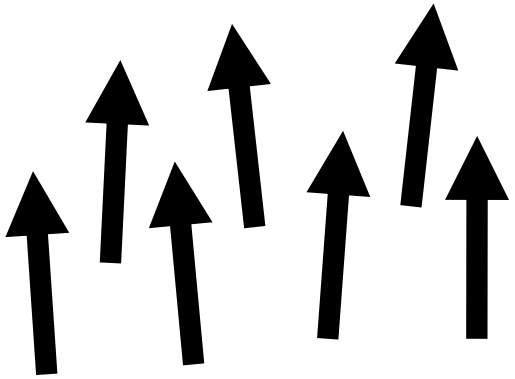
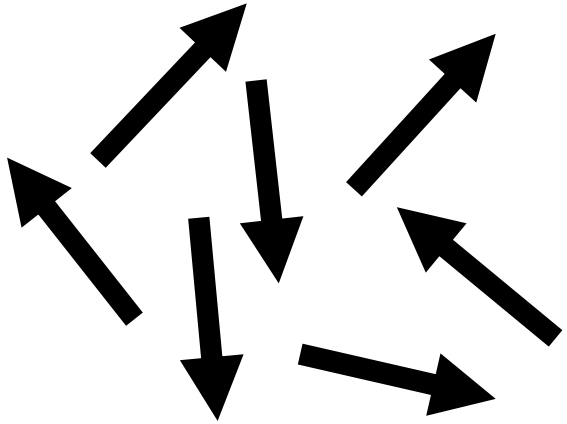
Lecture 7: Introduction to the Ising model



Ferromagnet
(low temperature)



Paramagnet
(high temperature)

Anton Souslov A.Souslov@bath.ac.uk

Content of this lecture

Brief reminder of ferromagnetism, and introduction to the Ising model

How to simulate the Ising model (Metropolis Monte Carlo algorithm)

Application of statistical mechanics to the Ising model (Boltzmann distribution)

How to use computer simulations to measure/predict physical observables such as energy or magnetisation, as a function of temperature (including a note on errors)

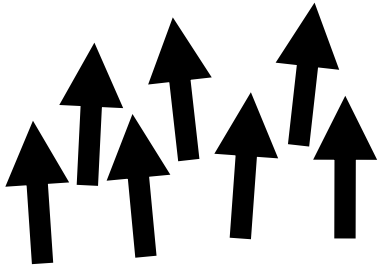
Ferromagnets

Electron spins in metals can lead to *ferromagnetism* (permanent magnets). The reason is that if the spins of electrons in nearby atoms align in order to lower their energy.

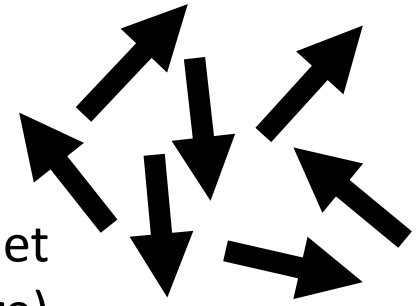
This means that at room temperature (and at lower temperatures), materials like iron prefer to have all their spins aligned.

At higher temperatures, systems prefer to increase their *entropy*, so all the spins point in random directions.

These high and low temperature regimes are separated by a special point, called a *phase transition.*

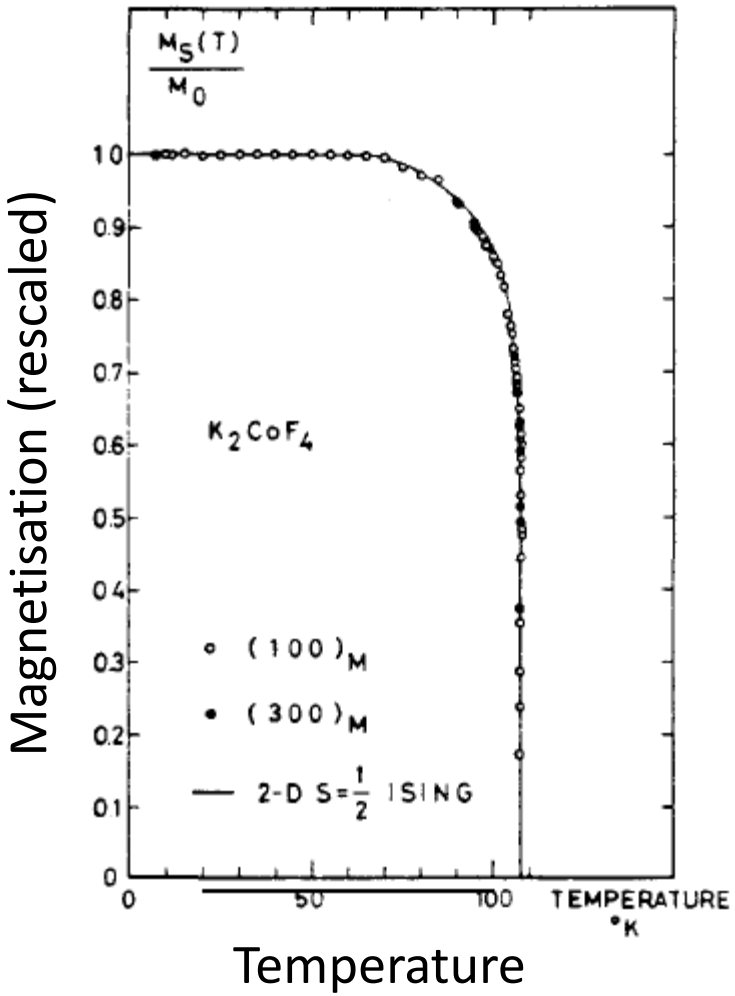


Ferromagnet
(low temperature)



Paramagnet
(high temperature)

Phase transition

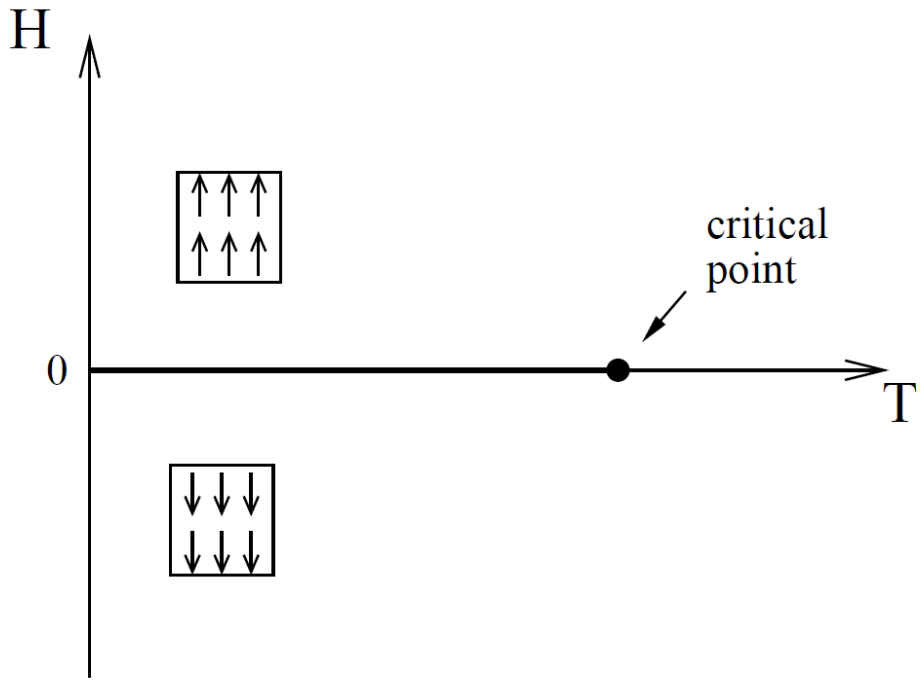


Experimental data for a magnetic material consisting of potassium, cobalt and fluorine

Sharp increase in magnetisation at the phase transition (approx 108K)

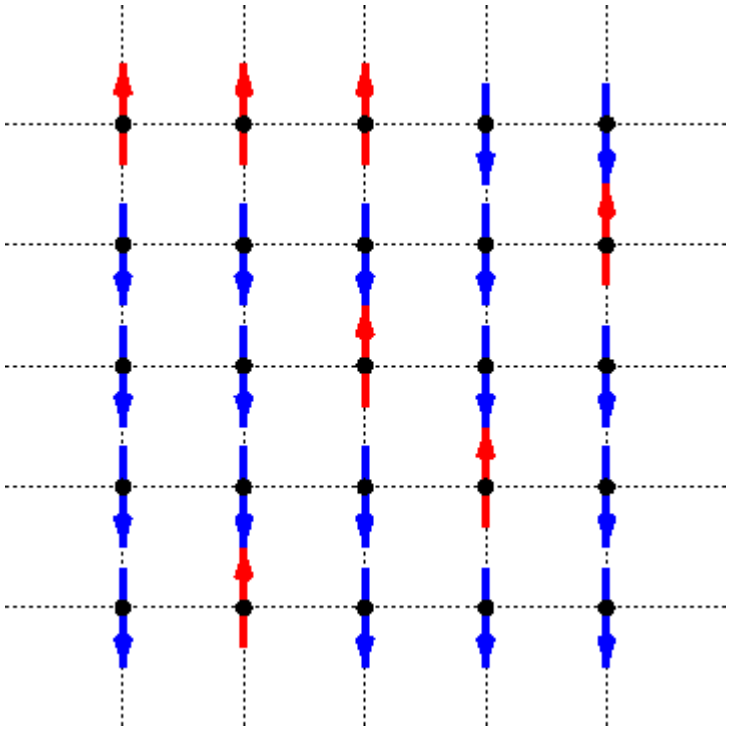
H Ikeda and K Hirakawa, Solid State Communications 14, 529 (1974)

Phase diagram

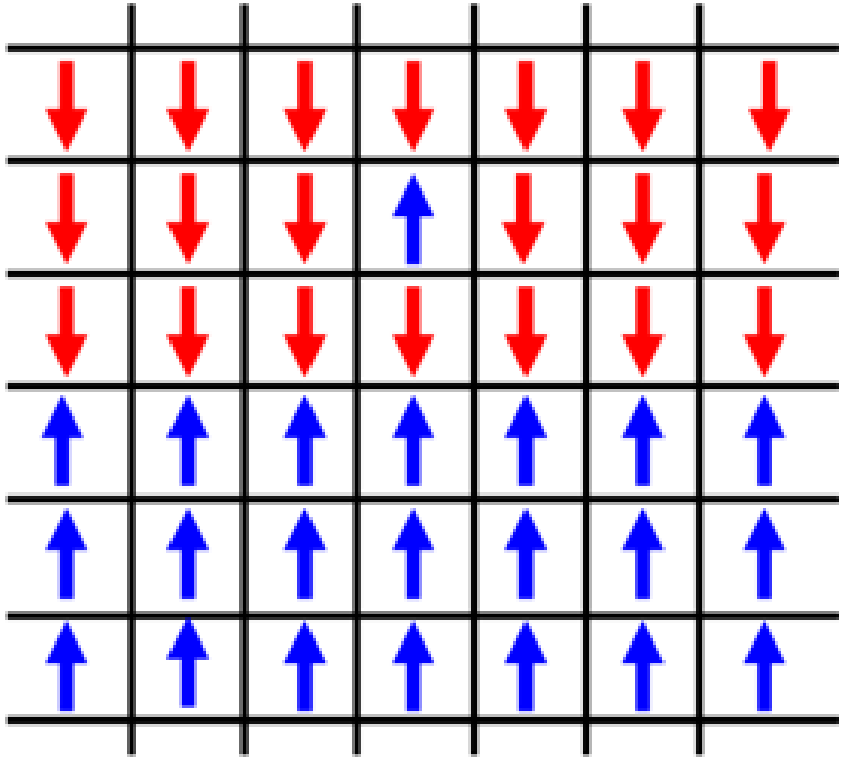


Up and down phases in a magnetic field-temperature phase diagram

Ising model of a ferromagnet



Mostly spin down
with some spin up

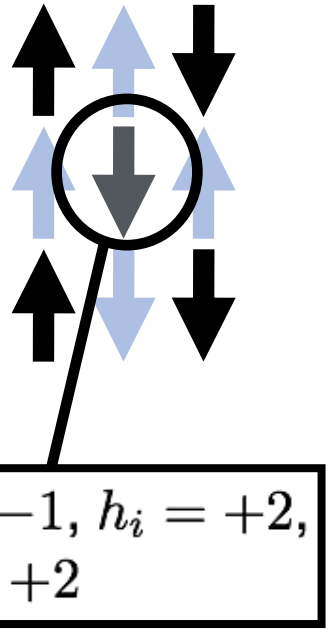


Domain wall between
spin down and spin up

Ising model

[E Ising, Zeitschrift fuer Physik A, **31**, 253 (1925)]

For simplicity, consider N spins on a square grid.
Let s_i be the state of spin i.
For simplicity, either $s_i = 1$ (up) or $s_i = -1$ (down)



Magnetisation $M = \frac{1}{N} \sum_i s_i$, is between -1 (all down) and $+1$ (all up)

The energy of each spin depends only on its nearest neighbours (n.n.) as $E_i = -h_i s_i$, with "local magnetic field"

$$h_i = J \sum_{\text{n.n. } j \text{ of } i} s_j$$

where J is the strength of the interaction.

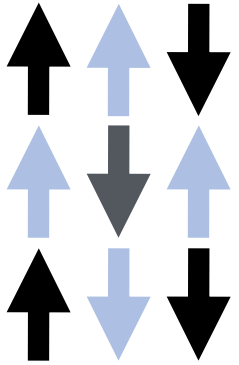
[see also the coursework handout]

Ising model

Repeated from previous page

The energy of each spin depends only on its nearest neighbours (n.n.) as $E_i = -h_i s_i$, with "local magnetic field"

$$h_i = J \sum_{\text{n.n. } j \text{ of } i} s_j$$



The total energy is $E = \frac{1}{2}\sum_i E_i$ The factor of $\frac{1}{2}$ is just for convenience, it means that we can write

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

where the sum runs over all pairs of nearest neighbours (with each pair counted once)

Physically, the system at low temperatures should have low energy, expect $M \approx \pm 1$.

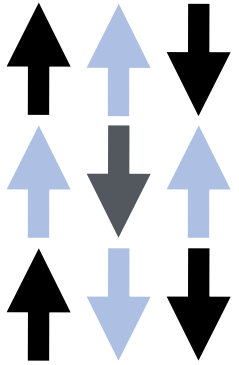
At high temperatures, symmetry means that up and down spins are equally likely, expect $M = 0$.

Ising model

Repeated from previous page

The energy of each spin depends only on its nearest neighbours (n.n.) as $E_i = -h_i s_i$, with "local magnetic field"

$$h_i = J \sum_{\text{n.n. } j \text{ of } i} s_j$$



The total energy is $E = \frac{1}{2}\sum_i E_i$ The factor of $\frac{1}{2}$ is just for convenience, it means that we can write

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

where the sum runs over all pairs of nearest neighbours (with each pair counted once)

$$E = -J \sum_{<ij>} s_i s_j - H \sum_i s_i$$

External field H

Ising model

In the coursework, the Ising model is studied by using:

1) Metropolis algorithm
   - Computational approach based on Monte Carlo simulations
   - More details in this lecture (see, also the coursework handout)

2) Theoretical solutions
   - Exact solution for 2d Ising model by L. Onsager (1944)
   - Mean-field (Curie-Weiss) theory
   - We'll see more details about these in the next lecture (see, also the coursework handout)

Both options have their benefits and limitations. One of your tasks in the coursework is to compare the numerical and theoretical results.

Metropolis Monte Carlo

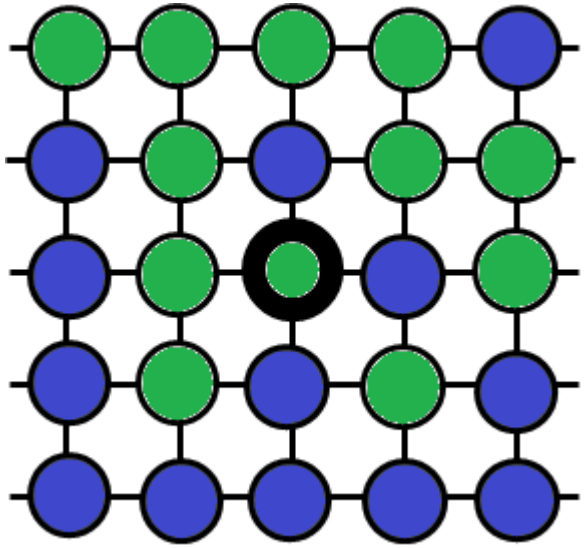
[N Metropolis *et al*, J. Chem Phys. **21**, 1087 (1953)]

We want to investigate the Ising model at *thermal equilibrium* (i.e. in a steady state given by the Boltzmann distribution)

Algorithm:

Pick randomly a spin site:

- Calculate the energy change $\Delta E_i = 2h_i s_i$ associated with the "flipping" the spin *i* (changing its colour)
- If $\Delta E_i < 0$, then flip the spin
- If $\Delta E_i > 0$ then flip the spin with probability $p_i = e^{-\Delta E_i/(k_B T)}$, where *T* is temperature



Repeat the process many times until thermal equilibrium is achieved

With this choice, the steady state of the model is consistent with the Boltzmann distribution

Boltzmann distribution

If we specify all the spins in the system, we say that the system is in a *microstate,* $S = \{s_1, s_2, \ldots, s_N\}$

In the equilibrium *macrostate* at a given temperature *T*, the system is in a microstate S with probability

$$p_B(S) = \frac{1}{Z(T)} e^{-E(S)/(k_B T)}$$

where $E(S)$ is the energy of the microstate and $Z(T) = \sum_S e^{-E(S)/(k_B T)}$ is the partition function (normalization constant)

Thermal equilibrium

Let's take a two microstate $S_1 = \{s_1, s_2, \ldots, si, \ldots, sN\}$ and $S_2 = \{s_1, s_2, \ldots, -si, \ldots, sN\}$ which are otherwise similar except the spin i is flipped, and that S_2 is higher in energy by ΔE.

Now, the probability of going from microstate S_1 to S_2 is

$$P(S_1 \rightarrow S_2) = pB(S_1) \times \frac{1}{N} \times e^{-\Delta E/(k_B T)}$$

probability of starting in state S_1

probability of choosing spin i

probability of accepting the move

On the other hand, the probability of going from microstate S_2 to S_1 is

$$P(S_2 \rightarrow S_1) = pB(S_2) \times \frac{1}{N} \times 1$$

because the state S_1 has lower energy.

Thermal equilibrium

The principle of *detailed balance* states that in thermal equilibrium the rate at which the system makes transitions from microstate S_1 to S_2 is equal to the rate at which the system makes reverse transitions

You can see that $P(S_1 \rightarrow S_2) = P(S_2 \rightarrow S_1)$ if

$$\frac{p_B(S_2)}{p_B(S_1)} = e^{-\Delta E/(k_B T)}$$

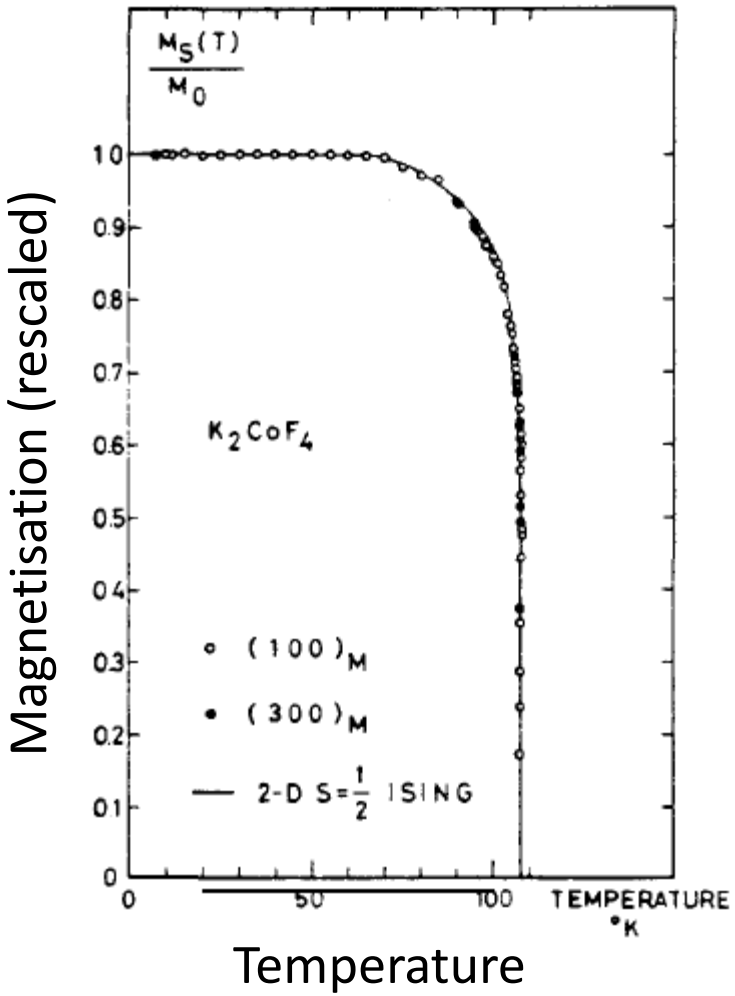
This indeed is true based on the definition of the Boltzmann distribution

$$p_B(S_1) = \frac{1}{Z(T)} e^{-E(S_1)/(k_B T)} \text{ and } p_B(S_2) = \frac{1}{Z(T)} e^{-E(S_2)/(k_B T)}$$

Hence the Metropolis algorithm obeys detailed balance

This can be used to prove that the method converges to the Boltzmann distribution

Ising model and real magnets



Experimental data for a magnetic material consisting of potassium, cobalt and fluorine (the *points* in the figure)

The *line* is a fit to results from an Ising model.

The model gets the shape of the curve precisely right…

H Ikeda and K Hirakawa, Solid State Communications 14, 529 (1974)

Outlook

Things to think about

It is clear that real magnetic materials are not as simple as the Ising model. Can we expect the model to agree with experiment?

Which quantities are most interesting to measure (and compare with experiment)?

Is there really a special temperature (phase transition) or can the system transform smoothly from M close to zero at high temperature to large M at low temperature?

Can we use theory to understand the model, and does this help us to understand the experiments?

Statistical Mechanics

Experimentally-observable quantities are obtained as averages.

For example, the average energy is

$$\langle E \rangle = \sum_S E(S) p(S) = \frac{1}{Z(T)} \sum_S E(S) \mathrm{e}^{-E(S)/k_\mathrm{B}T}$$

For the Ising model we can use our formula for the energy to write

$$p(S) = \frac{1}{Z(T)} \exp\left(-\beta_0 \sum_{\langle ij \rangle} s_i s_j\right)$$

where $\beta_0 = J/(k_\mathrm{B}T)$ is a dimensionless measure of the interaction strength.

Note: p is dimensionless, it can only depend on dimensionless variables such as β_0 (which can also be interpreted as an inverse temperature).

Ergodicity

So far, we explained that the system at equilibrium should be described by a Boltzmann distribution

Another important idea in statistical mechanics is that instead of averaging over many copies of a system (an *ensemble*), we can take averages over some long time period...

... we (usually) expect these two averages to be the same...

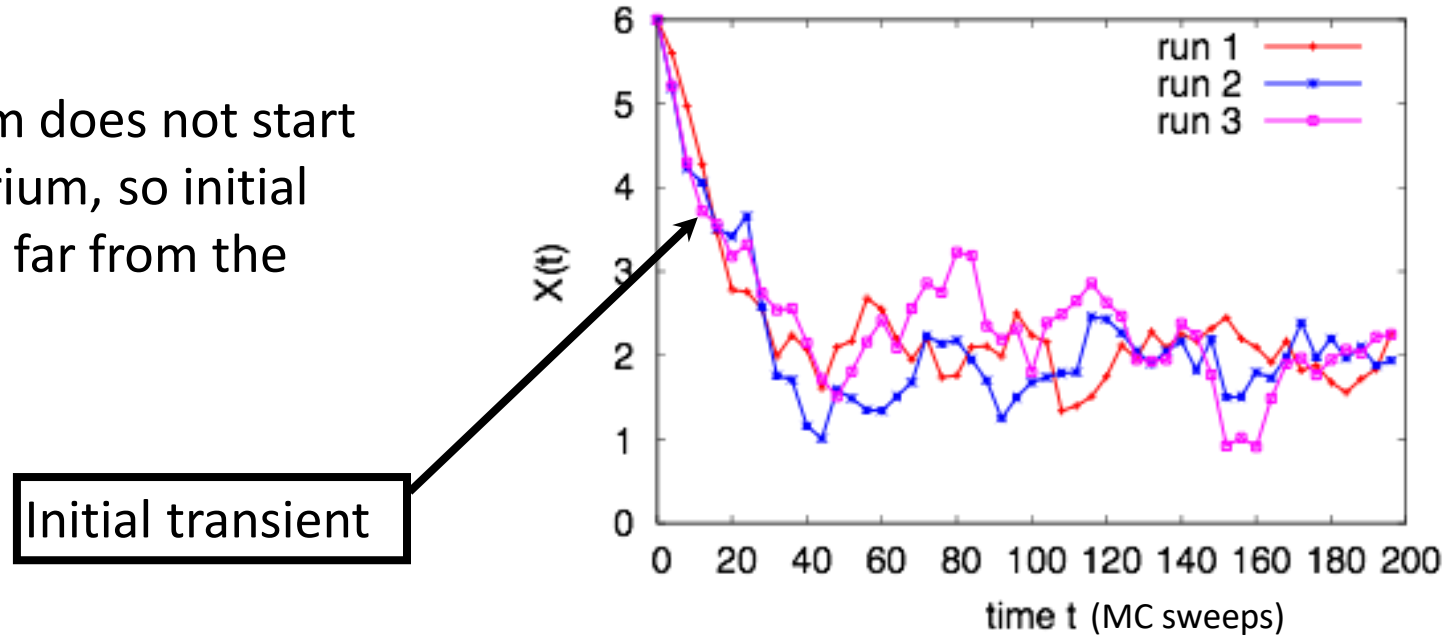
This is useful in *computational physics* because we can *simulate* the system over a long time, and use these data to estimate averages...

... e.g. measure how the (average) energy and magnetisation vary as a function of temperature

Ergodicity

Consider these example data where we measure some quantity X as a function of simulation time t, in three separate runs

The system does not start at equilibrium, so initial values are far from the average

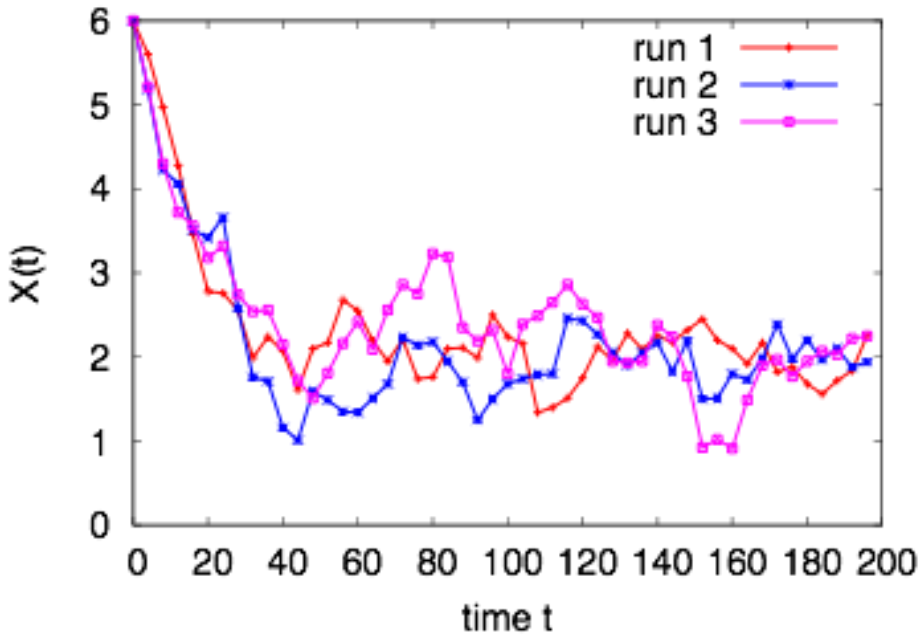


The idea of ergodicity is that if we ignore the transient, we can either average over different runs at the same time (e.g. t = 100) or we can average the data from a single runs at different times

[For example, average all the blue data for all times t > 50]

Time averages

Data points at nearby times are not independent (e.g. if one data point is above average, the next one is also likely to be above average)



To have an efficient estimate of the average, it is useful to have (more-or-less) independent measurements...

Suggested method for estimating averages: discard the first n_0 MC sweeps. Then take measurements every n MC sweeps. Do this until you have m measurements.

Overall you need to run for $n_0 + nm$ MC sweeps. For accuracy one should take n_0 and m large. For efficiency, it's good to have n large enough that your measurements are (roughly) independent

A note on errors...

Suggested method for estimating averages: discard the first n_0 MC sweeps. Then take measurements every n MC sweeps. Do this until you have m measurements.

Repeated from previous page

Your estimate of $\langle X \rangle$ will be

$$\overline{X} = \frac{1}{m} \sum_{i=1}^{m} X_i$$

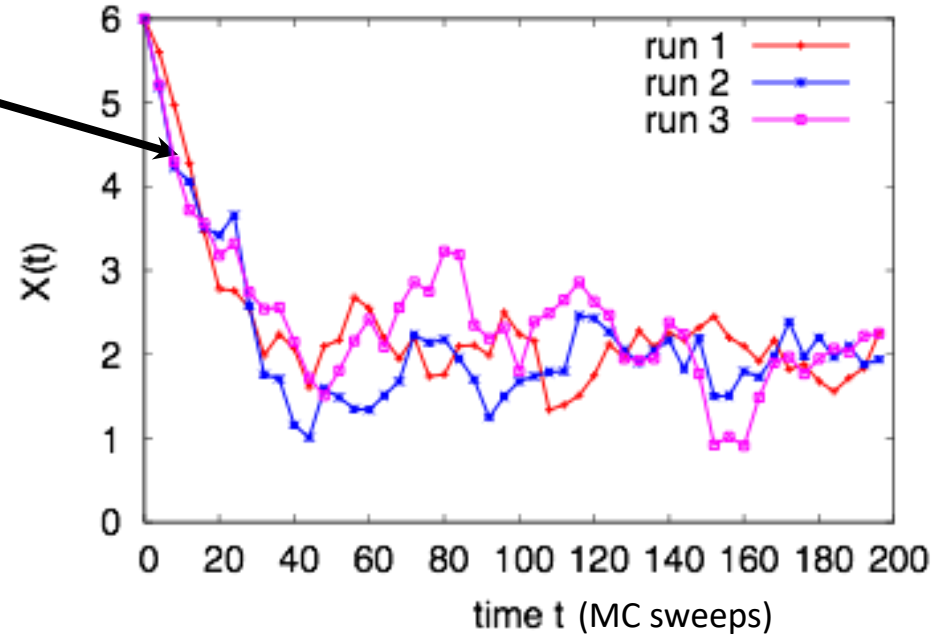
where X_i is the ith measurement.

If the measurements are independent then the standard error gives a good estimate of the uncertainty:

$$\overline{\sigma}_X = \frac{1}{\sqrt{m-1}} \sqrt{\frac{1}{m} \sum_{i=1}^{m} (X_i - \overline{X})^2}$$

But note: if measurements are not independent then $\overline{\sigma}_X$ is an underestimate of your uncertainty about the average.

Initial transients



Initial transients can also be interesting in themselves...

... if a system takes a long time to converge to its equilibrium state, this may be an indication that some interesting collective motion is happening...

... for example "coarsening", "aging"... slow transients in experiments can be compared with theories and models, to understand how different materials behave...

Note also: failing to exclude the transient when estimating averages can lead to *systematic errors*

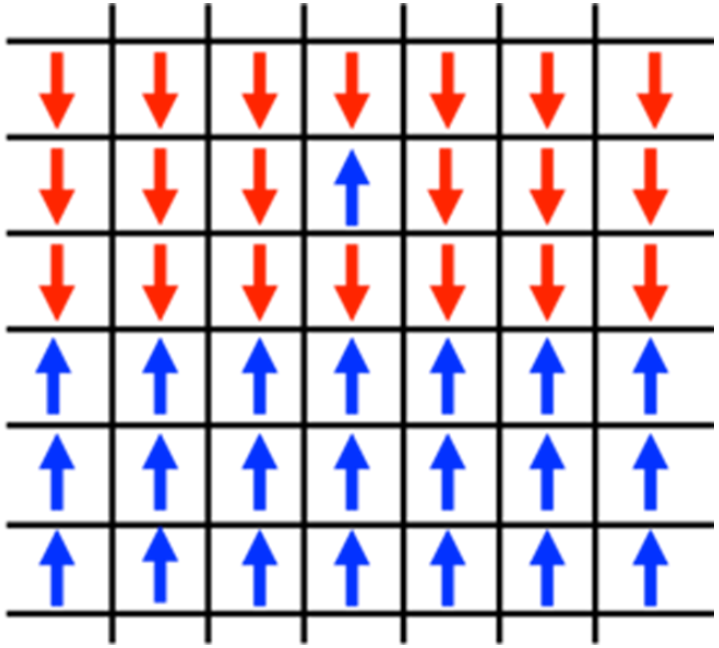
In general

The two dimensional Ising model is complicated enough to have non-trivial properties but simple enough to have an analytic solution

Ising model describes also other phase transitions (for example condensation) and other random systems that consist of elements that have two states (for example, neurons and neural networks in the brain)

Metropolis algorithm has many variants, for example Metropolis-Hastings algorithm which is used to sample multidimensional probability distributions

Summary



The Ising model is a very simple model of a magnet, in which nearby spins have low energy if they are aligned

The model has an equilibrium state described by the Boltzmann distribution

We can simulate the model using the Metropolis algorithm, and ergodicity means that we can use these simulations to estimate averages of observable quantities

When making such estimates and analysing their errors, we need to think about the initial transient and about using independent samples.