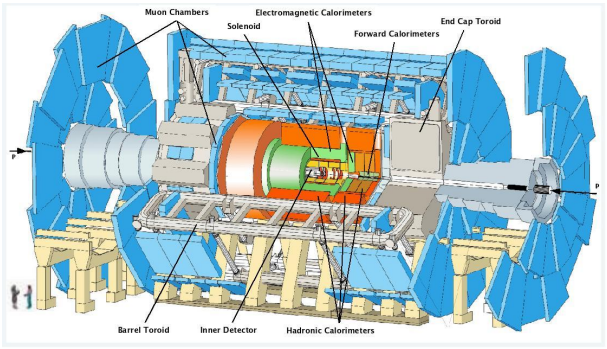
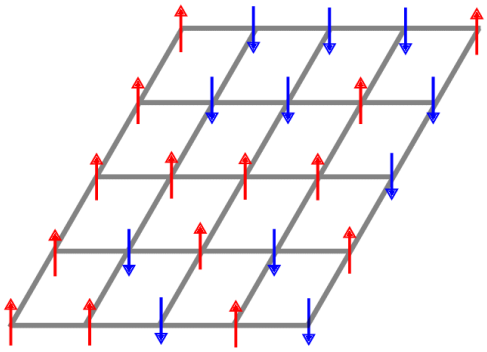
Lecture 7:

The Ising model



A magnet at Cern.

Credit: Cern



2D Ising model.

Credit: Sascha Wald

Ising model: Introduction

- Build-on previous lectures (random walks, cluster growth, percolation) by adding interactions between particles

  i.e. between occupied sites of the regular grid discussed in Lecture 7

- In addition, add a random component to mimic the effects of temperature on the system

  not surprisingly, this results in a system with more complex behaviour

  simulation mimics thermodynamic behaviour of a 'real' system

- We will use this Ising model as a model for ferro-magnetism

  and study the phase transition associated with ferro magnetism

Ising model: Introduction

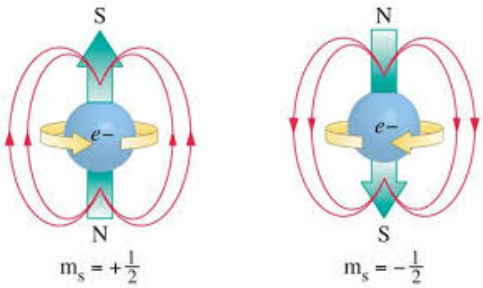


Illustration of the relation between an electron's spin and its magnetic moment. Credit: Princeton University

The physics! Electrons have a quantum mechanical property called *spin*. When spin is measured along *any* axis, its value is either $\hbar/2$ or $-\hbar/2$, where $2\pi\hbar$ is Planck's constant. An electron's spin is closely related to its magnetic moment - it is as if an electron is a tiny bar magnet with a North (N) and South (S) pole, with the N pole either pointing up or down. Just as is the case for bar magnets, the magnetic moments of two electrons close together create a force between them, such that they will preferentially line up anti-parallel. So we would expect the spins of two electrons close together to each other to be preferentially anti-aligned. However, there is more to it than that, because (*i*) electrons repel each other electrostatically since they have the same charge, and (*ii*) the Pauli exclusion principle, which states that no two electron can be in the same quantum mechanical state. So consider electrons arranged on a regular grid, and focus on a nearest-neighbour pair. When anti-aligned, they can be close together since they are in different quantum mechanical states, and hence they will repel each-other electrostatically. In contrast when aligned, they can never get close to each other because that would violate Pauli's exclusion principle, therefore the electrostatic repulsion between them is not very strong. The upshot of this is, that it is energetically favourable to be in the parallel spin state. The difference in energy (between parallel and anti-parallel) is mostly electrostatic in origin, and can be quite large (of order $\sim$ eV). This is much larger than the energy associated with the magnetic interaction. As a consequence, electron spins on a regular lattice will tend to be aligned in the same direction, with the combined magnetic moment of each electron adding to a large net magnetic moment - this is Ising's model for ferromagnetism, click here if you want to know more. In single atoms, the same phenomenon gives rise to Hund's rules for ordering orbitals in energy.

Ising model: Introduction

- Ising's model is a superb *toy model* to understand the physics of ferromagnetism
- Subject of E. Ising's PhD thesis (1920's)

Ising model: Mathematical model

we will restrict ourselves to a two dimensional (2D) Ising model

- Consider a 2D square lattice with spins at each lattice site
- Spins can have two values: $s_i = \pm 1$

  our convention here - see below for correct units
- Take into account only nearest neighbour interactions

  left-right, up-down. Nearest-neighbour interaction is good approximation because Pauli's exclusion principle only relevant if spins are close
- Write total energy due to electron interactions as

$$E = \sum_{i=1}^{N} E_i \,; \quad E_i = -\frac{J}{2} \sum_{j=i\pm 1} s_i \, s_j \,,$$

  Sum i runs over all N lattice sites on the square lattice, sum j runs over *neighbours* of i; factor $1/2$ to avoid double counting pairs. Unfortunately, the course book misses this factor of 2.
- J is the exchange constant, $J > 0$ for ferromagnets

Ising model: Mathematical model

- Look at units: $\tilde{J} \times (\tilde{s})^2$ has dimension of energy, where $\tilde{s}$ is physical spin with units $\hbar$, and $\tilde{J}$ is the exchange constant
- In our notation, $\tilde{s} = \frac{\hbar}{2} s$, so $\tilde{s} = \pm\frac{\hbar}{2}$ implies $s = \pm 1$
- Therefore $\tilde{J} = \tilde{J}(\frac{\hbar}{2})^2 s^2 \equiv J s^2$ and J has the dimension of energy
- Energy of lattice depends on whether spins are mostly aligned, or mostly random
  - If all spins are aligned, $E = -2JN$ - lowest energy state
  - If spins are random, $E \approx 0$

Ising model: Mathematical model

Consider a 2D lattice of spins, at a given temperature, T. Temperature means electrons can jiggle about:

if T is sufficiently high, spins can flip randomly

- Probability of spin flip from state 1 $\rightarrow$ state 2

  e.g from up to down, or vice versa

  is the *Boltzmann factor*

$$\mathcal{P}_{12} \propto \exp\left(-\frac{E_{12}}{k_B T}\right)$$

  $E_{12} \equiv E_2 - E_1$, the difference between the energy in the final state (*i.e.* state 2) and initial state (*i.e.* state 1); k_B is Boltzmann's constant

- if $E_2 < E_1 \rightarrow E_{12} < 0$, $\mathcal{P}_{12} > \mathcal{P}_{21}$ more likely to flip to lower energy state
- if $|E_{12}| \ll k_B\, T$, $\mathcal{P}_{12} \approx \mathcal{P}_{21}$ at high T, flips in either direction equally likely

Ising model: Mathematical model

Suppose we have a spin lattice at a given value of T. Spin may or may not flip. Which **macroscopic quantities** can we compute, and how are they related to the individual spin states?

- For a *given* spin configuration, called 'micro states'
  - Total energy: $E = -\frac{J}{2} \sum_{i=1}^{N} s_i \left(\sum_{j=i\pm1} s_j \right)$
  - Magnetisation: $M = \sum_i^N s_i$

    M is dimensionless, get physical magnetization by multiplying with electron's magnetic moment
- A given value of T can correspond to many micro state. The macroscopic state's properties are
  - $E = \sum_\alpha E_\alpha \mathcal{P}_\alpha$
  - $M = \sum_\alpha M_\alpha \mathcal{P}_\alpha$

  Weigh each micro state by its probability, $\mathcal{P}_\alpha$.

  Problematic because computational expensive: there are *very* many possible micro states (in fact, 2^N)
- Need good way of calculating these macroscopic values - we discuss two of them

Ising model: Mean Field Approximation

MFA - for Mean Field Approximation

- Elegant method - but its predictions are not very accurate

  is only an approximation

- MFA: Replace individual spins with average spin, $s_i = \pm 1 \rightarrow \langle s \rangle$

$$M = \sum_i s_i \longrightarrow M = \sum_i \langle s \rangle = N\langle s \rangle \equiv N\langle s_i \rangle$$

- Works well for infinitely large system where all spins are equivalent
- How can we compute this in practise?

Ising model: Mean Field Approximation

- Add an external magnetic field appears to be a detour, but wait & see!

$$E = -\frac{J}{2}\sum_{i=1}^{N}\left(\sum_{j=i\pm1} s_i s_j\right) - \mu H \sum_i s_i$$

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

- Apply this to a system with just one spin:

$$E_\pm = \mp \mu H$$

notice how $\pm \to \mp$: spin aligned with H has less energy than anti-aligned

- This has two micro states, with probabilities $\mathcal{P}_\pm = C \exp\left[\pm \frac{\mu H}{k_B T}\right]$
- Determine normalisation C by requiring $\mathcal{P}_+ + \mathcal{P}_- = 1$

$$\Longrightarrow C = \frac{1}{\exp\left(\frac{\mu H}{k_B T}\right) + \exp\left(-\frac{\mu H}{k_B T}\right)} = \frac{1}{2\cosh\left(\frac{\mu H}{k_B T}\right)}$$

- Therefore thermal average of the single spin:

$$\langle s_i \rangle = \mathcal{P}_+ - \mathcal{P}_- = \tanh \frac{\mu H}{k_B T}$$

Ising model: Mean Field Approximation

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

$$E = -\sum_i \left(\frac{J}{2} \sum_{j=i\pm 1} s_j + \mu H \right) s_i \equiv -\mu H_{\text{eff}} \sum_i s_i$$

- The effective magnetic field is therefore

$$H_{\text{eff}} = \frac{J}{2\mu} \sum_{j=i\pm 1} s_j + H$$

- Mean field approximation: set $s_j \to \langle s \rangle$ and $H \to 0$:

$$H_{\text{MFA}} = \frac{nJ}{2\mu} \langle s \rangle$$

Here, n is the number of nearest neighbours, $n = 4$ in our 2D case

- Combining this with $\langle s \rangle = \tanh \frac{\mu H_{\text{MFA}}}{k_B T}$ yields a non-linear equation for $\langle s \rangle$

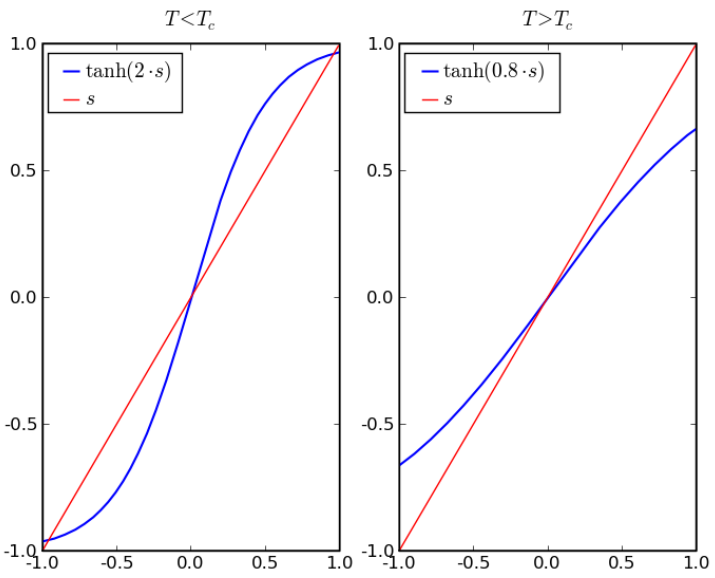
$$\langle s \rangle = \tanh \left(\frac{T_c}{T} \langle s \rangle \right) ; \quad T_c \equiv \frac{nJ}{2k_B} .$$

T_c is called the critical temperature

Ising model: Mean Field Approximation

numerical example, for $T = \frac{T_c}{2}$ ('low' T, left panel) and $T = \frac{T_c}{0.8}$ ('high' T, right panel)

- Notice the two different regimes:
  3 solutions $T < T_c$, left or 1 solution which $=0$ $T > T_c$, right



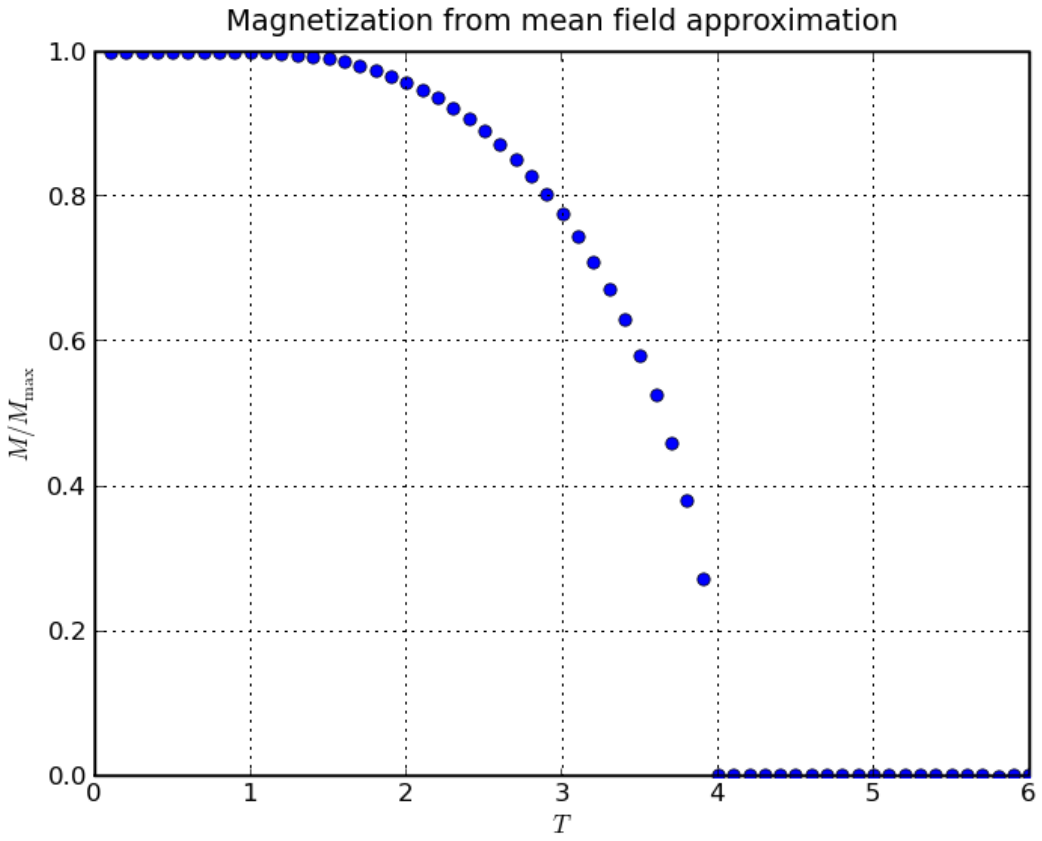
left panel: low T, magnetization, can be up, $\langle s \rangle = 1$, or down, $\langle s \rangle = -1$, or no magnetization, $\langle s \rangle = 0$

right panel: high T, no net magnetization, $\langle s \rangle = 0$

Ising model: Mean Field Approximation

Magnetization as a function of temperature

- Solve numerically $f(\langle s \rangle) = \langle s \rangle - \tanh \frac{T_c \langle s \rangle}{T} = 0$



Ising model: Mean Field Approximation

- When making plots: plot M in units of $M_{\max} = N$, and set $J = k_B$ for simplicity.
- Plots illustrates a phase transition at $T = T_c$ ($T_c = 2J/k_B = 2$) of *second order*

  meaning 1st derivative of order parameter, in this case magnetisation, is discontinuous at transition
- Around T_c: $\frac{\mathrm{d}M}{\mathrm{d}T} \to \infty$.
- Exact form of singularity from Taylor expansion of tanh:
$$\tanh x = x - \frac{x^3}{3} + \mathcal{O}(x^4)$$
- Therefore, around $T = T_c$:
$$\langle s \rangle = \frac{T_c}{T} \langle s \rangle - \frac{1}{3} \left(\frac{T_c}{T} \right)^3 \langle s \rangle^3$$

Ising model: Mean Field Approximation

- Examine behaviour around $T = T_c$: define $\eta \equiv \frac{T_c}{T} - 1$, with $0 < \eta \ll 1$

$$\langle s \rangle = (3\eta)^{1/2} \propto (T_c - T)^{1/2} \propto (T_c - T)^{\beta}$$

- Critical temperature and critical exponent:

$$T_c = \frac{nJ}{2k_B}; \quad \beta = \frac{1}{2}$$

- Exact analytical (non MFA) result is

$$T_c = \frac{2.27\,J}{k_B}; \quad \beta = \frac{1}{8}$$

for a square lattice with $n = 4$

- Will now turn numerical/simulation treatment

Ising model: Numerical treatment

- Strategy very similar to what's been done before: Use a random number generator to decide whether to flip a spin

  spin flip probability is Boltzmann factor

- Algorithm: loop over spins one at a time, decide whether it flips (compare $\mathcal{P}_{\text{flip}}$ with number from RNG), repeat until M equilibrates
- 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).

Ising model: Numerical treatment

this is called the *Metropolis* algorithm Layout of programme:

1. Initialise the lattice, *i.e.* choose s_i for each spin (either at random, or $s_i = 1 \forall i$, or similar)
2. Sweep over all spins
   At each step, decide whether or not to flip spin:
   - Calculate the system's energy $E = -J/2 \sum s_i s_j$
     - for current spin state, energy E_1
     - if spin were flipped, energy E_2
   - Calculate $\Delta E = E_2 - E_1$
     - $\Delta E < 0$: flip spin
     - $\Delta E \geq 0$: flip spin if

$$\exp\left(-\frac{\Delta E}{k_B T}\right) > \mathcal{R}$$

   where $\mathcal{R}$ is a random number $\in [0, 1]$
3. Repeat step 2 until magnetization in equilibrium at T_c, never in equilibrium

Ising model: Numerical treatment

why does Metropolis algorithm work: Detailed balance

- Consider spin flips between states 1 and 2 energy E_1, and $E_2 > E_1$
- Metropolis algorithm:
  - Probability spin flip $1 \to 2$ is $\mathcal{P}_{1\to 2} = 1$
  - Probability spin flip $2 \to 1$ is $\mathcal{P}_{2\to 1} = \exp\left(-\frac{E_1 - E_2}{k_B T}\right) \leq 1$

  Does this give the right answer?

- Analysis: Let W_1 be the fraction of spins in state 1 & W_2 for state 2
  The rate of transitions from $1 \to 2$ and vice versa is

$$\mathcal{R}_{1\to 2} = W_1\, \mathcal{P}_{1\to 2} = W_1\,; \;\; \mathcal{R}_{2\to 1} = W_2 \mathcal{P}_{2\to 1} = W_2\, \exp\left(-\frac{E_1 - E_2}{k_B T}\right)$$

the product of the fraction of spins in a given state times the probability that a spin flips

In thermal equilibrium, $\mathcal{R}_{1\to 2} = \mathcal{R}_{2\to 1}$, in which case $W_1/W_2 = \exp(-(E_1 - E_2)/k_B T)$ that is, states are occupied according to the Boltzmann distribution. Applying the Metropolis algorithm therefore drives systems to thermal equilibrium

Ising model: Numerical treatment

- Metropolis algorithm drives system to thermal equilibrium

$$\frac{W_1}{W_2} = \exp(-(E_1 - E_2)/k_B T)$$

W_1 and W_2 fraction of spin in states 1, and 2, with energies E_1 and E_2

- 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* by summing over micro-states with a Monte Carlo method.

Ising model: Numerical treatment

Sketch of Metropolis code

Initialise an $L \times L$ lattice with spins s_i.

Set all i spins constant, $s_i = 1$, or at random, $s_i = \pm 1$

Sweep over all spins

Sweep (meaning go) systematically through the lattice, line by line, column by column, and decide for each spin in turn whether it flips or not. Note that, to compute ΔE for a given flip, you **do not need to sum over all spins**

Impose periodic boundary conditions

spin at $(0, j)$ has neighbours at $(1, j)$ **and** $(L-1, j)$, in addition to $(0, j+1)$ and $(0, j-1)$. 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

Compute M so that you can plot M versus number of sweeps

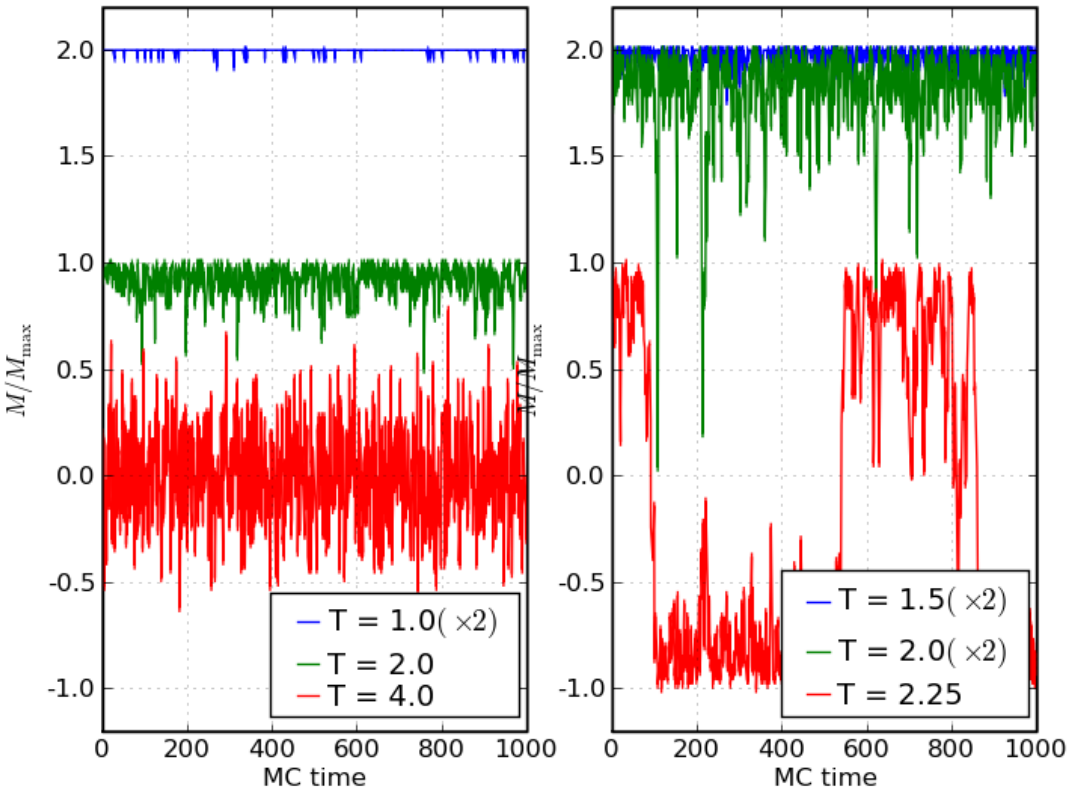
Ising model: Numerical treatment

- In workshop: **red-black sweeps** subtlety in sweeping over spin
  - Consider a chess-board: has red and black squares
  - when sweeping over spins:
    - sweep over red spins first first horizontally, then vertically
    - then sweep over all black spin first horizontally, then vertically
- this improves the rate at which the system thermalises

Ising model: Numerical treatment

Example of M as a function of sweep number

- At choosen T, sweeps on an 10×10 lattice



Ising model: Numerical treatment

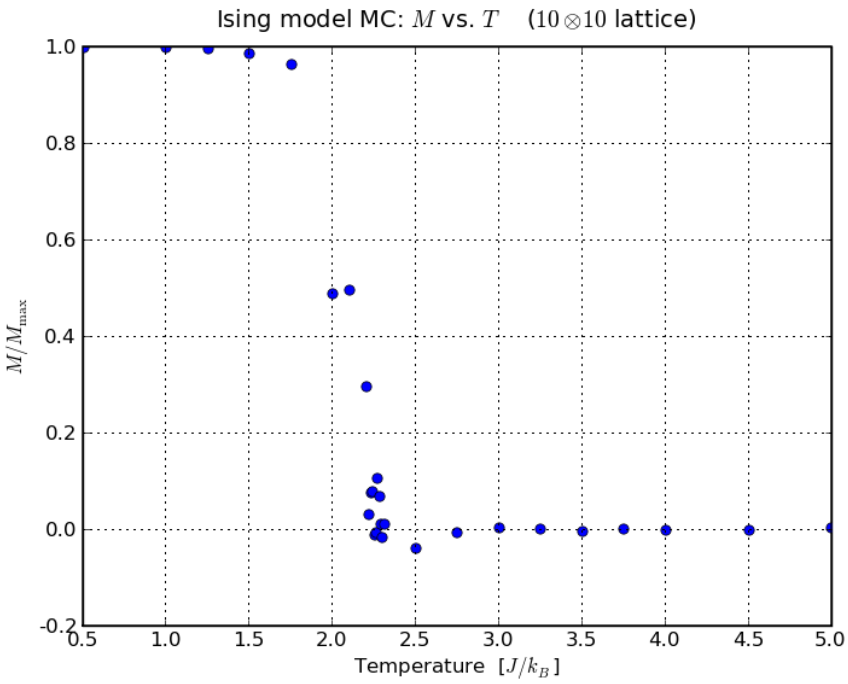
Analysis of result

- At low temperature ($T = 1$ or $T = 1.5 \ll T_c \approx 2$): system quite stable, with small fluctuations around $M = M_{\max}$
- At high temperature ($T = 4 \gg T_c \approx 2$): system has $M \approx 0$, with relatively large fluctuations around $M = 0$
- At intermediate temperatures ($T = 2$) we see very large fluctuations
- Close to the critical value ($T = 2.25 \approx T_c$) see even large fluctuations, with $M \approx 1$ for a large number of sweeps, followed by a jump to $M = -1$ for a large number of sweeps

Ising model: Numerical treatment

Phase transition - the MC look at things

- Analyse 10×10 lattice as function of temperature



As expected from MFA: when $T \ll T_c$: spins are aligned, $M \approx M_{\max}$

When $T \gg T_c$ spins are not aligned, $M \approx 0$. Second-order phase-transition around $T = T_c \approx 2J/k_B$

Ising model: Numerical treatment

Discussion

- Results above plotted when system is in equilibrium
- critical slowdown around critical point:
  The system's time to equilibrate diverges (never in equilibrium)
- Independent of this: Monte Carlo results in agreement with exact calculation and MFA calculation not very accurate but does describe generic behaviour correctly

Summary

- Simulation of a system with interactions here, between spins
- 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. Interestingly, numerical answers gets closer to MFA for larger I