$

Magnetization from mean field approximation

Discussion of results

- In plots use $M_{\mathrm{max}} = N$ for normalisation and $J = k_B$ to keep things simple.
- Phase transition at $T_c = 4$ - second order
  (1st derivative of order parameter magnetisation jumps)
- Around T_c: $\mathrm{d}M/\mathrm{d}T \to \infty$.
- Exact form of singularity from Taylor expansion of tanh:
  $$\tanh x = x - \frac{x^3}{3} + \mathcal{O}(x^4)$$
- Therefore, around $T = T_c$:
  $$\langle s \rangle = \frac{jJ}{k_B T} \langle s \rangle - \frac{1}{3} \left(\frac{jJ}{k_B T} \right)^3 \langle s \rangle^3$$

Quantifying the phase transition

- Non-trivial solution for:

$$\langle s \rangle = \sqrt{\frac{3}{T} \left(\frac{k_B T}{jJ} \right)^3} \left(\frac{jJ}{k_B} - T \right)^{1/2} \sim (T_c - T)^{\beta}$$

- Critical temperature and exponent:

$$T_c = jJ/k_B, \ \beta = 1/2.$$

- But exact results (analytically known):

$$T_c = 2/\ln(1 + \sqrt{2}) \approx 2.27, \ \beta = 1/8$$

for a square lattice with $j = 4$ and $J = k_B$.

- Will now turn numerical/simulation

Strategy of simulation

- Strategy very similar to what's been done before: Use the random number generator to evolve the system
- This time: RNG to describe interactions
- Necessary: Interactions in probabilistic language
- Algorithm will look like: Go over the spins, check whether they flip (compare $\mathcal{P}_{\text{flip}}$ with number from RNG), repeat to equilibrate.
- To calculate $\mathcal{P}_{\text{flip}}$: Use energy of the two micro-states (before and after flip) and Boltzmann factors.
- While running, evaluate observables directly and take thermal average (average over many steps).

Metropolis

A classical method for the program above

1. Initialise the lattice, i.e. fix all s_i
   (either at random, or $s_i = 1 \forall i$, or similar)

2. In each time step go through the entire lattice.
   For each spin decide whether it flips or not

   ▸ Calculate $E = -J \sum s_i s_j$ for both configs
   ▸ Determine characteristic "energy gain by flip"
     $E_{\text{flip}} = E_{\text{after}} - E_{\text{before}}$
   ▸ if $E_{\text{flip}} < 0$, the spin is flipped
   ▸ if $E_{\text{flip}} > 0$, the spin is flipped with probability
   $$\mathcal{P}_{\text{flip}} = \exp\left(-\frac{E_{\text{flip}}}{k_B T}\right)$$

3. Repeat with a huge number of time steps
   $\implies$ allow the system to equilibrate

Why Metropolis is correct: Detailed balance

- Consider one spin flip, connecting micro-states 1 and 2.
- Rate of transitions given by the transition probabilities $\mathcal{W}$
- If $E_1 > E_2$ then $\mathcal{W}_{1 \to 2} = 1$ and $\mathcal{W}_{2 \to 1} = \exp\left(-\frac{E_1 - E_2}{k_B T}\right)$
- In thermal equilibrium, both transitions equally often:
$$\mathcal{P}_2 \mathcal{W}_{2 \to 1} = \mathcal{P}_1 \mathcal{W}_{1 \to 2}$$
  This takes into account that the respective states are occupied according to the Boltzmann factors.
- In principle, all systems in thermal equilibrium can be studied with Metropolis - just need to write transition probabilities in accordance with detailed balance, as above.
- Metropolis algorithm simulates the canonical ensemble, summing over micro-states with a Monte Carlo method.

Some code specifics

<u>Initialise</u> the $L \times L$ lattice with spins s_i.

Take the spins either fixed (all $s_i = 1$) or at random (all $s_i = \pm1$)

A single time-step: sweep through the lattice
Go systematically through the lattice, line by line, spin by spin, and decide, whether the spin should flip or not. Important here: boundary conditions

Boundary conditions (finite-size lattices)
We use periodic boundary conditions. This means that the spins at the right edge of the lattice are taken as neighbours of spins at the left edge. For 2-D lattices this renders our lattice effectively a donut-shaped object. Such a treatment reduces finite-size effects, but one should keep in mind that correlations with a length larger than $\sqrt{2}L$ cannot be simulated.

Sweeping though the lattice

▶ Fix temperature, use a 10×10 lattice
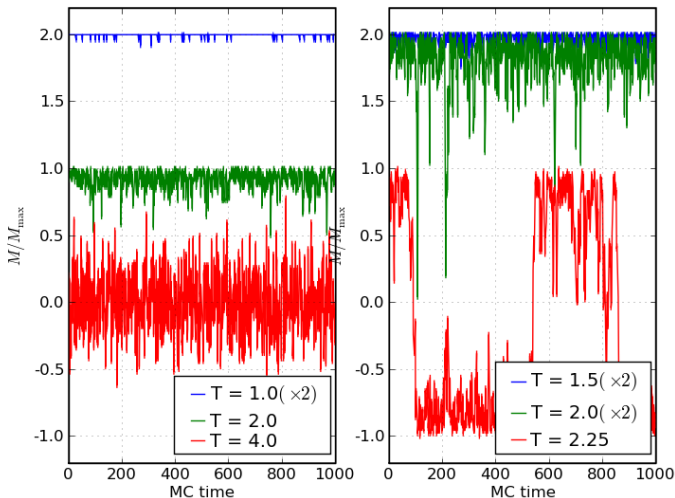
Discussion of the sweeps

- ▶ At low temperatures ($T = 1$): system quite stable, only small fluctuations, relative magnetisation around 1.
- ▶ At larger temperatures, but below T_c (T=2): larger fluctuations due to more favourable Boltzmann factor (10% anti-aligned), average magnetisation around 0.9.
- ▶ At large temperatures ($T = 4$): system disordered, no average magnetisation left.
- ▶ Around the critical temperature ($T = 2.25$): Huge fluctuations, after periods of stability, system jumps from sizable positive to negative magnetisation and vice versa.
- ▶ This is in agreement with fluctuation-dissipation theorem (next lecture).

Phase transition - the MC look at things

- Still on a 10×10 lattice

Ising model MC: M vs. T ($10 \otimes 10$ lattice)
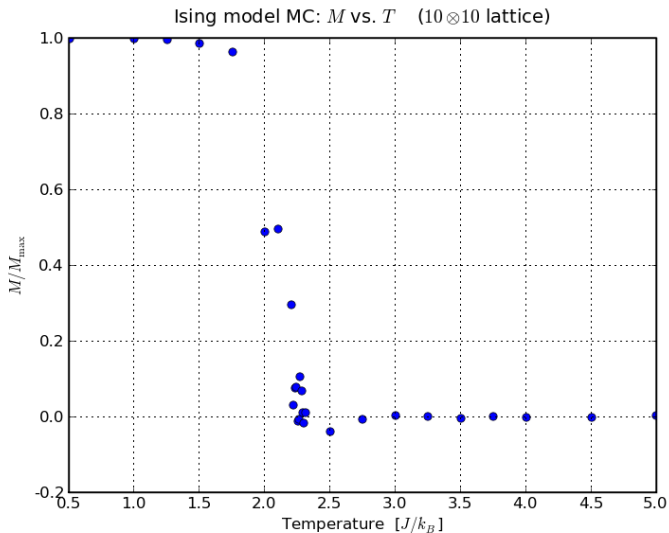
Some simulation nitty-gritty

- Results above after equilibrating the system, but
- critical slowdown around critical point:
  The system's time to equilibrate diverges.
- Independent of this: Monte Carlo results in agreement
  with exact calculation and in disagreement with the
  results from mean field approximation.

Summary

- First simulation of a system with interactions
- Used the Ising model as laboratory: well-defined, well-studied system, analytical results known, a favourite of the simulators
- A (simple) analytical approximation: mean field theory gives qualitatively correct results: existence of a phase transition, estimate of critical temperature
- Exact calculations (and simulation) agree and are quantitatively different from MFA.