Theory of Complex Systems
Lecture Notes

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Chapter 0

Introduction

1 Introduction to Complex Systems

The science of Complex Systems is providing radical new ways of understanding how a large collection of components – locally interacting with each other at small scales – can spontaneously self-organize to exhibit non-trivial global structures and behaviors at larger scales. The properties of the collection may not be understood or predicted from the full knowledge of its constituents alone. The system is not just the "sum" of the behaviour of each part. For example, it is impossible to predict where traffic jams will occur by only studying the behaviour of individual drivers.

Examples of complex systems include crowd movement, human economies, climate, nervous systems, cells and living things, as well as social systems or telecommunication infrastructures.

Complex systems are systems whose behavior is intrinsically difficult to model due to the dependencies, competitions, relationships, or other types of interactions between their parts or between a given system and its environment. Systems that are "complex" have distinct properties that arise from these relationships, such as non-linearity, emergence, spontaneous order, adaptation, organisation and pattern formation among others.

What do we want to know from a complex system?

- Link micro rules to macro behaviour:
  Understand how interactions at a microscopic level create a macroscopic behaviour.

- Uncover hidden patterns and the structure of the system.

- Predict the macroscopic behaviour of a system.

- Study the stability of the system.
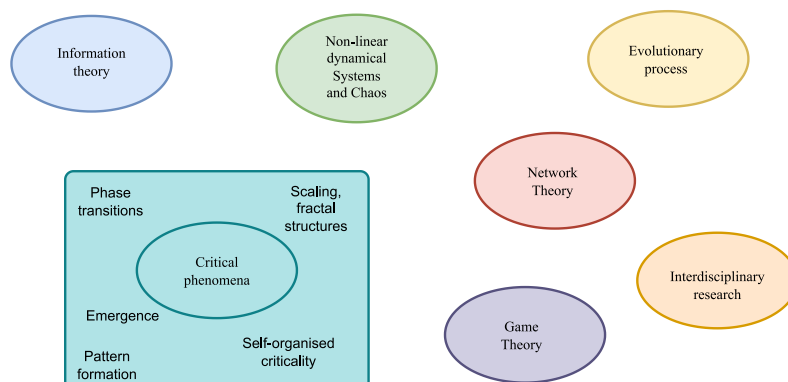
In this course, we will discuss a theory of complex systems with a main focus on phase transition, critical phenomena and emergence.

2 Introduction to Critical phenomena

The word "critical" is used in science with different meanings. Here we used it in the context of critical phenomena, in which the term "critical" describes a system that is at the border between order and disorder.

2.1 Phases and Phase Diagrams

2.1.1 Definitions

> **Phase:** A macroscopic state of a system that has physical properties that are uniform on a macroscopic length scale.

Scale	Physics/chemistry	Complex Systems
Microscopic	atomic scale	Scale of the individual component of the complex system
Macroscopic	'daily life scale'	Scale at which the system displays non-trivial collective behaviour

> **Phase transition:** When a system undergoes a drastic change in its macroscopic properties in response to a small change in the environment.

Thermodynamically, a phase transition occurs when there is a singularity in the free energy. The latter, as we will see, is the generator of many physical quantities. Therefore this drastic change is described theoretically by singularities in the physical quantities characterizing the system.

The phase of the system is determined by the values of a few parameters, such as the temperature and the pressure. We have chosen to represent the phase diagram in the $P - T$ plane, but there are not necessarily only two parameters that define the phase of a system.

2.1.2 Examples

Different phases of water. At atmospheric pressure, $P = 1[\text{atm}]$ ice turns to liquid water at exactly $0°$C.
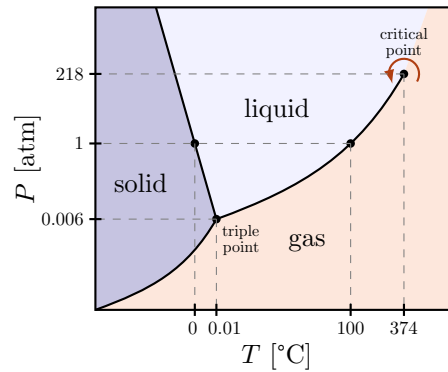
Figure 1: Phase diagram for water. The triple point corresponds to a coexistence of the three phases at this point. Beyond the critical point, there is no distinction between liquid and gas. It is possible to go from liquid to gas without crossing any boundary curve.

In figure 1 the solid-liquid coexistence curve continues indefinitely. No matter how high we make the pressure, there will always be two distinct phases and a transition between them. However in the liquid-gas coexistence curve there is an end point, called the **critical point**.

The existence of the liquid–gas critical point reveals a slight ambiguity in labelling the single phase regions. When going from the liquid to the gaseous phase, one usually crosses the phase boundary, but it is possible to choose a path that never crosses the boundary by going to the right of the critical point. Thus, the liquid and gaseous phases can blend continuously into each other (*supercitical fluid*).

Ferromagnetic-paramagnetic transition

context

We can think of a material composed of atoms that have a magnetic moment (like a 'tiny magnet'- due to unpaired electrons). Specifically we are interested in two types of material:

Paramagnetic material: barely behaves like magnet. It shows small attraction to magnets.
Ferromagnetic material: shows strong attraction to magnets (e.g. Iron, Cobalt, Nickel)

As we raise the temperature of a magnet, its magnetisation will vanish continuously at a critical temperature T_C (Curie Temperature). Intuitively, we can think of temperature as introducing noise to the system which leads the spins to point in a random direction and hence the sum of all these spin directions (magnetization) will be zero (paramagnetic phase).

Conversely, as we decrease the temperature of the material, a *spontaneous* magnetisation appears at T_c. Now all the spins are pointing to the same, but spontaneously chosen, direction (ferromagnetic phase).

(a) $T > T_c$: Paramagnetic phase. Each spin points in a random direction. Total magnetization $M = \sum_i s_i = 0$,

(b) $T < T_c$: Ferromagnetic phase. Every spin points to the same direction. Total magnetization $M = \sum_i s_i \neq 0$.
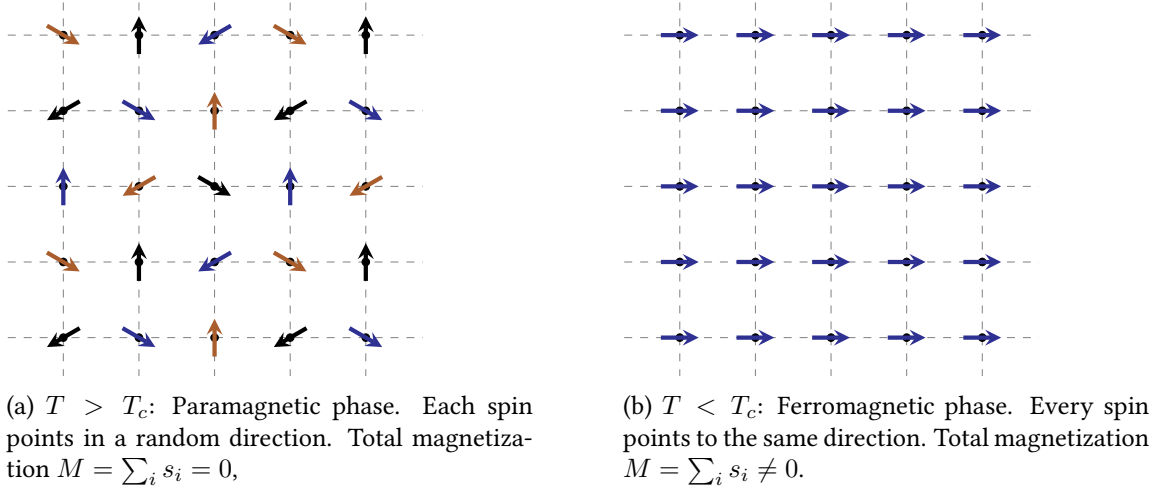
Figure 2: Paramagnetic vs. Ferromagnetic phase in a $2d$ lattice.

Later we will try to model this!

2.2 Thermodynamic potentials

Phases of system are characterized by thermodynamic functions.

A thermodynamic potential is a function of the parameters of the system and external constraints (e.g. pressure, temperature) that decreases during the evolution of the system until reaching a minimum equilibrium.

Common thermodynamic potentials:

Potential		Fixed	Differential	First derivatives	
Internal energy	U	V,S	$\mathrm{d}U = T\mathrm{d}S - p\mathrm{d}V$	$T = \left(\frac{\partial U}{\partial S}\right)_V$	$p = -\left(\frac{\partial U}{\partial V}\right)_S$
Free energy	$F = U - TS$	V,T	$\mathrm{d}H = T\mathrm{d}S + V\mathrm{d}p$	$T = \left(\frac{\partial H}{\partial S}\right)_p$	$V = \left(\frac{\partial H}{\partial p}\right)_S$
Enthalpy	$H = U + pV$	P,S	$\mathrm{d}F = -S\mathrm{d}T - p\mathrm{d}V$	$S = -\left(\frac{\partial F}{\partial T}\right)_V$	$p = -\left(\frac{\partial F}{\partial V}\right)_T$
Gibbs free energy	$G = H - TS$	P,T	$\mathrm{d}G = -S\mathrm{d}T + V\mathrm{d}p$	$S = -\left(\frac{\partial G}{\partial T}\right)_p$	$V = \left(\frac{\partial G}{\partial p}\right)_T$

For many simple models of complex systems we are interested in systems with

- fixed size (volume)

- fixed temperature (level of noise)

so we will be mainly working with the Free energy.

2.3 Classification of phase transitions – Critical Phenomena

There is a classification of phase transitions, due originally to Ehrenfest. When the nth derivative of a thermo-dynamic potential (usually the Free energy F or the Gibbs free energy G) is discontinuous, we say we have an nth order phase transition. In practice, most of the times we deal with 1st (discontinuous) and 2nd (continuous) phase transitions. For example, the **liquid-gas** transition releases latent heat $\Delta Q = T_0\Delta S$, which means that the entropy $S = -\frac{\partial F}{\partial T}$ is discontinuous. It is therefore a **first order phase transition** . The volume is also a first differential of G and this also shows a discontinuous jump.
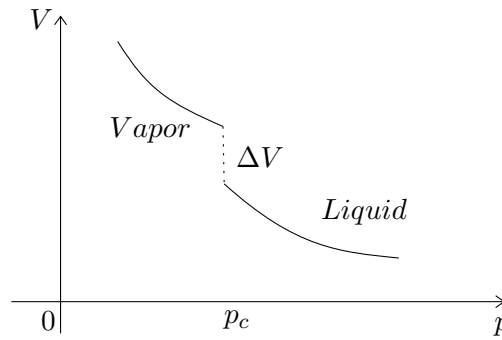
> **Discontinuous (1st order) phase transitions**: At the transition the system has discontinuities in most physical properties. The transition shows a latent heat.

In most cases these transitions happen with **no precursors, no hint** that a change is about to occur.

> **Example**: Water vapor at $101°$C has no little droplets of water inside.

- G (or F) is continuous

- $V = \left(\frac{\partial G}{\partial p}\right)_T$ and $S = -\left(\frac{\partial G}{\partial T}\right)_p$ are discontinuous.

By Ehrenfest's classification, a second-order phase transition has no latent heat because the entropy does not show a disconinuity (and neither does the volume - both being first differentials of G or F). But quantities like the heat capacity and compressibility (second differentials of G) do.

> **Continuous (2nd order) phase transitions**: Continuous change in the entropy (no latent heat). Close to the critical point the system is subject to extremely large susceptibility to external factors and distant parts of the system show strong correlations.

- G (or F) is continuous

- The magnetization $M = -\left(\frac{\partial G}{\partial h}\right)_T$ and $S = -\left(\frac{\partial G}{\partial T}\right)_h$ are continuous.

- The magnetic susceptibility $\chi(T) = -\left(\frac{\partial^2 G}{\partial h^2}\right)_T$ is discontinuous.

Since there are mainly two cases of phase transitions, we no longer use the Ehrenfest classification (i.e. order of phase transition = order of the lowest derivative of the thermodynamic potential showing a discontinuity). Instead, we determine a phase transition from the continuity/discontinuity of the Entropy S (i.e. the presence of latent heat).

> - The liquid-gas phase transition is a first-order transition, except at the critical point where the phase transition involves no latent heat and is a continuous phase transition.
> - A ferromagnet such as iron, loses its ferromagnetism when heated to the Curie temperature T_C. This phase transition is continuous, since there is no latent heat. Furthermore, the magnetization (which serves as the order parameter of the system as we will see later) is a first differential of the Gibbs function and does not change discontinuously at T_C.

In the context of phase transition, the term critical phenomena describes a system at the border between order and disorder, which is characterized by an extremely large susceptibility to external factors and strong correlation between distant parts of the system. Continuous phase transitions are often synonymous with critical phenomena.

2.4   Example of a microscopic model of critical phenomena: the Ising model

To appreciate some of the intriguing properties of phase transitions, it is helpful to consider a very simple model that can exhibit a phase transition. We will now refer to the 'tiny magnet' that we introduced in section 2.1.2 as spin, i.e. we replace each atom of the material by just the spin. We then assume a set of these spins arranged on a d-dimensional regular lattice, and also that each spin can be in one of only two states $s_i = \pm 1$. We are interested in modeling ferromagnetism, so let's suppose that the interaction between the spins is such that it costs less energy for a site to be in the same state as its neighbours ('peer pressure to conform'). The interactions are short-ranged; spins interact only with their nearest neighbors.

Hamiltonian of Ising Model

$$H = -J \sum_{\langle i,j \rangle} s_i s_j.$$

with $J > 0$, $s_i = \pm 1$ and $\langle i, j \rangle$ denoting the nearest neighbors.

The energy between two neighbour spins is:

$$E_{ij} = -Js_i \cdot s_j = \begin{cases} -J & \text{if spins are aligned } \uparrow\uparrow, \downarrow\downarrow \\ +J & \text{if spins are anti-aligned } \uparrow\downarrow, \downarrow\uparrow \end{cases}.$$

Since the system is always trying to go towards states of lower energy, and E_{ij} is smaller if the spins are aligned, we have achieved a ferromagnetic behavior! Spins tend to align. If instead we had $J < 0$ we would have antiferromagnetic interactions (neighboring spins opposite aligned).

Note:

If we replace the binary spins by continuous, normalised vectors $\mathbf{s}_i$ we get the **Heisenberg model**.

The **state probability** is given by the *Boltzmann factor*

$$P(s_1, \ldots, s_N) = \frac{e^{-\beta H}}{\mathcal{Z}}.$$

Where $\beta = 1/k_b T$ the inverse temperature $\rightarrow$ controls the level of 'noise' in the system, and

$$\mathcal{Z} = \sum_{s_1, \ldots s_N} e^{-\beta H}$$

the partition function which ensures the normalisation of the probability. Notice, that being a sum over all possible configurations of the system, it contains all the information about the system.

From the latter, we can define the free energy:

$$F = -k_b T \log \mathcal{Z}.$$

Chapter 1

From Microscopic to Macroscopic description of a complex system

1 From Micro to Macro description of a Complex Systems at Equilibrium

In this lecture, we are interested in understanding how to connect the microscopic description of a complex system to its macroscopic behavior at equilibrium.

1.1 Microstates VS Macrostates of a Complex System

When observing physical systems, we don't see the system in all its little microscopic states. Instead we see it in a 'macrostate', in which we measure macroscopic observables.

Example:

	Gas in a box	Voting
Microstate	exact position, speed of all the molecules	single vote of every person
Macrostate	system characterized by pressure, temperature, energy	average orientation of group, correlations between people.

We are interested in how the properties of the system at a microscopic level gives rise to its macroscopic properties.

Microstates: They are characterized by $\mathbf{s}$ = vector of all the characteristics of each constituent of the system, and $P(\mathbf{s})$ = probability to observe the system in state $\mathbf{s}$ at equilibrium.

e.g. $\mathbf{s}$ =position and speed of each molecule (in the gas system), or the value ± 1 of each spin (in the Ising model)

Macrostates: Composed of the most probable microstates and characterized by macroscopic observables.

> **Macroscopic observables**
> $$\langle A \rangle = \sum_{\mathbf{s}} A(\mathbf{s}) P(\mathbf{s})$$

where $\sum_{\mathbf{s}}$ denotes the sum over all the microstates, $A(\mathbf{s})$ is the observable at the microscopic level and $P(\mathbf{s})$ is the probability to observe the system in the microstate.

Given that the **total magnetisation per spin**, for N total spins is,

$$M(\mathbf{s}) = \sum_{i=1}^{N} s_i = M_\uparrow - M_\downarrow$$

Some macroscopic observables for the Ising system would be

- Average energy of the system $\langle E \rangle = \sum_{\boldsymbol{s}} E(\boldsymbol{s}) P(\boldsymbol{s})$

- Average total magnetization $\langle M \rangle = \sum_{\boldsymbol{s}} M(\boldsymbol{s}) P(\boldsymbol{s})$

Gibbs' postulate $U = \langle E \rangle$
- U : Internal energy of the system (Thermodynamics)
- $\langle E \rangle$: Ensemble average of the energy over all microstates (Statistical Physics)

1.2 Entropy: Thermodynamic and statistical
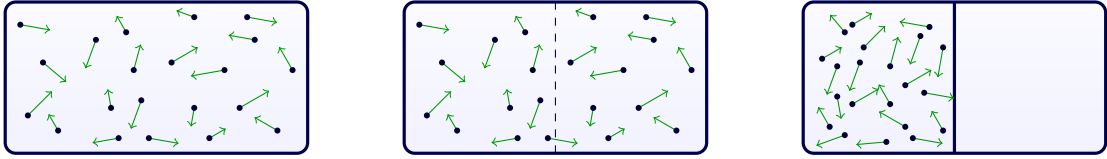
Figure 1.1: Isolated system with particles. $V =$ fixed, $N =$ fixed (no exchange of particles), $\Delta Q = 0$ (no exchange of heat). In the middle picture, we imagine a virtual wall partitioning the system. On the right picture we literally partition the system.

Postulate of statistical thermodynamics:
In an isolated system, all microstates are equiprobable.

Focusing on the middle picture with the virtual wall splitting the system, from the above postulate, we can argue that each particle has a probability $1/2$ to be on the left side of the virtually partitioned box.

Then the probability to see two particles on the left side is $\frac{1}{2} \cdot \frac{1}{2} = \frac{1}{4}$ the probability to see three particles on the left side $\frac{1}{2} \cdot \frac{1}{2} \cdot \frac{1}{2} = \frac{1}{8}$ and so on. The probability to see all the particles N on the left, like the right picture in 1.1, is then $\frac{1}{2^N}$ and we can see that this probability goes to zero if $N \to \infty$.

The probability to observe N_L particles on the left is

$$P(N_L) = \frac{1}{2^N} \binom{N}{N_L} \xrightarrow{N \to \infty} \mathcal{N}\left(\mu = \frac{N}{2}, \sigma^2 = \frac{N}{4}\right).$$

Notice that

$$\frac{\sigma}{\mu} = \frac{\sqrt{N}}{N} = \frac{1}{\sqrt{N}}.$$

As $N \to \infty$ the fluctuations of N_L around $N/2$ become undetectable (the Gaussian becomes steeper and steeper).

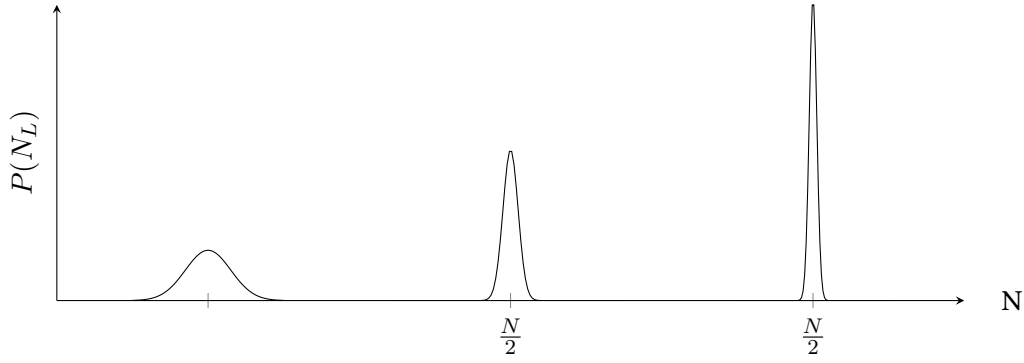This means that macroscopically, in the thermodynamic limit $N \to \infty$, we will see the middle picture of fig. 1.1, with the particles being equally distributed in the left and right domain of the box.

1.2.1 Statistical definition of Entropy

Boltzmann's entropy formula For an isolated system

$$S = k_B \log \Omega \tag{1.1}$$

Where Ω the number of microstates of the system.
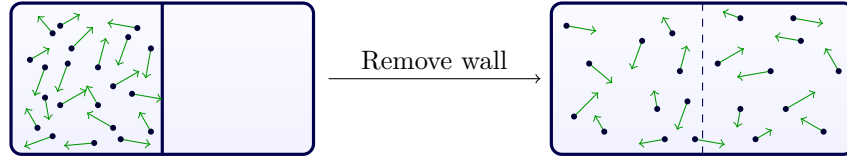
Figure 1.2: Boxes of particles separated by a real wall (left) vs. a virtual wall (right).

Consider again the box separated by a partition into two equal volumes, with all the atoms being on the left. If we remove the partition, the particles will start to occupy the whole box[1] and the thermodynamic entropy will increase $S_F > S_I$. We are interested in the origin of this increase.

Microscopically, removing the partition induces a big increase in the volume that the particles can occupy. Hence, there is a huge increase in the number of microstates $\Omega \propto V^N$.

This expansion from the half left part of the box to the whole box is formally **irreversible**. There is no way to get the gas back into the initial chamber without doing any work. Microscopically, there is a very tiny probability that all particles will come back to the left ("Microscopic reversibility").

1.2.2 Shannon Entropy

Shannon Entropy[a]:
$$S = -k_B \sum_{\boldsymbol{s}} P(\boldsymbol{s}) \log P(\boldsymbol{s}) \tag{1.2}$$

where $k_B = 1.38 \cdot 10^{-23} J \cdot K^{-1}$ the Boltzmann constant.

---
[a]Also called Gibbs entropy, due to the dimensionful factor k_B which ensures the thermodynamic nature of the entropy.

From the above defintion we can can see that we have

---
[1]This is known as 'Joule expansion'.

- a **minimal** when we only have one microstate with probability 1 and all the others with probability 0.

  Then $S = 0$: no uncertainty at all. Observing the state doesn't provide any information about the system, since we knew from the beginning to which state the system would be.

- a **maximal** when all the microstates have the same probability $P(\boldsymbol{s}) = \frac{1}{\Omega}$, where Ω the total number of microstates.

  Then $S = k_B \log \Omega$: maximum uncertainty.

- Other distributions $P(\boldsymbol{s})$ will result to entropy between these two values.

In fact, we can prove that the two definitions for entropy that we gave so far ((1.1), (1.2)) are equivalent!

In particular, for an isolated system, all the microstates have the same probability $P(\boldsymbol{s}) = \frac{1}{\Omega}$. Then the Shannon entropy is

$$
\begin{aligned}
S &= -k_B \sum_{i=1}^{\Omega} \frac{1}{\Omega} \log\left(\frac{1}{\Omega}\right) \\
&= -k_B \log\left(\frac{1}{\Omega}\right) \\
&= k_B \log(\Omega).
\end{aligned}
$$

The last line is the Boltzmann's entropy formula.

1.3 Boltzmann distribution

We will often consider systems in contact with a thermostat at fixed temperature **T**. The system exchanges energy with the thermostat and the latter acts as a constant source of energy, which allows to control the temperature, or the 'noise' level of the system.

In this case, the state probabilities $P(\boldsymbol{s})$ are given by the

> **Boltzmann distribution**
>
> $$
> P(\boldsymbol{s}) = \frac{e^{-\beta E(\boldsymbol{s})}}{\mathcal{Z}}.
> $$
>
> where
> - $E(\boldsymbol{s})$ is the energy of the system in the microstate $\boldsymbol{s}$
> - $\beta = \frac{1}{k_B T}$ is the inverse temperature. Contols the noise level of the system.
> - $\mathcal{Z}$ the normalization factor (partition function).

Theromstat T
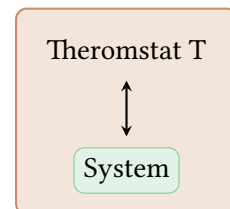
System

↪ States with the same energy have the same probability to occur.

↪ System has a larger probability to be in states with lower energy.

↪ There is a **competition** between the energy of the system and thermal energy.

  – In the limit $T \to 0$ ($\beta \to \infty$): The system is governed by the minimal $E(\boldsymbol{s})$, since it gives the maximum probability $\sim e^{-\beta E(\boldsymbol{s})}$ (all the other states are infinitely less probable). In this case, we have **order** .

– In the limit $T \to \infty$ ($\beta \to 0$) : $P(\boldsymbol{s}) \sim e^{-\beta E(\boldsymbol{s})} \to 1$ for all states. All the states have the same probability, independently of their energy. In this case, we have **disorder** . No interaction is able to order the system.

Example: Ising model

Remember that the energy is given by $E(\boldsymbol{s}) = -J \sum_{\langle i,j \rangle} s_i s_j$ where $\langle i, j \rangle$ denotes the interaction between neighbor spins only.

The minimal energy is $E_{min} = -J N_{pairs}$ which is reached when all the spins are aligned (all up or all down).

Here, the competition between $E(\boldsymbol{s})$ and $k_B T$ means:
- The energy of interaction $E(\boldsymbol{s})$ between the spins tends to align them → Wins at small temperatures.
- The thermal noise has a disordering effect → Wins at large temperatures/noise.

∗ Remember figure 2.

1.4   Free energy

Definition(s):

Thermodynamics $F = U - TS$. A thermodynamical potential for a system with V, T constant.

Statistical Physics $F = -k_B T \log \mathcal{Z}$. All the properties of the system are encoded in $\mathcal{Z}$.

Some useful relations we have seen so far:

1. Gibbs' postulate $U = \langle E \rangle = \sum_{\boldsymbol{s}} E(\boldsymbol{s}) P(\boldsymbol{s})$

2. Shannon entropy $S = -k_B \sum_{\boldsymbol{s}} P(\boldsymbol{s}) \log P(\boldsymbol{s})$

3. Boltzmann distribution $\log P(\boldsymbol{s}) = -\beta E(\boldsymbol{s}) - \log Z$

We can obtain all the thermodynamic quantities of interest from $\mathcal{Z}$ (equivalently F). For example, differentiating the above logarithmic expression of the Boltzmann distribution with respect to β, we get the internal energy

$$U = \langle E \rangle = -\frac{\partial \log Z}{\partial \beta}.$$

2   Tutorials: Complex systems out-of-equilibrium – Markov Processes

This part comes from the tutorials T0 and T1. In these tutorials, we learn how to describe the evolution of a complex systems following a continuous-time Markovian process out-of-equilibrium, by writing down a master equation.

2.1   Poisson process

Poisson processes are used as mathematical models for a wide range of phenomena, such as the arrival of customers at a place, the radioactive decay of atoms, the spiking time of neurons, or the occurrence of rare mutations in DNA. They can describe the number $N(t)$ of events in time intervals t. The occurence of a new event is random, and **independent** of the previous events, so Poisson processes fall into the larger category of Markovian (memoryless) processes.
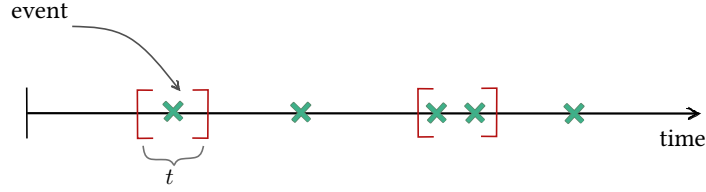
🏠 See tutorial TCS0.

Summary

If $N(t)$ follows a Poisson process, with parameter $\lambda > 0$, then:
- the probability to observe k events in a given time interval t is given by the Poisson distribution:

$$\mathbb{P}[N(t) = k] = \frac{\mu^k \exp(-\mu)}{k!}, \quad \text{where} \quad \mu = \lambda t \tag{1.3}$$

λ represents the event rate.
- Small interval (δt) probabilities:

$$P(N(\delta t) = 0) = 1 - \lambda \delta t + o(\delta t) \tag{1.4}$$
$$P(N(\delta t) = 1) = \lambda \delta t + o(\delta t) \tag{1.5}$$
$$P(N(\delta t) \geq 2) = o(\delta t). \tag{1.6}$$

Specifically eq. (1.5) shows that if the time interval goes to zero, the probability also goes to zero, with a rate proportional to δt. Additionally, as λ increases, the probability that we have an arrival on δt increases (hence the attribute event rate).
- the distribution of the waiting time τ between two events is the exponential distribution :

$$P(\tau) = \lambda \exp(-\lambda \tau) \tag{1.7}$$

2.2 Markov Chains and Master Equation

🏠 See tutorial T1 for details.

The concept of Markov chains is central to Monte Carlo simulations. They can be used to create a sequence of configurations, distributed according to a probability distribution P.

Starting from an initial state $\mathbf{s}_0$, at time $t = 0$, a chain of states is generated:

$$\mathbf{s}_0 \to \mathbf{s}_1 \to \cdots \to \mathbf{s}_n \to \mathbf{s}_{n+1} \to \ldots \tag{1.8}$$

A transition matrix w_{ij} gives the transition probabilities of going from a state $\mathbf{s}_i$ to a state $\mathbf{s}_j$ in one step of the Markov process. Specifically,

The probability that the system jumps from $\mathbf{s}$ to $\mathbf{s}'$ during dt is given by

$$w(\mathbf{s} \to \mathbf{s}') \, dt . \tag{1.9}$$

Consequently, the probability to find the system in a state $\mathbf{s}$ at time $t + dt$ is given by

$$p(\mathbf{s}, t + dt) = p(\mathbf{s}, t) + \sum_{\mathbf{s}' \neq \mathbf{s}} p(\mathbf{s}', t) \, w(\mathbf{s}' \to \mathbf{s}) \, dt - \sum_{\mathbf{s}' \neq \mathbf{s}} p(\mathbf{s}, t) \, w(\mathbf{s} \to \mathbf{s}') \, dt \tag{1.10}$$

Subtracting $p(\mathbf{s}, t)$ and diving by dt on both sides leads to an equation that gives the time evolution of the probability $p(\mathbf{s}, t)$ to find the system in state $\mathbf{s}$ at time t, which is called the Master equation.

Master equation:

$$\frac{\mathrm{d}\,p(\mathbf{s},t)}{\mathrm{d}t} = \sum_{\mathbf{s}'\neq\mathbf{s}} p(\mathbf{s}',t)\,w(\mathbf{s}'\to\mathbf{s}) - \sum_{\mathbf{s}'\neq\mathbf{s}} p(\mathbf{s},t)\,w(\mathbf{s}\to\mathbf{s}')\,. \qquad (1.11)$$

At **equilibrium**, $\frac{\mathrm{d}\,p(\mathbf{s},t)}{\mathrm{d}t} = 0$, which gives:

$$\sum_{\mathbf{s}'} p_{st}(\mathbf{s}')w(\mathbf{s}'\to\mathbf{s}) = \sum_{\mathbf{s}'} p_{st}(\mathbf{s})w(\mathbf{s}\to\mathbf{s}')\,, \quad \text{where} \quad p_{st}(\mathbf{s}) : \text{ the stationary probability }. \qquad (1.12)$$

The goal is to determine the transition matrix w, so that we asymptotically reach the desired (equilibrium) probability distribution $P(\mathbf{s})$, i.e. $p_{st}(\mathbf{s}) = P(\mathbf{s})$

A sufficient (but not unique) solution is the

detailed balance condition:

$$P(\mathbf{s}')w(\mathbf{s}'\to\mathbf{s}) = P(\mathbf{s})w(\mathbf{s}\to\mathbf{s}')\,. \qquad (1.13)$$

Transition probabilities between any two states in the chain is equal in both directions.

2.3   Macroscopic observables

Definition of ensemble average – see tutorial on Metropolis algorithm.

2.4   Example: simple model of car traffic – TASEP

⌂ See tutorial TCS0.

3   Tutorial: from out-of-equilibrium to equilibrium description: the Metropolis algorithm

⌂ See TCS1 for details.

The simplest Markov Chain Monte Carlo algorithm (MCMC) is the Metropolis algorithm.

Staring from a randomly sampled initial state (out-of-equilibrium) at time $t = 0$, we consider very short time increments dt (typically, for an Ising model it is common to take $dt = 1/n$, where n is the total number of sites), and during each time step dt we perform the two operations:

– from a current state $\mathbf{s}$ of the system, sample a random new state $\mathbf{s}'$;

– the new state is accepted with probability $\Pi(\mathbf{s}\to\mathbf{s}')$.

The choice for $\Pi(\mathbf{s}\to\mathbf{s}')$ introduced by Metropolis et al. is:

$$\Pi(\mathbf{s}\to\mathbf{s}') = \begin{cases} 1, & \text{if}\quad H(\mathbf{s}') \leq H(\mathbf{s}) \\ \exp\left[-\beta(H(\mathbf{s}') - H(\mathbf{s}))\right], & \text{otherwise}\,. \end{cases} \qquad (1.14)$$

Chapter 2

Examples of Critical Phenomena in Complex Systems at Equilibrium

1   The Ising Model

Now we are ready to model the paramagnetic-ferromagnetic phase transition and study various interesting phenomena. For this, we will use the simple but feature rich, Ising model. We have seen already that the Hamiltonian (energy) of the model is given by,

$$H = -J \sum_{\langle i,j \rangle} s_i s_j \tag{2.1}$$

with scalar spins $s_i = \pm 1$ and $J > 0$.
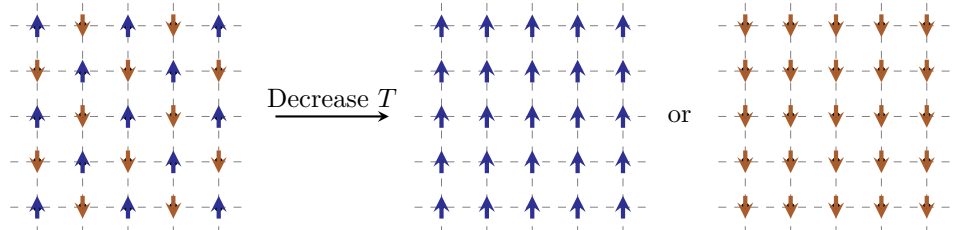
Figure 2.1: Left: Ising spins randomly aligned in high temperature $T > T_c$ (paramagnetic material). Right: spins aligned (all up or all down) in low temperature $T < T_c$ (ferromagnetic material).

1.1   Spontaneous magnetization

As the temperature is lowered below a certain critical temperature T_c, the model displays a **spontaneous emergence of magnetization** , even in the absence of an external magnetic field. We would like to explain this emergent phenomenon through the microscopic interactions. For this, we will first consider a system with no interactions, but subject to an external magnetic field.

1.1.1   System of non-interacting spins ($J = 0$): No spontaneous magnetization

The Hamiltonian (energy) of the system is

$$E(\boldsymbol{s}) = -h \sum_{i=1}^{N} s_i \qquad s_i = \pm 1 \tag{2.2}$$

where h the constant external magnetic field.

Since the spins are non-interacting, the problem is independent of the underlying lattice and dimensionality.
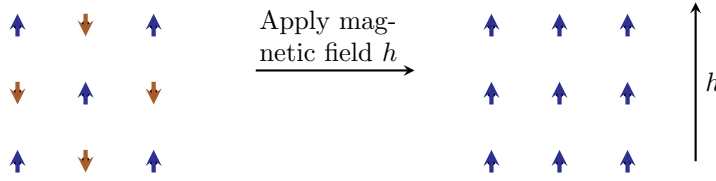
The probability distribution of the microstates is

$$P(\boldsymbol{s}) = \frac{e^{-\beta E(\boldsymbol{s})}}{\mathcal{Z}}.$$

Now the behaviour of the system is determined by the **competition** between

- the external field h, which tends to align spins

- the thermal energy $k_B T$, which tends to disorganise spins.

⇨ In the limit $\frac{h}{k_B T} \to 0$: the thermal energy 'wins' over the external field. The most probable microstates are spins randomly pointing up and down . The average magnetization and energy is

$$\langle M \rangle = 0 \qquad \text{adding random spin vectors results to } 0$$
$$\langle E \rangle = 0 \qquad E \sim h.$$

⇨ In the limit $\frac{h}{k_B T} \to \pm\infty$ the external field 'wins' over the thermal energy. Now the most probable microstates are those where all the spins are aligned in the same direction with the external field h .The average magnetization and energy is

$$\langle M \rangle = \begin{cases} N & h > 0 \\ -N & h < 0 \end{cases}$$
$$\langle E \rangle = -N|h|.$$

> Notice that the above quantities scale with the system size N. This means that they are **extensive** quantities. We can make them **intensive** by defining
>
> $$m = \frac{\langle M \rangle}{N} \quad \epsilon = \frac{\langle E \rangle}{N}.$$

A natural question to ask is whether there is a phase transition. In section 2 we mentioned that a phase transition occurs when there is a singularity in the free energy. So our next goal is to calculate the free energy $F = k_B T \log \mathcal{Z}$, essentially by calculating the partition function $\mathcal{Z}$.

$$\mathcal{Z}(T, h) = \sum_{\boldsymbol{s}} e^{-\beta E(\boldsymbol{s})}$$
$$= \sum_{s_1=-1}^{+1} \exp\left(\beta h s_1\right) \sum_{s_2=-1}^{+1} \exp\left(\beta h s_2\right) \cdots \sum_{s_N=-1}^{+1} \exp\left(\beta h s_N\right)$$
$$= \left(2\cosh(\beta H)\right)^N.$$

Then,

$$F = -k_B T \log \mathcal{Z} = -N k_B T \log(2 \cosh(\beta H)).$$

Since $F \sim N$, it is an extensive quantity. So again we can make it intensive by dividing by N:

$$f(T, h) = \frac{F(T, h)}{N} = -k_B T \log(2 \cosh(\beta H)) \tag{2.3}$$

which is the free energy per spin.
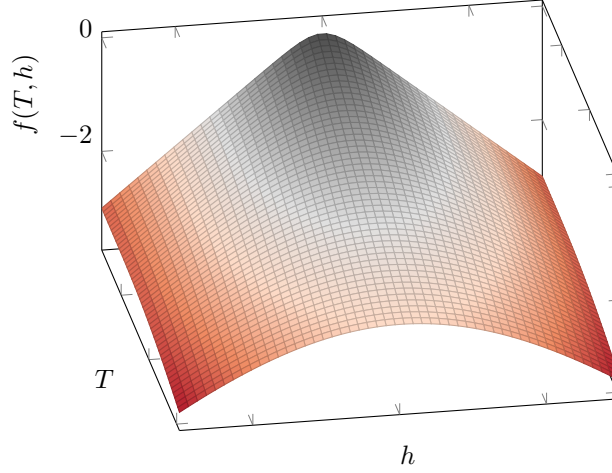
Figure 2.2: $f(T, h) = -k_B T \log(2 \cosh(\beta h))$.

We can confirm that f is analytic everywhere (except the origin), so there is **no phase transition**.

We can also calculate the magnetization by differentiating with respect to the applied field h (i.e. querying how much the free energy changes as the external field changes, at a given temperature):

magnetisation per spin: $m(T, h) = -\left(\frac{\partial f}{\partial h}\right)_T$

Here,

$$m(T, h) = -\left(\frac{\partial f}{\partial h}\right)_T = \tanh(\beta h).$$
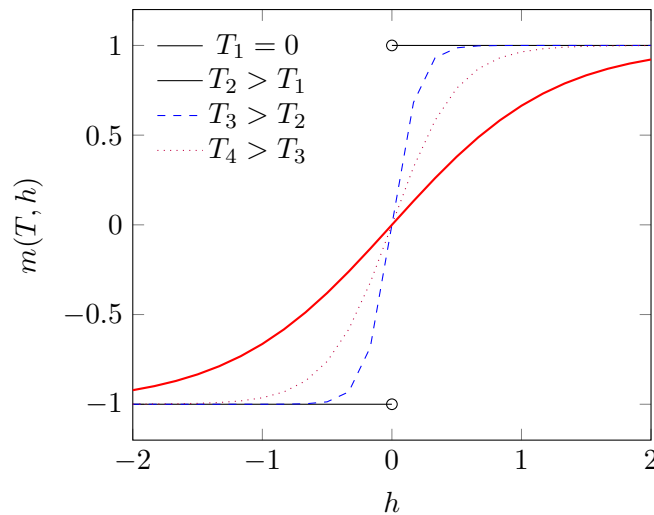
We can summarize the above diagram with the following table:

	$H \neq 0$	$H = 0$
High T	a strong h must be applied to align the spins	$m(T,0) = 0$
Small T	spins align more easily	$m(T,h)$ becomes steeper as $T \to 0$
T = 0	all the spins are aligned with h	$\lim\limits_{h \to 0^{\pm}} m(T,h) = \pm 1$ (step function)

We conclude, that for a system with non-interacting spins, there is **no spontaneous magnetisation** in zero magnetic field for any temperature.

1.1.2 Systems of interacting spins, with no external field ($H = 0$): Spontaneous magnetization

Now let's consider again the case of nearest-neighbor interactions, in the absence of a magnetic field. The Hamiltonian (energy) is

$$E(\boldsymbol{s}) = -J \sum_{\langle i,j \rangle} s_i s_j.$$

- At high temperatures $\frac{J}{k_B T} \ll 1$: The **thermal energy dominates**; spins are randomly up or down and hence the magnetization $m(T) = 0$.

- At low temperatures $\frac{J}{k_B T} \gg 1$: The **interaction term dominates**; spins tend to align with each other to minimize the total energy.

- At T=0: The configuration with the minimal energy is with all the spins aligned
  $E_{min} = -J N_{pairs}$. However there are two ways with which we can achieve this configuration: either **all spins up** ($m(T) = +1$), or **all spins down** ($m(T) = -1$). This means that, initially, we have a **symmetry** between up and down. The system will inevitably 'choose' one of these two possible states, which results to a **spontaneous symmetry breaking**.

  At which point is determined whether the system at $T = 0$ will have all spins up or down? There must be a critical temperature T_c where this happens. Indeed, when the thermal energy $k_B T$ and the interaction energy J are comparable there is a phase transition from a disordered (paramagnetic) high-temperature phase to an ordered (ferromagnetic) low-temperature phase.

If it is a continuous phase transition, we expect a continuous but abrupt pick-up of a magnetisaztion at the critical temperature. A similar behaviour is observed in the

> **Order parameter**: Quantity that distinguishes two different phases. It is zero in the disordered phase and non-zero in the ordered phase.

> E.g.
> - In the **Ising model** the order parameter is the **magnetisation**.
> - In the **water** phase transition, the order parameter is the **density** .

We had a similar type of transition at the *critical point* of the phase diagram of water (see 1). After some critical temperature we could 'go-around' the critical point without undergoing a phase transition and we had a *supercritical fluid*.
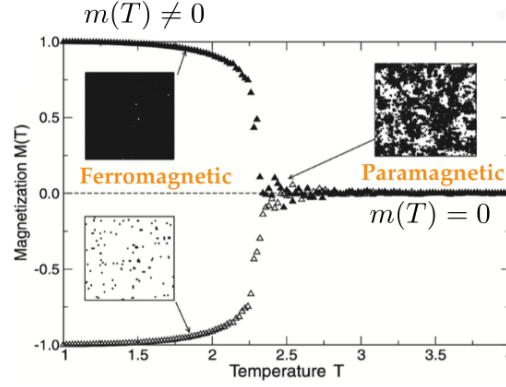
Figure 2.3: Magnetisation vs. temperature diagram. At $T > T_c$, $m(T) = 0$ (disorder) whereas for $T < T_c$, $m(T) \neq 0$ (order). At $T \to 0$ $m(T) = \pm 1$. In the images, white pixels indicate down spins and black pixels up spins.

1.1.3 Symmetry breaking

Let's consider again the system with no external field ($h = 0$)

$$E(\boldsymbol{s}) = -J \sum_{\langle i,j \rangle} s_i s_j.$$

The probability distribution is $P(\boldsymbol{s}) = e^{-\beta E(\boldsymbol{s})}/\mathcal{Z}$.

Next, we consider a microstate $\boldsymbol{s}$ and one with all the spins flipped, $-\boldsymbol{s}$:

⇨ Both have the same energy $E(\boldsymbol{s}) = E(-\boldsymbol{s})$, hence same probability distribution $P(\boldsymbol{s}) = P(-\boldsymbol{s})$

⇨ but opposite magnetisation $M(\boldsymbol{s}) = M(-\boldsymbol{s})$

Then the average total magnetization is $\langle M \rangle = \sum_{\boldsymbol{s}} M(\boldsymbol{s})P(\boldsymbol{s}) = 0$ for every temperature T, as for each state, there is a symmetric state with same probability but opposite magnetization. This is contradicting to the above analysis, no phase transition is occurring now!

Let's try a different approach. We will add an external magnetic field h, and then take the limit $h \to 0$.

$$E(\boldsymbol{s}) = -J \sum_{\langle i,j \rangle} s_i s_j - h \underbrace{\sum_{i=1}^{N} s_i}_{M}, \qquad P(\boldsymbol{s}) = \frac{e^{-\beta E(\boldsymbol{s})}}{\mathcal{Z}}.$$

Now, $E(\boldsymbol{s}) - E(-\boldsymbol{s}) = -2hM(\boldsymbol{s})$, so $\frac{P(\boldsymbol{s})}{P(-\boldsymbol{s})} = \exp\left(2\beta h M(\boldsymbol{s})\right)$.

Recall that M **is an extensive quantity**, but $m(\boldsymbol{s}) = \frac{M(\boldsymbol{s})}{N}$ is intensive. We can rewrite

$$\frac{P(\boldsymbol{s})}{P(-\boldsymbol{s})} = \exp\left(2\beta h N m(\boldsymbol{s})\right).$$

If we first take the limit $h \to 0$ and then assume the thermodynamic limit $N \to \infty$, we obtain the previous result: $P(\boldsymbol{s}) = P(-\boldsymbol{s})$.

However, if we first take the thermodynamic limit and then take the field to go to zero (assuming that we start with a state $\boldsymbol{s}$ such that $M(\boldsymbol{s}) > 0$):

$$\lim_{h \to 0^{\pm}} \lim_{N \to \infty} \frac{P(\boldsymbol{s})}{P(-\boldsymbol{s})} \begin{cases} \infty, & \text{for } h \to 0^+ \longrightarrow \text{ configurations with } M(\boldsymbol{s}) > 0 \text{ have probability } 1 \\ 0, & \text{for } h \to 0^- \longrightarrow \text{ configurations with } M(\boldsymbol{s}) < 0 \text{ have probability } 1 \end{cases}.$$

A tiny field h, breaks the symmetry among the spin configurations.

The important notice here is that the **order of the limits matters**.

> Non-commuting limits indicate a **spontaneous symmetry breaking**

> E.g. in the Ising model,
>
> $$\lim_{h \to 0^\pm} \lim_{N \to \infty} \langle M \rangle = 0$$
> $$\lim_{N \to \infty} \lim_{h \to 0^\pm} \langle M \rangle := N m_0 \neq 0 \rightarrow \textbf{spontaneous magnetisation}$$
>
> where m_0 is the order parameter (magnetisation per spin)

Above T_c the magnetization is zero in any case. **Below T_c:**

- In a finite size system, temporal average of the magnetisation over a sufficiently long time will give zero, since the system will spend equal time in m and $-m$ configurations.

- In a infinite size system, there is a spontaneous symmetry breaking. The system will spend all its time in only one phase, determined by the initial conditions.

1.2 Phase Transition in the Ising model

1.2.1 Control Parameter and Order Parameter

> **Order parameter**: Quantity that distinguishes two different phases. It is zero in the disordered phase and non-zero in the ordered phase.

> Examples:
> - In the **Ising model** the order parameter is the **magnetisation**.
> - In the **water** critical phase transition, the order parameter is the **difference in density** between the coexisting liquid and the gas phases.

1.2.2 1D Ising model

> **Ising model in magnetic field**: We consider a small field $h \neq 0$
>
> $$E(\boldsymbol{s}) = -J \sum_{i=1}^{N} s_i s_{i+1} - h \sum_{i=1}^{N} s_i \qquad s_i = \pm 1.$$

Since in the end we care about the thermodynamic limit $N \to \infty$, we can impose periodic boundary conditions $s_{N+1} = s_1$. The boundary does not matter in an infinite size system.
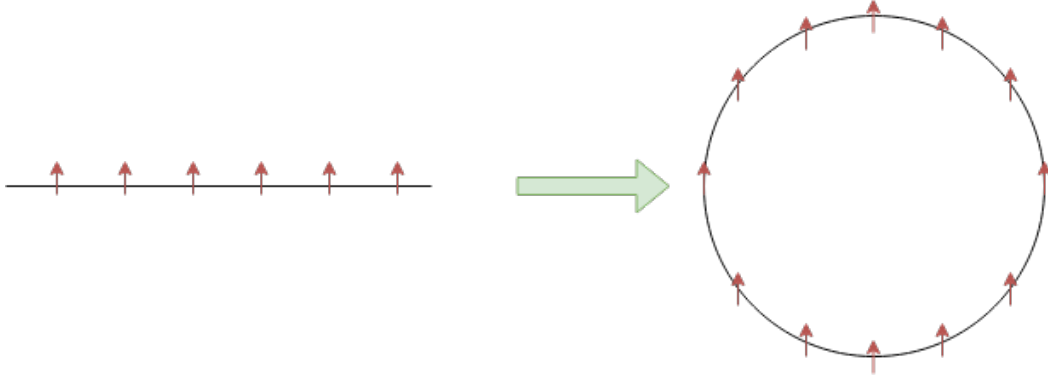
Figure 2.4: Open vs periodic boundary conditions.

The **Partition function** can be then calculated explicitly:

$$\mathcal{Z} = \sum_{\boldsymbol{s}} e^{-\beta E(\boldsymbol{s})}$$

$$= \sum_{\boldsymbol{s}} \exp\left(\beta J \sum_{i=1}^{N} s_i s_{i+1} + \beta h \sum_{i=1}^{N} s_i\right)$$

there is a symmetry in $i, i+1$, due to periodic boundary conditions

$$= \sum_{\boldsymbol{s}} \exp\left(\beta J \sum_{i=1}^{N} s_i s_{i+1} + \beta \frac{h}{2} \sum_{i=1}^{N} (s_i + s_{i+1})\right)$$

$$= \sum_{\boldsymbol{s}} \exp\left(\beta J s_1 s_2 + \beta \frac{h}{2}(s_1 + s_2)\right) \ldots \exp\left(\beta J s_N s_1 + \beta \frac{h}{2}(s_N + s_1)\right).$$

We notice that each exponential has a similar form, so we define the **Transfer matrix (2×2)** :

$$t_{s_i s_{i+1}} = \exp\left(\beta J s_i s_{i+1} + \beta \frac{h}{2}(s_i + s_{i+1})\right).$$

$$\boldsymbol{T} = \begin{pmatrix} t_{1,1} & t_{1,-1} \\ t_{-1,1} & t_{-1,-1} \end{pmatrix} = \begin{pmatrix} e^{(\beta J + \beta h)} & e^{-\beta J} \\ e^{-\beta J} & e^{(\beta J - \beta)} \end{pmatrix}.$$

Then, we can rewrite the partition function in a more compact form,

$$\mathcal{Z} = \sum_{\boldsymbol{s}} \prod_{i=1}^{N} t_{s_i s_{i+1}}$$

$$= \sum_{s_1 = \pm 1} \cdots \sum_{s_N = \pm 1} t_{s_1 s_2} \ldots t_{s_{N-1} s_N} t_{s_N s_1}$$

$$= \sum_{s_1 = \pm 1} \cdots \sum_{s_N = \pm 1} \underbrace{\left(\sum_{s_2 = \pm 1} t_{s_1 s_2} t_{s_1 s_3}\right)}_{(\boldsymbol{T}^2)_{s_1 s_3}} \ldots t_{s_{N-1} s_N} t_{s_N s_1}.$$

Where in the last step we used the following property of matrix multiplication

$$(AB)_{ij} = \sum_{k=1}^{n} A_{ik} B_{kj}.$$

Similarly, performing all the sums over the spins $s_2, s_3, \ldots s_{N-1}$, we get

$$
\begin{aligned}
\mathcal{Z} &= \sum_{s_1=\pm 1} \sum_{s_N=\pm 1} (\boldsymbol{T}^{N-1})_{s_1 s_N} \, t_{s_N s_1} \\
&= \sum_{s_1=\pm 1} (\boldsymbol{T}^N)_{s_1 s_1} \\
&\equiv \mathrm{Tr}(\boldsymbol{T}^N).
\end{aligned}
$$

In 1d, the partition function of the **Ising model**, can be calculated using the transfer matrix $\boldsymbol{T}$ as,

$$
\mathcal{Z} = \mathrm{Tr}(\boldsymbol{T}^N).
$$

Since we know the form of the transfer matrix,

$$
\boldsymbol{T} = \begin{pmatrix} e^{(\beta J + \beta h)} & e^{-\beta J} \\ e^{-\beta J} & e^{(\beta J - \beta h)} \end{pmatrix}.
$$

We can diagonalize this matrix, so that:

$$
\mathcal{Z} = \mathrm{Tr}(\boldsymbol{T}^N) = \lambda_+^N + \lambda_-^N \qquad \text{where } \lambda_\pm \text{ the eigenvalues of } \boldsymbol{T}.
$$

The eigenvalues are solutions of the charachteristic polynomial given by $\det(\boldsymbol{T} - \lambda \boldsymbol{I})$

$$
\lambda_\pm = e^{\beta J} \left(\cosh(\beta h) \pm \sqrt{\sinh^2 \beta h + \exp(-4\beta J)} \right).
$$

Special cases:

$$
\boldsymbol{J = 0}: \quad \lambda_+ = 2\cosh(\beta h), \qquad \lambda_- = 0 \; \rightarrow \qquad \text{recover } \mathcal{Z} = (2\cosh \beta h)^N \; \checkmark
$$

$$
\boldsymbol{h = 0}: \quad \lambda_+ = 2\cosh(\beta J), \qquad \lambda_- = 2\sinh(\beta J) \; \rightarrow
$$

$$
\mathcal{Z} = (2\cosh \beta J)^N \left(1 + (\tanh \beta J)^N \right) \xrightarrow{N \to \infty} (2\cosh \beta J)^N \quad \because \tanh \beta J < 1
$$

In general, in the **thermodynamic limit** $N \to \infty$.

$$
\mathcal{Z}(T, h) \sim \lambda_+^N \qquad \text{as } \frac{\lambda_-}{\lambda_+} < 1.
$$

Free energy

$$
\begin{aligned}
F(T, h) &= -k - BT \log \mathcal{Z} \\
&= -k_B T \log \lambda_+^N \qquad \text{for } N \to \infty \\
&= -N k_B T \left[\beta J + \log \left(\cosh \beta h + \sqrt{\sinh^2 \beta h + \exp(-4\beta J)} \right) \right]
\end{aligned}
\tag{2.4}
$$

which has a similar graph with that of figure 2.2; it is analytic everywhere, except at $(T, h) = (0, 0)$.

Limit $h \to 0$

Notice that $\cosh x = \frac{1+e^{-2x}}{2e^{-x}}$

$$f(T,0) = \frac{F(T,0)}{N} = -k_B T \log(2\cosh\beta J)$$
$$= \begin{cases} -k_B T \log 2, & T \to \infty \\ -J, & T \to 0 \end{cases}.$$

The equivalent form of the free energy is

$$F = Nf = \langle E \rangle - TS.$$

- For $T \to \infty$: All the spins are randomly oriented. The energy is zero and the free energy is determined by the maximization of S: $\to S = Nk_B \log 2$

- For $T \to 0$: All the spins are aligned. The entropy S is zero and the free energy is determined by the minimization of $\langle E \rangle \to \langle E \rangle = -NJ$

Average magnetization

Having found the free energy, we can compute any physical quantity of interest.

The **average magnetization** is given by

$$m(T,h) = -\left(\frac{\partial f}{\partial h}\right)_T.$$

From the derived expression for the free energy (2.4), we can compute

$$m(T,h) = -\left(\frac{\partial f}{\partial h}\right)_T = \frac{\sinh\beta h}{\sqrt{\sinh^2\beta h + \exp\left(-4\beta J\right)}}.$$
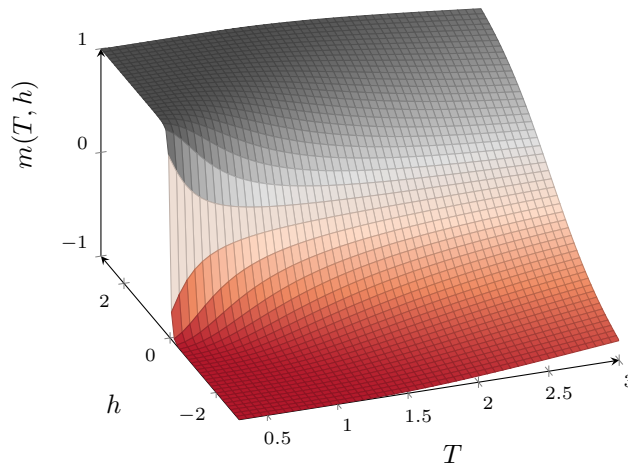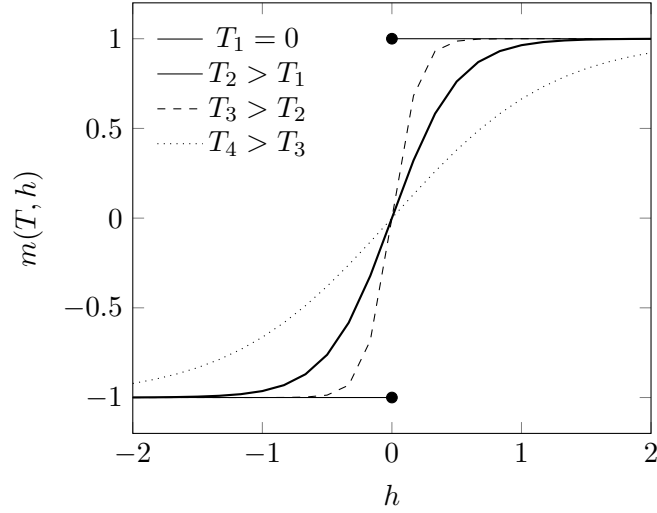

Figure 2.5: $m(T,h)$

$$m_0(T) = \lim_{h\to 0^\pm} m(T,h) = \begin{cases} 0, & T > 0 \\ \pm 1, & T = 0 \end{cases}.$$

This means that we have a **spontaneous magnetization** at $(T_c, h_c) = (0,0)$

1.2.3 2d Ising

In the case of a 2d Ising model, there is still an exact solution for $h = 0$. In fact, Onsager [4] (1944) proves the existence of a critical phase transition at

$$k_B T_c = \frac{2J}{\log\left(1 + \sqrt{2}\right)} \simeq 2.269 J.$$

The average magnetization per spin for $h \to 0^+$ is

$$m_0(T) = \begin{cases} 0 & T \geq T_c \\ \left(1 - \sinh^{-4}\left(\frac{2J}{k_B T}\right)^{1/8}\right) & T < T_c \end{cases}$$

$$= \begin{cases} 0 & T \geq T_c \\ \left(4\sqrt{2}\ln\left(1 + \sqrt{2}\right)^{1/8}\left(\frac{T_c - T}{T_c}\right)^{1/8}\right) & T \to T_c^- \end{cases} \tag{2.5}$$
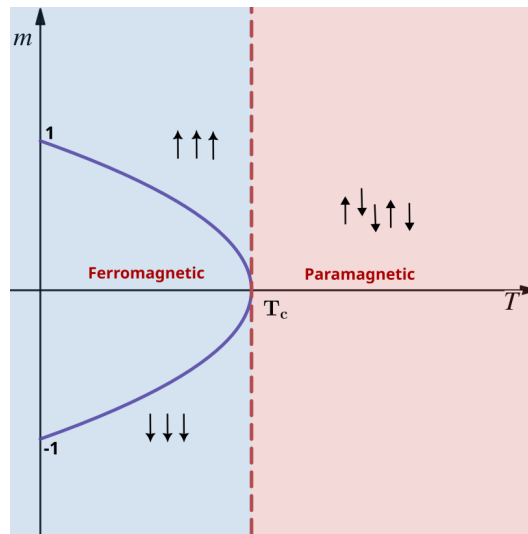

Figure 2.6: Phase diagram of 2d Ising model with $h \to 0^+$.

There is a phase transition at T_c. At $T < T_c$ the system will be either in the positive magnetization regime or in the negative one (spontaneous symmetry breaking).

In general, it is difficult to derive exact solutions in the case of non-zero external field and in higher dimensions. There are though different techniques which allow us to get approximate results:

- Mean-field theory

- Landau theory

- Renormalisation group

1.3 Properties at the critical point: Infinite clusters of Correlated Spins

1.3.1 The correlation length diverges at T_c

Correlation function

The **spin-spin correlation function** is defined as:

$$g(s_i, s_j) = \langle (s_i - \langle s_i \rangle)(s_j - \langle s_j \rangle) \rangle$$
$$= \langle s_i s_j \rangle - \langle s_i \rangle \langle s_j \rangle.$$

It describes how correlated are the two variables s_i and s_j, i.e. how the average value $\langle s_i s_j \rangle$ differs from the value it would get if s_i and s_j were independent.

In particular, note that if s_i and s_j are independent, then one would have that $\langle s_i s_j \rangle = \langle s_i \rangle \langle s_j \rangle$, which would then give a correlation $g(s_i, s_j) = 0$.

Notice that in every lattice point, $\langle s_i \rangle = \langle s_j \rangle = m$, the magnetization. We can also exploit the translational invariance of the Ising model and write the correlation function in terms of the relevant distance between the spins r.

$$g(s_i, s_j) = g(r) = \langle s_i s_{i+r} \rangle - m^2, \qquad \text{where } r = |j - i|.$$

Let's calculate the correlation function in the case of a zero external magnetic field.

$$g(s_i, s_j) = \langle s_i s_{i+r} \rangle - m_0^2(T) \qquad \text{for } h = 0..$$

At $T = 0$, all the spins are aligned $\Rightarrow g(s_i, s_j) = 0$ (no fluctuations).

We saw that in the 1d Ising model, $m_0(T) = 0$ for any finite temperature $T > 0$. Hence,

$$g(s_i, s_j) = \langle s_i s_{i+r} \rangle$$
$$= \frac{1}{\mathcal{Z}} \sum_{\{s_i\}} s_i s_{i+r} e^{-\beta E_{\{s_i\}}}.$$

Let's assume for now that the interaction couplings are local $J \to J_i$, i.e. they depend on the lattice site.

$$E_{\{s_i\}} = -\sum_{i=1}^{N} J_i s_i s_{i+1}.$$

Then the partition is

$$\mathcal{Z} = \sum_{\{s_i\}} e^{-\beta E_{s_i}}$$
$$= \prod_{i=1}^{N} 2 \cosh(\beta J_i).$$

Then from the observation that

$$\frac{\partial}{\partial J_k} \exp\left(\beta \sum_{i=1}^{N} J_i s_i s_{i+1}\right) = \beta s_k s_{k+1} \exp\left(J_i s_i s_{i+1}\right)$$

we can construct the correlation function:

$$
\begin{aligned}
g(s_i, s_j) &= \frac{1}{\mathcal{Z}} \sum_{\{s_i\}} \exp\left(\beta \sum_{i=1}^{N} J_i s_i s_{i+1}\right) s_i s_{i+r} \\
&= \frac{1}{\mathcal{Z}} \sum_{\{s_i\}} \exp\left(\beta \sum_{i=1}^{N} J_i s_i s_{i+1}\right) s_i s_{i+1} s_{i+1} \ldots s_{i+r-1} s_{i+r-1} s_{i+r} \\
&= \frac{1}{\mathcal{Z}} \frac{1}{\beta^r} \frac{\partial^r}{\partial J_i \partial J_{i+1} \ldots \partial J_{i+r-1}} \sum_{\{s_i\}} \exp\left(\beta \sum_{i=1}^{N} J_i s_i s_{i+1}\right) \\
&= \frac{1}{\mathcal{Z}} \frac{1}{\beta^r} \frac{\partial^r}{\partial J_i \partial J_{i+1} \ldots \partial J_{i+r-1}} \prod_{i=1}^{N} 2 \cosh \beta J_i \\
&= \frac{(2 \cosh \beta J)^{N-r} (2\beta \sinh \beta J)^r}{(2 \cosh \beta J)^N \beta^r} \qquad \text{restoring } J_i = J \\
&= \tanh^r \beta J.
\end{aligned}
$$

So, for the 1d Ising model, with $h = 0$,

$$g(r) = \langle s_i s_{i+r}\rangle = \tanh^r \beta J = \exp\left(r \log\left(\tanh(\beta J)\right)\right) \qquad (2.6)$$

We can rewrite the latter as

$$g(s_i, s_j) = \exp\left(-r/\xi\right), \qquad (2.7)$$

with

$$\xi(T, 0) = -\frac{1}{\log(\tanh \beta J)}, \qquad (2.8)$$

the **correlation length**. We see that the spin-spin correlation only depends on the relative distance between spins r and **decays exponentially** with the correlation length at zero external field.

Correlation length. From (2.7), we can interpret the correlation length as a measure of how fast the correlation function vanishes. The behaviour of (2.8) in the various limits is the following

$$
\xi(T, 0) = \begin{cases} 0 & T \to \infty \\ \frac{\exp(2\beta J)}{2} & T \to 0^+ \\ 0 & T = 0 \end{cases}.
$$

The correlation length diverges as $T \to 0^+$, i.e. as the system is closer to the critical temperature $T_c^{1D} = 0$.

1.3.2 The susceptibility diverges at T_c

Susceptibility per spin

> **Susceptibility**: sensitivity of the magnetization to changes in the external field at fixed temperature
>
> $$\chi(T, h) = \left(\frac{\partial m}{\partial h}\right)_T.$$

So in our case,

$$\chi(T, h) = \left(\frac{\partial m}{\partial h}\right)_T = \beta \frac{\cosh \beta h \exp\left(-4\beta J\right)}{\left[\sinh^2 \beta h + e^{-4\beta J}\right]^{3/2}}.$$

In zero external field $h = 0$:

$$\chi(T, 0) = \beta \exp\left(2\beta J\right) \to \begin{cases} \beta & T \to \infty \\ \beta e^{2\beta J} & T \to 0 \end{cases}.$$

For $T \to 0$, the susceptibility diverges exponentially.

> **Fluctuation-dissipation theorem**: The variance of the magnetisation is related to the susceptibility per spin through,
>
> $$\frac{\langle M^2 \rangle - \langle M \rangle^2}{N} = k_B T \chi.$$

This means that the variance of the magnetization diverges at $T \to 0$.

1.3.3 Phase transition at the microscopic scale

Qualitatively, we can understand the phase transition microscopically, in terms of clusters of spins.

> **Clusters of correlated spins**: Chain of spins with the same orientation.

Temp.	'wins'	Corr. length	Behaviour
$T \gg T_c$	Thermal energy	0	disordered spins
$T \ll T_c$	Local spin-spin interactions	size of spin-spin interaction	aligned spins
$T = T_C$	competition	diverges	huge fluctuations

- At $T \gg T_c$ spins are randomly orientated with no correlations.

- As T is lowered, the spin-spin interactions start to become more important and so larger and larger clusters of correlated spins form. However, as long as the correlation length is finite, there is an equal probability of having clusters of spin up or spin down and therefore the total magnetization is zero (in an infinite system).

- At T_c, the correlation length diverges and a "macro-cluster" of correlated spins emerges. This cluster is in fact a fractal; it contains clusters of all possible sizes. This non-local effect gives rise to a spontaneous magnetization as T passes T_c.
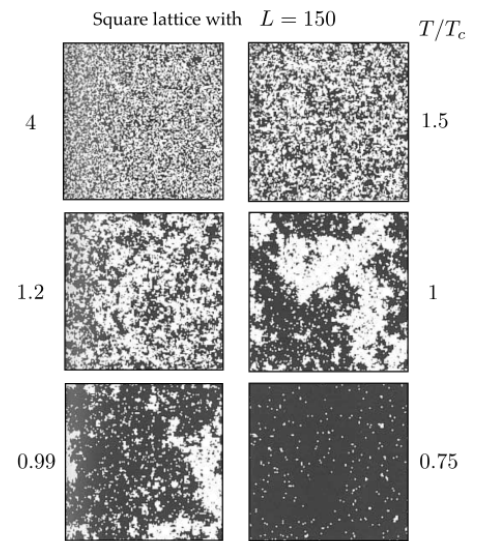
Figure 2.7: Microstates of the 2d Ising model in zero external field, at different temperatures T/T_c.

- At $T \ll T_c$, almost all spins are aligned. Now the non-zero correlation length gives rise to (small) fluctuations away from the fully aligned state.
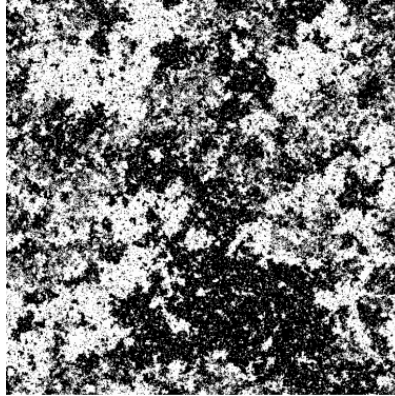

Figure 2.8: 2d Ising model close to T_c. At criticality the system is scale invariant $\rightarrow$ it has a fractal structure; it contains clusters of all sizes of opposite spins.

2 Percolation

Percolation provides one of the simplest model undergoing a phase transition.

To 'percolate' means to 'trickle through' something. This could be water through a coffee machine or viruses infecting an entire population. Percolation typically exhibits universality; close to the phase transition, it allows us to describe phenomena that are different as coffee filtering and the spreading.

Take some squared paper and black out a portion of the squares randomly. Consider the clusters of adjacent black squares.
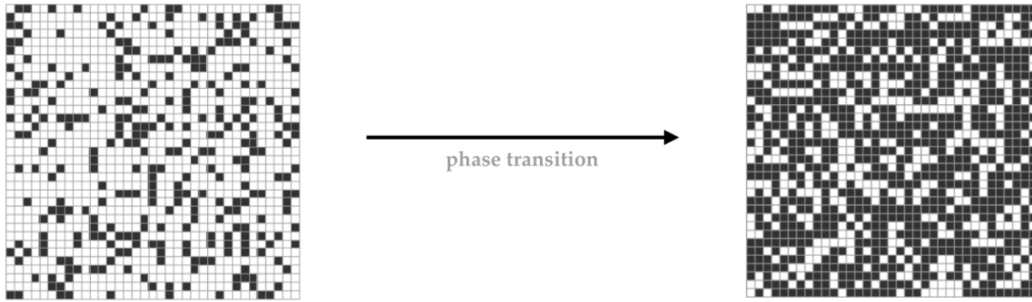
Left: If a small portion of the squares is blacked out, it's unlikely that the cluster extends across opposite sides of the paper.
Right: If a large portion of the squares is blacked out it is likely that the cluster "percolates" across the paper.

There is a fraction of randomly blacked out squares that marks a phase transition from a non-percolating cluster to a percolating one.

2.1 Site percolation on a lattice

We consider a $2d$ lattice of $L \times L$ sites.

We define:

- p = **occupation probability** = probability that a site is occupied.

- **cluster** = group of nearest-neighboring occupied sites

- s = **cluster size** = number of sites in a cluster.

We say that the cluster is percolating if the cluster is infinite. At finite systems, clusters that span the lattice from left/top to right/bottom are good candidates.

Behaviour for different probability values

- For $p = 0$, the lattice will be empty.

- For $p = 1$, all the sites will be occupied $\rightarrow$ 1 big cluster of size L^2.

- For $0 < p < 1$, each realization will be different, but we expect the size of the largest cluster to increase with p.

p=0.10	p=0.55	p=0.58	p=p$_c$=0.5927	p=0.65	p=0.90
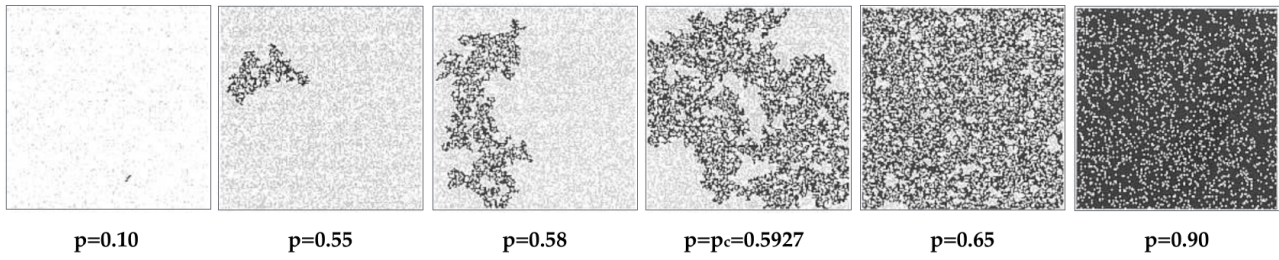
Percolation parameters

1. Intensive parameter: $p =$ occupation probability.

2. Order parameter: $\begin{cases} \theta(p) = & \text{percolation probability, i.e. probability that there is a cluster of infinite size.} \\ P_\infty(p) = & \text{probability that any given site belongs to the percolation cluster.} \end{cases}$

   These should equal to 1 in the percolating phase and 0 before the phase transition.

More generally, we are interested in the probability distribution of cluster sizes s, or simply in the frequency of occurrence of clusters of size $s : N(s,p)$

Other questions:

⇨ **Size** : How much space does the percolating cluster occupy? What is the probability that a site belong to the percolating cluster?

⇨ **Geometry** : What is the geometry of the percolating cluster? Does it have a fractal structure?

⇨ **Finite clusters** What are the distribution of sizes of the finite clusters? What is the probability that a given site belongs to a cluster of size s?

2.1.1 Site percolation in d=1
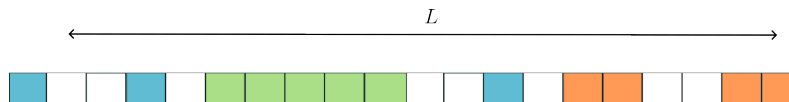
We define the following useful quantities:

$$N(s,p) = \text{cluster size frequency = number of clusters of size s.}$$

s	N(s,p)
1	3
2	2
5	1

$$n(s,p) = \frac{N(s,p)}{L} = \text{cluster size density = density of clusters of size s.}$$

$$sn(s,p) = \text{probability that a given site belongs to a cluster of size s.}$$

$$n(s,p) = \text{probability that a given site belongs to the left hand side of a cluster of size s.}$$

$$n(s,p) = \underbrace{p^s}_{\substack{\text{prob. that s} \\ \text{sites are occupied}}} \cdot \underbrace{(1-p)^2}_{\substack{\text{prob. that} \\ \text{boundary sites} \\ \text{are not occupied.}}}$$

This relation can be rewritten as:

$$n(s,p) = (p_c - p)^2 \exp\left(\ln p^s\right)$$
$$= (p_c - p)^2 \exp\left(s \ln p\right)$$
$$= (p_c - p)^2 \exp\left(-\frac{s}{s_\xi}\right).$$

where s_ξ the cutoff cluster size, i.e. the characteristic cluster size.

$$s_\xi = -\frac{1}{\ln p} = \frac{-1}{\ln\left(p_c - (p_c - p)\right)} \xrightarrow{p \to p_c = 1} \frac{1}{p_c - p} = (p_c - p)^{-1} \qquad \qquad \ln(1-x) = -x + \mathcal{O}(x^2).$$

> The **critical exponent** σ gives the power law behaviour of the cutoff cluster size s as $p \to p_c$
>
> $$\sigma_\xi \propto |p_c - p|^{-1/\sigma} \qquad p \to p_c.$$

So for the 1d percolation, $\sigma = 1$.

For $p < p_c$ the probability that a site belongs to *any* cluster, is simply the probability p that it is occupied. Since the probability that a site belongs to a cluster of size s is $sn(s,p)$, the probability that a site belongs to **any** cluster is

$$\sum_s s\,n(s,p) = p \qquad p < p_c$$

How large is a cluster

The probability that an **occupied** site belongs to a cluster of size s is

$$w(s,p) = \frac{s\,n(s,p)}{p} = \frac{s\,n(s,p)}{\sum_s s\,n(s,p)}.$$

Then, the **mean** cluster size is

$$\begin{aligned}
\chi(p) &= \sum_{s=1}^{\infty} s\,w(s,p) \\
&= \sum_{s=1}^{\infty} \frac{s^2 n(s,p)}{p} \\
&= \frac{(1-p)^2}{p} \sum_{s=1}^{\infty} s^2 p^s \\
&= \frac{(1-p)^2}{p} \left(p\frac{d}{dp}\right)\left(p\frac{d}{dp}\right)\left(\sum_{s=1}^{\infty} p^s\right).
\end{aligned}$$

Using the formula for the geometric series and acting twice with the operator $p\frac{d}{dp}$, we obtain

$$\chi(p) = \frac{1+p}{1-p} = \frac{p_c + p}{p_c - p} \xrightarrow{p \to p_c} \frac{2p_c}{p_c - p} \propto (p_c - p)^{-1}.$$

> The **critical exponent** γ gives the power law for the mean cluster size, near p_c
>
> $$\chi(p) \propto |p_c - p|^{-\gamma} \qquad p \to p_c.$$

For the 1d percolation $\gamma = 1$.

We see that both the characteristic cluster size and the mean cluster size diverge for $p \to p_c$

Correlation function

> The **correlation function** $g(r)$ is the probability that a site at position r from an occupied site belongs to the same finite cluster

By definition $g(r = 0) = 1$ (occupied site).

In $1d$, for a site at position r to be occupied and belong to the same (finite) cluster with an occupied site at $r = 0$, this site and all the $(r - 1)$ intermediate sites must be occupied:

$$g(r) = p^r$$
$$= \exp\left(r \ln p\right)$$
$$= \exp\left(-r/\xi\right)$$

where

$$\xi = -\frac{1}{\ln p} = -\frac{1}{\ln\left(p_c - (p_c - p)\right)} \rightarrow \frac{1}{p_c - p} = (p_c - p)^{-1}, \qquad p \rightarrow p_c = 1.$$

ξ is the **correlation length**, which also diverges for $p \rightarrow p_c$.

> The **critical exponent** ν gives the power law of the correlation length, near p_c :
>
> $$\xi \propto |p_c - p|^{-\nu} \qquad p \rightarrow p_c.$$

Universality

It turns out that the critical occupation probability p_c is **non-universal**. It depends on the lattice details and the occupation rule (e.g. site or bond percolation).

However, the critical exponents are **universal**. They are insensitive to the details of the lattice, but they do depend on the dimensionality of the lattice.

Exponent	Quantity	d=1	d=2	d=3	d=4	d=5	$d \geq 6$	Bethe
β	$P_\infty(p) \propto (p - p_c)^\beta$	0	5/36	0.4181(8)	0.657(9)	0.830(10)	1	1
γ	$\chi(p) \propto \|p - p_c\|^{-\gamma}$	1	43/18	1.793(3)	1.442(16)	1.185(5)	1	1
ν	$\xi(p) \propto \|p - p_c\|^{-\nu}$	1	4/3	0.8765(16)	0.689(10)	0.569(5)	1/2	1/2
σ	$\sigma_\xi(p) \propto \|p - p_c\|^{-1/\sigma}$	1	36/91	0.4522(8)	0.476(5)	0.496(4)	1/2	1/2
D	$\sigma_\xi \propto \xi^D$	1	91/48	2.523(6)	3.05(5)	3.54(4)	4	4

∗ The Bethe lattice corresponds to an infinite-dimensional lattice.

2.2 Critical exponents and Universality

> **Universality**: two systems, microscopically completely different, can exhibit precisely the same critical behaviour, close to their phase transition. We then say that they belong to the same universality class.
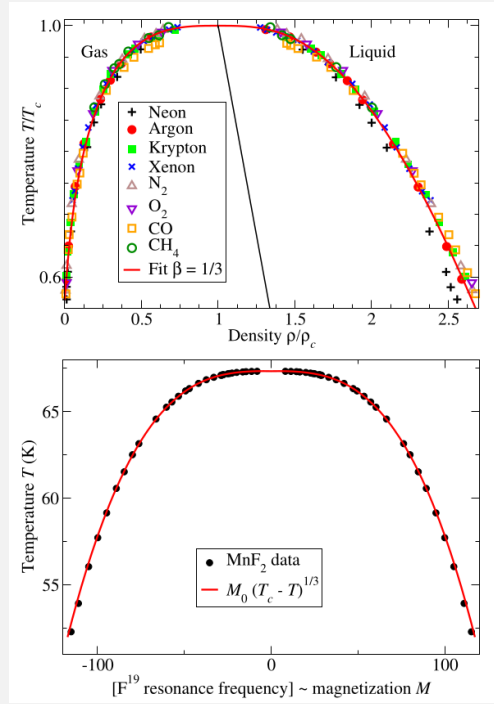
Note: Universality originates from the *Renormalization Group*.

> E.g. Universality at the **liquid-gas critical point** and at the **ferromagnetic-paramagnetic critical point**.

Order parameters close to criticality:

$$\frac{\Delta\rho}{\rho_c} = \frac{\rho_L - \rho_G}{\rho_c} = 2\rho_0 \left(1 - \frac{T}{T_c}\right)^\beta \qquad \begin{cases} \rho_0 = 1.75 \\ \beta = 1/3 \end{cases}$$

$$\langle M \rangle = M_0 T_c \left(1 - \frac{T}{T_c}\right)^\beta \qquad \beta = 1/3.$$

Both the magnet and liquidg-gas critical point have order parameters that vary as $\left(1 - \frac{T}{T_c}\right)^\beta$ with $\beta = 1/3$. The two systems belong to the same universality class, along with the 3D Ising model. β is an example of a **critical exponent**, which in this case, characterises the scaling behaviour close to the critical point.

∗ The liquid-gas coexistence curves are tilted, but we can define a shifted, effective density so that the graph is symmetric like in the case of the magnet.

Chapter 3

Mean-field theory

1 Mean-field (MF) approximation

1.1 Introduction to the MF approximation

1.1.1 The general idea

Systems with many degrees of freedom are generally hard to solve exactly. We saw that the 1d Ising model and 2d Ising model in zero external field can be described with closed, analytic forms, but often we need to describe systems in higher dimensions or with more complex interactions. Mean Field Theory (MFT) is an *approximation* method which allows us to reduce many-body interactions to a one-body interaction. This is done by approximating the effect of each individual part of the system by a single *averaged* effect, or in other words, we replace all the interactions by an effective 'mean' field. This drastically simplifies the calculations.

In the context of the Ising model, this method gives a good qualitative insight to the phase transitions in dimensions $d > 1$. In particular, the theory correctly predicts a phase transition at a finite temperature T_c for $h = 0$.

In practice, the idea of MFT is to expand the (spin) fields around their mean values, plus some fluctuations around them:

$$s_i = \langle s_i \rangle + \epsilon_i, \qquad \text{with} \quad |\epsilon_i| \ll |\langle s_i \rangle|,$$
$$\epsilon_i = s_i - \langle s_i \rangle.$$

We will prove that this corresponds to a system of **non-interacting spins**, subject to an **effective field** of strength $H + Jqm$, where $m = \langle s_i \rangle$ and q the number of nearest neighbors. Spins act as **independent**, but immersed in an average local field created by their neighbors: $H_{loc} = q \times Jm$.

1.1.2 Example: Mean-field Ising model

Mean-field Ising model: It corresponds to a system of non-interacting spins, immersed in an effective field of strength $H + Jqm$ where $m = \langle s_i \rangle$ and $q = $ number of nearest neighbors.

Let's prove this:

$$s_i = \langle s_i \rangle + \epsilon_i \qquad\qquad |\epsilon_i| \ll |\langle s_i \rangle|,$$
$$= \langle s_i \rangle + (s_i - \langle s_i \rangle)$$

$$.$$

Interaction energy:

$$E_{int}(\boldsymbol{s}) = -J \sum_{\langle i,j \rangle} \left[\langle s_i \rangle + (s_i - \langle s_i \rangle) \right] \left[\langle s_j \rangle + (s_j - \langle s_j \rangle) \right]$$

$$= -J \sum_{\langle i,j \rangle} \left(\langle s_i \rangle \langle s_j \rangle + \langle s_i \rangle s_j + \langle s_j \rangle s_i - 2\langle s_i \rangle \langle s_j \rangle + \underbrace{(s_i - \langle s_i \rangle)(s_j - \langle s_j \rangle)}_{\epsilon_i \epsilon_j} \right)$$

Neglect

$$= J \sum_{\langle i,j \rangle} \langle s_i \rangle \langle s_j \rangle - 2J \sum_{\langle i,j \rangle} \langle s_j \rangle s_i \qquad i \leftrightarrow j$$

$$= N \frac{Jm^2 q}{2} - qJm \sum_{i=1}^{N} s_i.$$

Mean field approximation consists of neglecting second order fluctuations $\sim \epsilon^2$.

Then we can write the **total energy** as

$$E(\boldsymbol{s}) = E_{int}(\boldsymbol{s}) - h \sum_{i=1}^{N} s_i$$

$$= N \frac{Jm^2 q}{2} + \sum_{i=1}^{N} E(s_i) \qquad \text{with } E(s_i) = - \underbrace{(qJm + h)}_{\text{Local effective field}} s_i.$$

Since $E(s_i)$ has only a single spin variable s_i, it means that we have non-interacting spins, but each spin s_i is now immersed to this new local effective field created by its neighbors.

A nice property of non-interacting/independent spins is that we can replace the joint probability distribution by a product of the probability distributions for each spin!

$$P(\boldsymbol{s}) = P(s_1, s_2, \ldots s_N) = \prod_{i=1}^{N} P(s_i).$$

where

$$P(s_i) = \frac{e^{-\beta E(s_i)}}{\mathcal{Z}_i} \qquad \text{with } \begin{cases} E(s_i) = -(qJm + h)s_i \\ \mathcal{Z}_i = 2 \cosh\left(\beta(qJm + h)\right) \end{cases}.$$

1.2 Computing the order parameter – Self-consistency relation

1.2.1 Self-consistency relation for m

Average magnetisation per spin:

$$m = \langle s_i \rangle = \mathbb{P}(s_i = 1) - \mathbb{P}(s_i = -1) = \frac{e^{-\beta E(1)} - e^{-\beta E(-1)}}{e^{-\beta E(1)} + e^{-\beta E(-1)}}.$$

Substituting the expression for $E(s_i)$, we get the following **self-consistency relation**

$$m = \tanh\left(\beta(qJm + h)\right) \tag{3.1}$$

1.2.2 Solving the self-consistency relation

This is an implicit function, but we can investigate its solutions graphically by ploting both the functions of m on the RHS and on the LHS of Eq. (3.1). First, we consider the case of a zero external field $h = 0$. Depending on the slope of the RHS at $m = 0$, there might be one or three solutions (see Fig. 3.1 and 3.2). The slope of the $\tanh$ function is given by

$$\frac{d}{dm} \tanh(\beta q J m)\Big|_{m=0} = \frac{qJ}{k_B T}.$$

We want to compare this with the slope of the diagonal of the graph $y = m \rightarrow \frac{dy}{dm} = 1$

As the following graph illustrates,

- if $\quad \dfrac{qJ}{k_B T} < 1 \quad$ only one solution exists at $m = 0$

- if $\quad \dfrac{qJ}{k_B T} > 1 \quad$ three solutions exist at $m = 0, m = \pm m_0$.

We can define the critical temperature as the temperature for which the slope equals to 1 :
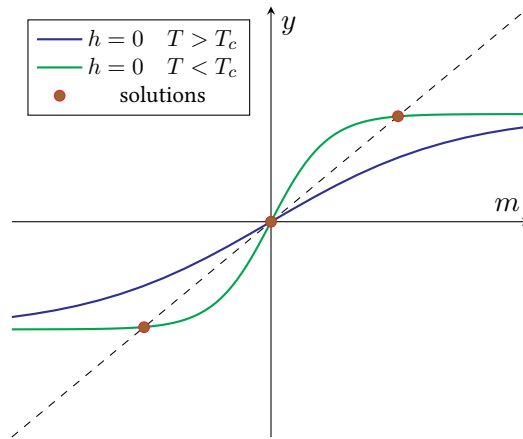
$$T_c = \frac{qJ}{k_B} \tag{3.2}$$

Figure 3.1: Graph of consistency equation (3.1) for $h = 0$. The solutions correspond to the intersection of $y = \tanh(\ldots)$ and the diagonal $y = m$. $m = 0$ is always a solution. Whether other solutions exist depends on the slope of $y = \tanh(\ldots)$ at $m = 0$. If the slope is larger than 1 (slope of diagonal) two new solutions appear.

For $h > 0$, the graphs are translated up to the y axis. Now there is only one solution both for $T < T_c$ and for $T > T_c$ (similarly for $h < 0$). This indicates that there must be a phase transition.
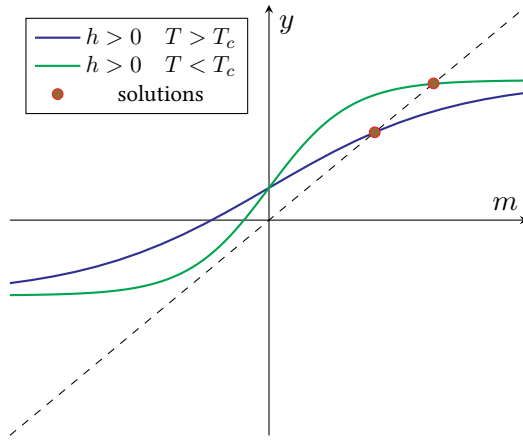
Figure 3.2: Graph of consistency equation (3.1) for $h > 0$. Only one solution, m_+ exists.

1.2.3 Stability of the solutions

We are also interested in the stability of these solutions. A first approach is to consider the graph of $h > 0$ and continuously take the field h to go to zero. The solution at m_+ persists and when $h = 0$ will coincide with $+m_0$. This means that m_+ will be a stable solution. Similarly, if we did the same starting from the $h < 0$ graph, we would find that m_- should also be a stable solution, coinciding with $-m_0$ at $h = 0$.

However in order to check if our prediction is correct, we have to compute the **free energy**.

Free energy:

$$F = -k_B T \log \mathcal{Z}$$

$$\mathcal{Z} = \exp\left(-\frac{\beta N J m^2 q}{2}\right) \prod_{i=1}^{N} \left[2 \cosh\left(\beta(qJm + h)\right)\right].$$

(3.3)

If we plot this expression for different values of h and T, we get the following pictures:
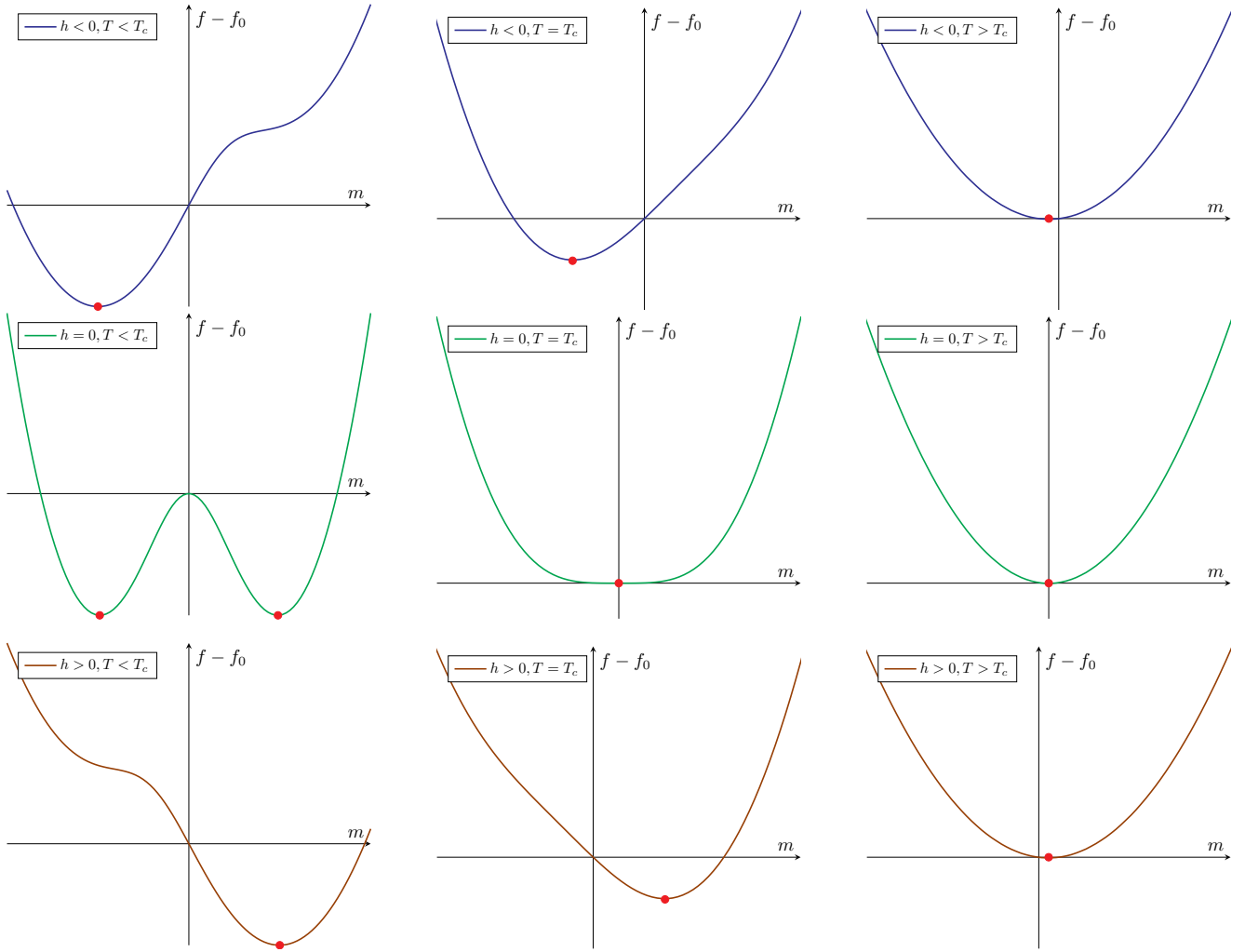
Figure 3.3: Plots of the free energy for $h < 0$ (first row), $h = 0$ (second row) and $h > 0$ (third row) and for different temperatures with respect to the critical one T_c. The red dot indicates the (global) minimum of the free energy, in which the system is realized. You can interactively explore these graphs by this app.

Indeed, m_+ is a stable solution for $h > 0$ and $T < T_c$, since it corresponds to the global minimum of the free energy, in which the system is realized. Similarly for m_- for $h < 0$. $m = 0$ is a stable solution only for $h = 0$ and $T \geq T_c$ (marginally stable for $T = T_c$). We will discuss more about the information that we can extract from these plots, in the following chapter.

1.3 Critical temperature and critical exponents: How good is the mean-field approximation?

Critical temperature: As we saw, the critical temperature predicted by the mean-field approximation is

$$T_c = \frac{qJ}{k_B}$$

where q the number of nearest neighnors. q depends on the dimensionality of the model though.

- For **d=1** : $q = 2 \rightarrow T_c = \frac{2J}{k_B}$, whereas we expect $T_c = 0$. So for $d = 1$, the approximation is not good.

- For **d=2** : $q = 4 \rightarrow T_c = \frac{4J}{k_B}$, whereas the value predicted by Onsager is $k_B T_c = \frac{2J}{\log(1+\sqrt{2})} \simeq 2.269J$. We predict a larger value for T_c. Intuitively this makes sense, because in the mean-field procedure we neglect

fluctuations of second order and higher . However, the fluctuations are the ones that probe the system to undergo a phase transition. Neglecting them, means that we consider a system that has a tendency to remain longer in the ferromagnetic phase, and thus we predict a higher critical temperature.

Critical exponents: What will actually determine the validity of the mean-field approximation, is whether it predicts correctly the critical exponents of the model, i.e. the scaling behaviour close to criticality. The derivation of the critical exponents is done by Taylor expanding the free energy for $h = 0$, and for small values of m, i.e. close to the critical temperature T_c (where $m = 0$). From the derivatives of the free energy we can generate any physical quantity of interest.

🏠 See exercises.

	Exponent	MF theory	d=2	d=3
$C \sim |T - T_c|^{-a}$	α	discont.	$\ln|T - T_c|$	0.01 ± 0.01
$M_0 \sim (T_c - T)^\beta \quad (T < T_c)$	β	0.5	0.125	0.312 ± 0.003
$\chi \sim |T - T_c|^{-\gamma}$	γ	1	1.75	1.250 ± 0.002

The critical exponents get better in higher dimensions. In fact, the mean-field approximation is **exact** in infinite dimensions d.

At first, we might think that this is because of the increasing number of neighbors q in higher dimensions. However, the critical exponents are **universal**, i.e. they do not depend on the underlying lattice (and therefore the number of nearest neighbors). The agreement between mean-field exponents in higher dimensions is rather a result of the unimportance of fluctuations in higher dimensions, in which mean-field theory is based on.

2 Landau Theory

2.1 Introduction: Taylor expansion of the free energy close to the critical point

A more fundamental approach to find the minima of the free energy and calculate all of its physical derivatives is by Taylor expanding it in powers of the order parameter. In the case of the Ising model, that would be the magnetization per spin m.

Let's try to apply this in equation (3.3) of the free energy that we derived from the mean-field approximation. Using that $T_c = \frac{qJ}{k_B}$, the free energy per spins is,

$$f = \frac{k_B T_c}{2} m^2 - k_B T \log \left[2 \cosh \left(\frac{T_c}{T} m + \frac{h}{k_B T} \right) \right].$$

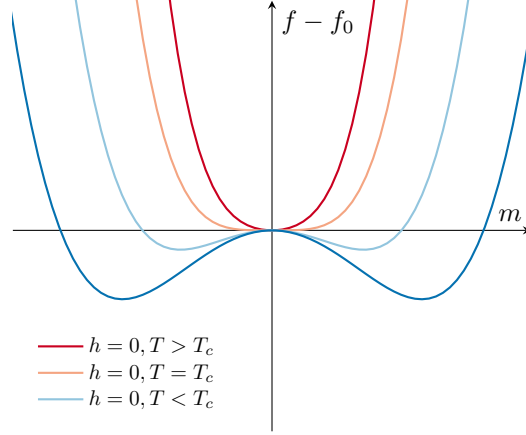Some useful Taylor expansions:

$$\log(1 + x) = x - \frac{x^2}{2} + \frac{x^4}{4} + \mathcal{O}(x^4)$$

$$\cosh x = 1 + \frac{x^2}{2!} + \frac{x^4}{4!} + \mathcal{O}(x^4)$$

$$\Rightarrow \log \cosh x = \frac{x^2}{2} - \frac{x^4}{12} + \mathcal{O}(x^4).$$

We expand around $(T_c, h = 0)$ up to fourth order in m, by setting $x = \frac{T_c}{T}m + \beta h$:

$$f = f_0 + \frac{k_B T_c}{2}m^2 - k_B T \left[\frac{1}{2}\left(\frac{T_c}{T}m + \beta h\right)^2 - \frac{1}{12}\left(\frac{T_c}{T}m + \beta h\right)^4 \right]$$

$$f = f_0 - hm + \frac{k_B}{2}(T - T_c)m^2 + \frac{k_B T}{12}m^4 + \mathcal{O}(m^4) \qquad T \to T_c$$

(3.4)

where $f_0 = -k_B T \log 2$, the pure entropy-part of the free energy, remaining when $T \to \infty$ $(m = 0)$.

This expansion of the free energy, preserves all the information required to extract the critical exponents that determine the behaviour of the mean-field Ising model close to the critical point $(T, h) = (T_c, 0)$.

If we were to expand only up to second order, we would not observe the phase transition, i.e. the transition from one to two minima after some critical temperature T_c.
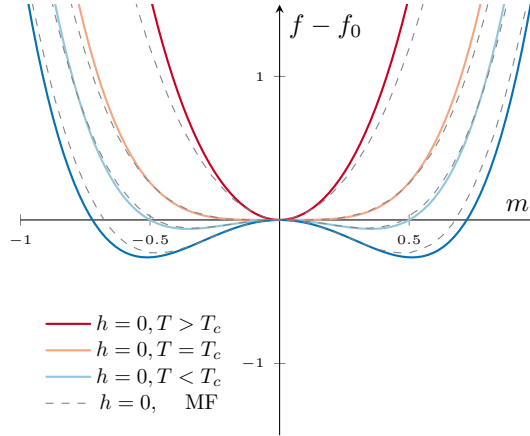

Figure 3.4: Graphs obtained from mean field theory vs. free energy expansion

We can rewrite the free energy expansion (3.4) as

$$f = f_0 - hm + \underbrace{a_2(T - T_c)}_{\substack{\text{positive if } T > T_c \\ \text{negative if } T < T_c}} m^2 + a_4 m^4 + \mathcal{O}(m^4)$$

(3.5)

with

$$f_0 = -k_B T \log 2, \qquad a_2 = \frac{k_B}{2}, \qquad a_4 = \frac{k_B T}{12} > 0.$$

Note that it is important that the last term of our expansion $(a_4 m^4)$ is positive, since f should be bounded from below. Only then there is a minimum where the physical system is going to be realized. If $a_4 < 0$, for large values of m, f will be decreasing indefinitely, and no minima will be able to be formed.

Landau approximation of the Ising model: corresponds to a 4-th order expansion of the free energy per spin in the order parameter m.

2.2   Critical exponents

Since we have an expression for the free energy, we can calculate any quantity of interest! Let's check that we can recover the critical exponents for various quantities.

By requiring that the free energy is minimized, we can obtain the magnetization per spin,

$$\frac{\partial f}{\partial m} = 0 \Rightarrow \underbrace{-h + 2a_2(T - T_c)m + 4a_4 m^3}_{\bullet} = 0.$$

For $h = 0$,

$$m_0^2 = -\frac{a_2}{2a_4}(T - T_c)$$
$$m_0 \sim (T_c - T)^\beta \quad \text{for } T < T_c$$
$$\Rightarrow \quad \beta = 1/2 \tag{3.6}$$

For the susceptibility $\chi = \left(\frac{\partial m}{\partial h}\right)_{h=0}$,

$$\lim_{h \to 0}\left(\frac{\partial \bullet}{\partial h}\right)_T = -1 + 2a_2(T - T_c)\chi + 12a_4 m_0^2 \chi = 0$$

$$\Rightarrow \chi = \frac{1}{2a_2(T - T_c) + 12a_4 m_0^2}$$

$$= \begin{cases} \frac{1}{k_B}(T - T_c)^{-1}, & T \to T_c^+ \\ \frac{1}{2k_B}(T - T_c)^{-1}, & T \to T_c^- \end{cases} \quad \Rightarrow \quad \gamma = -1.$$

$$\chi \sim |T - T_c|^{-\gamma}$$

We obtain the same results for the critical exponents.

2.3   Landau Theory for continuous phase transitions

We can generalize the above expansion for any system undergoing a continuous phase transition. Since the order parameter grows continuously from zero at the critical point, Landau suggested that, the free energy (being analytic near the critical point) can be Taylor expanded in terms of the order parameter , which is small near the phase transition. From this expansion we can extract information for the system's behaviour close to the critical point.

A compact way to write the expansion, for an order parameter η:

$$f(T, h, \eta) = \sum_{k=0}^{\infty} a_k(T, h)\eta^k \qquad \text{for } (T, h) \to (T_c, h_c).$$

By exploiting the symmetries of the problem we can find constraints for the coefficients $a_k(T, h)$.

E.g. In the Ising model at $h = 0$, we know that there is a $\mathbb{Z}_2$ symmetry, i.e. $f(T, 0, -m) = f(T, 0, m)$ since it doesn't make any difference if the spins will point all up or all down below the critical temperature.

This means that f is **even** and therefore

$$a_k(T, 0) = 0 \quad \text{for } k \text{ odd .}$$

Only even powers of the order parameter m will be present in the expansion.

Another remark is that close to the phase pransition, the order parameter m is small, which allows us to neglect higher order terms. In particular,

$$f(T, 0, m) = a_0(T, 0) + a_2(T, 0)m^2 + a_4(T, 0)m^4$$

is the simplest expansion that contains a phase transition.

Moreover, we can always constrain the last coefficient of the expansion to be positive, so that f has a minimum. Here,
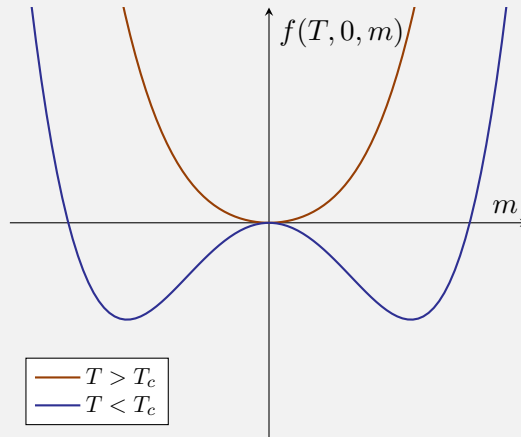
$$a_4(T, 0) > 0.$$

Finally, plugging all these to a graphical calculator we can confirm that

If $a_2(T, 0) > 0$ for $T > T_c \longrightarrow$ there is only one minimum, at **m=0**

If $a_2(T, 0) < 0$ for $T < T_c \longrightarrow$ there two non-zero symmetric minima, at $\boldsymbol{m = m_\pm}$

$$\Rightarrow \quad a_2(T, 0) = \tilde{a}_2(T - T_c) \quad \text{with } \tilde{a}_2 > 0.$$

For $T > T_c$ ($m = 0$) the only remaing term is $a_0(T, 0) = f_0(T)$, the entropic part of the free energy.

Landau description of **continuous phase transitions**

$$\boldsymbol{h = 0}: \quad f(T, 0, m) = f_0(T) + \tilde{a}_2(T - T_c)m^2 + a_4(T, 0)m^4$$
$$\boldsymbol{h \neq 0}: \quad f(T, h, m) = f_0(T) - hm + \tilde{a}_2(T - T_c)m^2 + a_4(T, h)m^4.$$
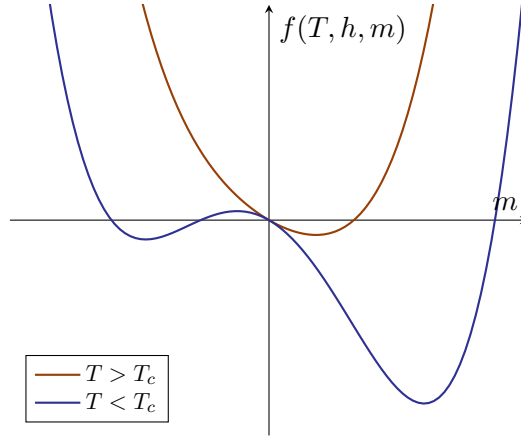
Figure 3.5: Free energy with a non-zero external field.

Notice that with the extra $-hm$ term, the graph of the free energy is tilted.

2.4 Validity of the mean-field theory: Ginzburg criterion

Landau's theory is a mean-field theory. In the mean-field approximation we assume that we can neglect fluctuations of the energy:

$$E(\boldsymbol{s}) = \underbrace{-(Jqm + h) \sum_{i=1}^{N} s_i + \frac{NJqm^2}{2}}_{E_0(\boldsymbol{s})} + \Delta E(\boldsymbol{s})$$

where $E_0(\boldsymbol{s})$ is the mean-field energy, whereas the spin-spin interaction is contained in

$$\Delta E(\boldsymbol{s}) = -\frac{Jq}{2} \sum_{i=1}^{N} (s_i - \langle s_i \rangle)(s_j - \langle s_j \rangle).$$

Fluctuations are negligible if $|\Delta E(\boldsymbol{s})| \ll |E_0(\boldsymbol{s})|$. In zero external field,

$$|\Delta E(\boldsymbol{s})| = \frac{Jq}{2} \sum_{i=1}^{N} g(s_i, s_j) = \frac{Jq}{2} k_B T \chi$$

$$|E_0(\boldsymbol{s})| = \left| -JqNm^2 + \frac{NJqm^2}{2} \right|$$

$$= \frac{Jq}{2} Nm^2.$$

So we want

$$Nk_B T\chi \ll (Nm)^2 = \langle M \rangle^2.$$

From the fluctuation-dissipation theorem, the quantity $Nk_B T\chi$ is the variance of the total magnetisation $\langle M^2 \rangle - \langle M \rangle^2$. Therefore, we arrive to the following criterion

$$\frac{\sqrt{\langle M^2 \rangle - \langle M \rangle^2}}{\langle M \rangle} \ll 1 \tag{3.7}$$

which is known as the Ginburg criterion. In the case of the mean-field Ising model, this results to an upper critical dimension:

$$d > 4.$$

Above this dimension, the mean-field theory gives correct predictions for the critical exponents, as a result of the 'unimportance' of fluctuations in higher dimensions.

Due to this criterion, Landau's theory is quantitatively inconsistent with experiments (where $d < 4$). However, it gives a good **qualitative** description of the phase transitions.

2.5 Landau Theory for discontinuous phase transitions

Landau's theory is also possible to describe discontinuous phase transitions. For example the Liquid to Solid water transition can be modeled by

$$f - f_0 = a(T - T_c)\rho^2 + c\rho^3 + \frac{1}{2}b\rho^4 \tag{3.8}$$

where all the coefficients are positive. Graphically this corresponds to an abrupt transition from one global minimum to another.
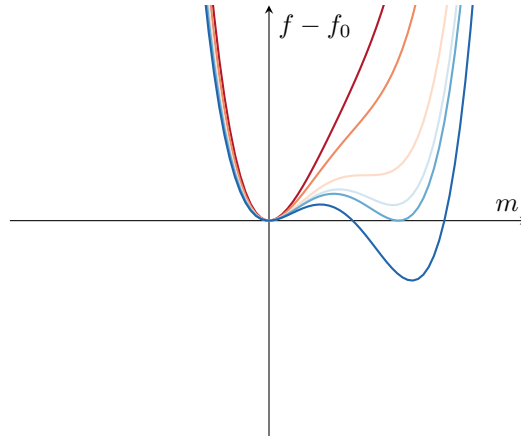

Figure 3.6: Free energy for a discontinuous phase transition. The colors indicate the change of the temperature; from $T \gg T_c$ (red line) to $T < T_c$ (dark blue line).

Notice that due to the odd power term $c\rho^3$ the graph is asymmetric.

A symmetric function would be

$$f - f_0 = a_0(T - T_c)m^2 + \frac{1}{2}\beta m^4 + \frac{1}{3}\gamma m^6 \tag{3.9}$$

with $a_0 > 0$, $\beta < 0$ and $\gamma > 0$. This again leads to an abrupt transition from one global minimum (at $m = 0$) to two minima at $m = \pm m_*$
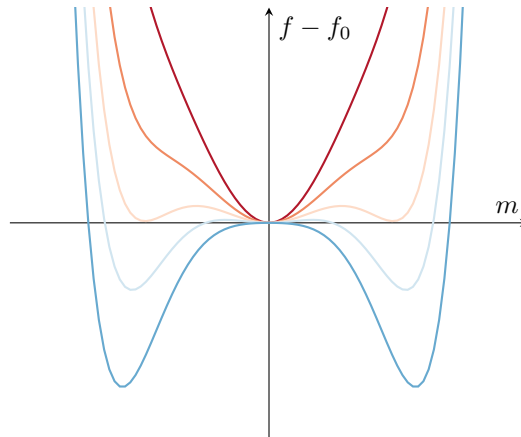

Figure 3.7: Free energy for a discontinuous phase transition. Symmetric case.

3 Tutorial: Application to the TASEP model

🏠 See TCS 3 for details

The mean-field approximation is widely used in the context of the modeling of many complex systems. We will use it in chapter 5 in the models of epidemic spreading and of opinion dynamics (see TCS 5).

Chapter 4

Scale Invariance and Universality

1 Emergent behaviors in the simple example of random walks: scale-invariance and universality

1.1 Introduction: properties of critical phenomena

At a continuous phase transition, the systems displays:

- **Universality:** two systems, microscopically completely different, can exhibit precisely the same critical behavior near their critical point;

- **Scale Invariance:** the system "looks" the same at all scales; it has the same statistical properties at all scales.

> **Scale invariance**: the system remains the same (in the statistical sense) at all scale.
>
> See for instance these videos: scale invariance of a **percolating cluster here** or scale invariance in the **critical Ising model here**.

1.2 Fractals: notion of self-similarity and fractal dimension

1.2.1 Self-similarity and fractals

Self-similar object: is exactly or approximately similar to a part of itself. This is a typically properties of fractals; see example of the Sierpiński triangle in Fig. 4.1. In nature, there are many things that are statistically self-similar, such as for examples Romanesco broccoli, Frost crystals, High-voltage breakdown within a block of acrylic glass, etc.
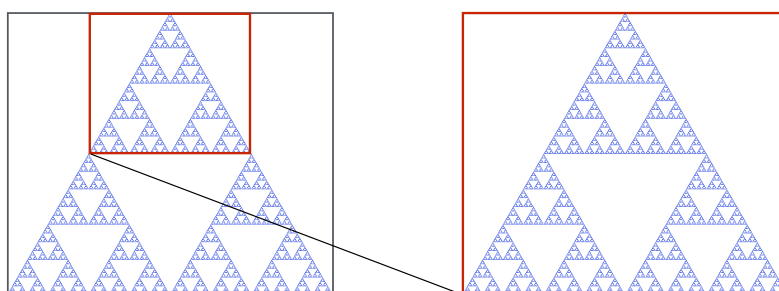

Figure 4.1: Sierpiński triangle.

You can find examples of simulation of simple models that generate statistically self-similar objects on the Complexity Explorables website: here. Most common types of models are:

- **Iteration process:** in which elements of a structure are replaced by a smaller version of the whole structure. See example here. For instance, you can see there how to build the Sierpiński triangle iteratively.

- **Lindenmayer Systems:** Statistical iterative system: how fractal patterns observed in natural systems, particularly structural properties of some plants. See example here.

- **Stochastic cellular:** automaton generating fractal growth patterns. See example here. (Note that again here there is a (deterministic) rule that can reproduce the Sierpiński triangle).

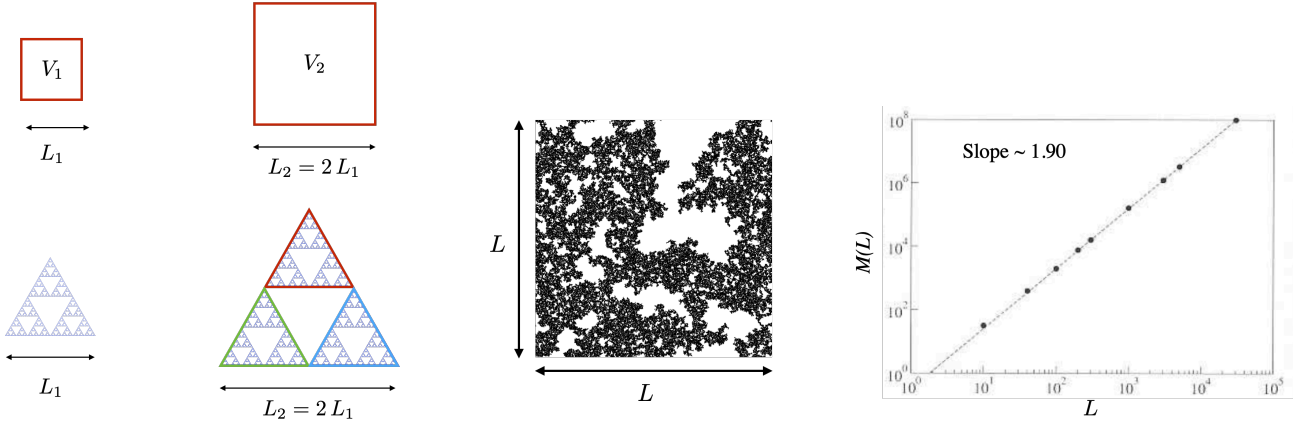Figure 4.2: Fractal dimension. Right: 2D site percolation.

1.2.2 Fractal dimension

In usual object, one expects that the mass (or volume) of the object scales as $M \propto L^d$, where d is the dimension of the object and L a typical size of the object along one direction. Another way to express this is that one expects that the density of the object doesn't depend on the scale at which we are looking at it. For example in Fig. 4.2 Top, we take two square boxes, one with mass M_1 and length of the side L_1 and the other one with mass M_2 and length $L_2 = 2 L_1$. If the second box is just a scaled-up version of the first box then one expect that the density of the two boxes to be the same, i.e. that $\frac{M_2}{L_2^d} = \frac{M_1}{L_1^d} = \rho$.

> **To summarize for a usual object:** of dimension d, if we scale the object by a factor λ, then mass (or volume) of the object is scaled by a factor λ^d:
>
> $$\text{if} \quad L_2 = \lambda \, L_1 \,, \qquad \text{then} \quad M_2 = \lambda^d \, M_1 \,. \tag{4.1}$$

Let's try to extend this scaling to fractal object. For instance, if we take two Sierpiński triangles, one of side length L_1 and the other one with side length $L_2 = 2 L_1$, then we see that the second triangle contains three of the first triangles (see Fig. 4.2 Bottom). Assume that we give a small weight to the lines in each triangles, then this means that the total mass of the second triangles would be three times the mass of the first triangle: $M_2 = 3 M_1$ (or same argument with total length of lines in each triangle). Consider that we extend the scaling $M_2 = \lambda^{d_F} M_1$ to this fractal object, where d_F is a constant "dimension" that must be defined, then we get (with $\lambda = 2$ in this example):

$$(M_2 =) \qquad 2^{d_F} M_1 = 3 M_1 \,. \tag{4.2}$$

Taking the logarithm on both side of the equation, we obtain a non-integer dimension:

$$d_F = \frac{\log 3}{\log 2} \simeq 1.58 \,, \qquad 1 < d_F < 2 \,, \tag{4.3}$$

50

which is larger than 1 (the dimension of lines, from which the triangle is drawn) and smaller than 2 (the dimension of the plane, in which the Sierpinski triangle is drawn). One way to see this is that the lines in the Sierpinski triangle are "so dense" that they start to cover more than 1 dimension of the space, almost becoming like a 2d-surface, but not quite yet.

We also observe now that the density of the fractal object depends on the scale at which we are "looking at" it, as:

$$\rho_2 = \frac{M_2}{L_2^d} = \frac{\lambda^{d_F} M_1}{\lambda^d L_1^d} = \frac{1}{\lambda^{d-d_F}} \rho_1 \,, \tag{4.4}$$

where d is the dimension of the space in which the object is embedded (in this case $d = 2$) and d_F is the fractal dimension of the object (in this case $d_F = \frac{\log 3}{\log 2} < 2$).

> **To summarize, a fractal object:** can have a non-integer dimension d_F; in which case, if we scale the object by a factor λ, then mass (or volume) of the object is scaled by a factor λ^{d_F}:
>
> $$\textbf{if } L_2 = \lambda L_1 \,, \qquad \textbf{then } M_2 = \lambda^{d_F} M_1 \,. \tag{4.5}$$

1.2.3 Fractal dimension of the percolating cluster at criticality

Example of the site percolation on a 2D lattice. The critical point is around $p_c \sim 0.59$. In this case, the "mass" of the percolating cluster can be measured as the number of sites occupied by the percolating cluster at criticality. We perform one simulation of a very large system at the critical point p_c. We then look at smaller windows of size $L \times L$ and count how many sites are occupied by the percolating cluster: this number can be consider as the mass $M(L)$ of the percolating cluster in the window of size L. If the cluster is indeed fractal, we will observe that $M(L)$ shouldn't scale as L^2, but with some smaller power L^{d_F}. A numerical experiment (see Fig. 4.2 Right) gives $d_F \simeq 1.90$.

1.3 Random walks

1.3.1 Universality and emergent behavior

Two types of emergent behaviors:

- An individual random walk, after a large number of steps, becomes fractal or scale invariant;

- The endpoint of the random walk has a probability distribution that obeys a simple continuum law, the diffusion equation.

Both of these behaviors are independent of the microscopic details of the walk: they are universal.

1.3.2 One dimensional random walk

See derivation in the correction of the tutorial.

Consider a one-dimensional random walker on the continuous 1d-line. At time $n = 0$, the walker starts from the origin, $X_0 = 0$. Then, at each time step, the walker goes to the next position X_{i+1} by doing a jump r_i that is randomly sampled from a probability distribution $P(r_i)$:

$$X_{i+1} = X_i + r_i \,. \tag{4.6}$$

The values of r_i can be positive (the walker goes to right) or negative (the walker goes to left), and the absolute values of r_i gives the length of the jump.

When the distribution $P(r_i)$ of the jump length of the walk has a finite mean $\langle r_i \rangle$ and a finite variance $\sigma_{r_i}^2$, the position of the walker after a large number N of steps goes to a Gaussian distribution with mean $\langle X_N \rangle = N \langle r_i \rangle$ and variance $\sigma_{X_N}^2 = N \sigma_{r_i}^2$.

Independent and Identically Distributed random variables (or, i.i.d. random variables):

For any variable X_N defines as the sum of N independently and identically distributed (i.i.d.) random variables r_i for which σ_{r_i} is finite, we have that:

- the mean of X_N is equal to N times the mean of r_i:

$$\langle X_N \rangle = N \langle r_i \rangle ; \tag{4.7}$$

- the variance of X_N is equal to N times the variance of r_i:

$$\sigma_{X_N}^2 = N \sigma_{r_i}^2 = N \left(\langle r_i^2 \rangle - \langle r_i \rangle^2 \right) . \tag{4.8}$$

As a consequence, the standard deviation of the final positions of a 1-dimensional random walk defined by X_N always grows as $\sqrt{N}$, as long as σ_{r_i} is finite (no matter the detailed shape of the distribution of r_i).

1.3.3 Continuous 1-dimensional random walk: Fokker-Planck equation – Diffusion equation

See derivation in the correction of the tutorial.

One-dimensional diffusion equation:

$$\frac{\partial P}{\partial t}(x, t) = D \frac{\partial^2 P}{\partial x^2}(x, t) . \tag{4.9}$$

where D is the diffusion constant.

One-dimensional Fokker-Planck equation: For small values of ℓ and dt, we obtain the equation:

$$\frac{\partial P}{\partial t}(x, t) = -v \frac{\partial P}{\partial x}(x, t) + D \frac{\partial^2 P}{\partial x^2}(x, t) , \tag{4.10}$$

where $D = \ell^2 / (2\, dt)$ is a constant diffusion coefficient and $v = (2p - 1)\, \ell / dt$ is a constant drift.

Comments:

- The diffusion constant D is the same as in the diffusion equation (4.9). In fact if we take $p = 1/2$ we obtain $v = 0$ and recover Eq. (4.9).

- For $p > 1/2$, the drift is positive $v > 0$, which means that the walker would tend to drift towards larger values of x (towards the right of the x-axis). This is compatible with a probability to jump to the right that is larger than one half, $p > 1/2$. Similarly, if $p < 1/2$, then the walker would tend to drift towards the left.

1.3.4 Anomalous diffusion – Lévy flights

When the variance of the jump distribution is infinite (e.g., heavy tailed distribution), the walker may look like it behaves like a Brownian walker over very short periods of times, but it will sometimes perform extremely long jumps (because the probability that such jumps occur is much less rare than when the variance is finite – see figure). Such walks are called Lévy walks. The distribution of the position of the walker after a large number of steps is not a Gaussian anymore and it is not described by the Fokker-Planck equation anymore. However,

in this case there is still universality: all the walks whose jump distribution has a heavy tail that decays as $\frac{1}{r^{\alpha+1}}$ (with $\alpha \leq 2$) will converge to a Lévy distribution with the same exponent α and will be described by the same fractional Fokker-Planck equation.

2 Real-Space Renormalization

> **Scale invariance**: A physical system is said to exhibit scale-invariance if it remains unchanged (in a statistical sense) by a coarse-graining operation.

In previous chapters we saw that at a critical point the correlation length ξ diverges. The statistical fluctuations extend on all scales of the system and trying to solve the dynamics of the system by considering only a finite number of degrees of freedom fails. Since $\xi \to \infty$, there is no characteristic scale, and the system is self-similar, it looks the same at all scales.

However, the absence of a characteristic scale, enables us to approach phase transitions in a more general way, via the *renormalization group*[1] (RG). It provides a theoretical scheme for studying critical phenomena and especially, their universal properties and scaling laws.

The physical intuition behind the RG derives from the observation that the natural description of physics generally changes with the scale at which observations are made.

Its main idea is to simplify the study of the system at criticality, by replacing the original microscopic degrees of freedom , by a smaller set of effective degrees of freedom (see Fig. 4.3).

Reducing the "density of degrees of freedom" can be realized in the following way. Suppose that the original system is a system of spins arranged in a lattice of spacing a. The new effective degrees of freedom, might be spins with spacing $2a$. This reduction in the degrees of freedom can be carried out repeatedly; starting with a lattice spacing a, after 1 step the spacing is $2a$, after 2 steps, $4a$ etc.

---

[1]It is worth mentioning that is is not a group in a mathematical sense; for example the transformations of the RG are irreversible which violates one of the basic properties of a group.
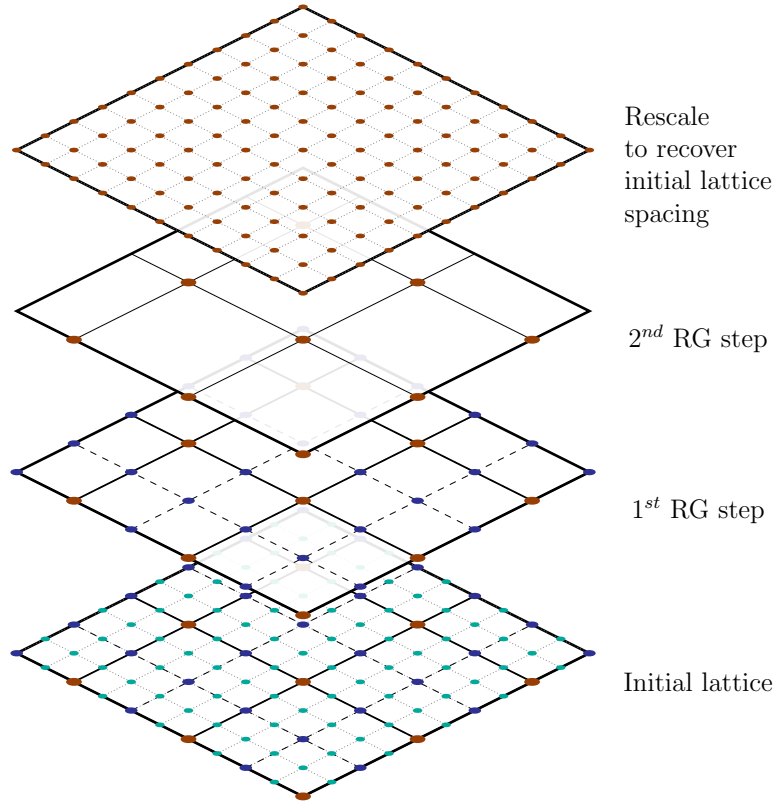
Figure 4.3: Sequence of a renormalization group transformation in real space; from the original, initial lattice with lattice spacing a and (spin) variables s_i, to new lattice spacings $a' = ba$ (1st step), $a'' = ba'$ (2nd step), with block spin variables σ_i. Finally, a scale transformation restores the original lattice spacing a.

In the 1960's a famous paper by Kadanoff [3] on critical phenomena contained an intuitive discussion of the idea of thinning the degrees of freedom (DOFs). Kadanoff assumed that one could discuss blocks of spins in a ferromagnet as if they were single effective spins interacting according to some effective dynamics.

This way, we eliminate all strongly coupled DOFs and obtain an effective system with relatively simple uncorrelated DOFs. This method is called **coarse graining** , and it is the base of the RG.

> **Real-space renormalization group procedure:**
>   1. Divide the lattice into blocks of linear size b (in terms of the lattice constant a) with each block containing at least a few sites.
>   2. Replace each block of sites by a single block site of size b which is occupied with probability $R_b(p)$ according to the RG transformation.
>   3. Rescale all lengths by the factor b, to restore the original lattice spacing.
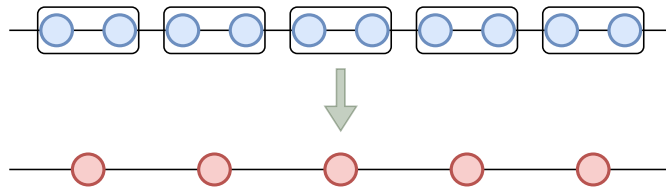

Figure 4.4: Grouping degrees of freedom in 1d as part of the coarse graining procedure.

Chapter 5

Examples of critical phenomena in Complex systems out-of-equilibrium

Until now, phase transitions were studied in the equilibrium framework. Next, we would like to examine them dynamically, out-of-equilibrium, when the system is evolving over time.

1 Example of complex systems out-of-equilibrium: Epidemic spreading

Lecture by Wout Merbis.

> 🏠 See T4 for details

2 Example of complex systems out-of-equilibrium: Opinion dynamics

2.1 Tutorial: The Voter model

> 🏠 See T4 for details

2.2 Seminar: Opinion polarization in social networks

See recorded seminar by Fernando P. Santos on *the impact of link recommendation algorithms in opinion polarization*.

3 Tutorial: Stability analysis

Bifurcation theory is a mathematical framework closely related to the study of phase transitions. The difference is that in bifurcation theory the object of study are dynamical systems , while for phase transitions we look at the behaviour of the free energy. For one-dimensional systems, it is possible to define a bifurcation potential $U(x)$ such that

$$\dot{x} = \frac{\mathrm{d}x}{\mathrm{d}t} = -\frac{\mathrm{d}U(x)}{\mathrm{d}x} \, . \tag{5.1}$$

The local minima of such a potential are equivalent to the steady states of the corresponding dynamical system.

As an example, consider

$$\dot{x} = \mu x^2 + x \,. \tag{5.2}$$

In bifurcation analysis, μ is considered to be parameter we can change . As a function of μ interesting things can happen to the nature of the solutions. The steady state solution is given by setting $\dot{x} = 0$, or $\mu x^2 + x = 0$. The steady-state solutions are therefore $x_0 = 0$ and $x_0 = -\frac{1}{\mu}$. To find the stability of this solution, one typically expands around the steady-state solution by writing $x(t) = x_0 + \epsilon(t)$ and plugging this back into the equation. For this system we find

$$\frac{d}{dt}(x + \epsilon) = \dot{x} + \dot{\epsilon} = \mu(x_0 + \epsilon)^2 + (x_0 + \epsilon) = \mu x_0^2 + x_0 + \epsilon(2\mu x_0 + 1) + \mu\epsilon^2 \,. \tag{5.3}$$

Since $\dot{x} = \mu x_0^2 + x_0$ is a solution to $\dot{x} = 0$, the only remaining terms are those involving ϵ. Since ϵ is assumed to be small, we only keep the terms proportional to ϵ. This is called linearizing the equation . We now have an equation for the evolution of small perturbations to the steady-state solution in the form of

$$\dot{\epsilon} = (2\mu x_0 + 1)\epsilon \,. \tag{5.4}$$

Solving for $\epsilon(t)$ we find

$$\epsilon(t) = \epsilon(0) \exp([2\mu x_0 + 1]t) \,. \tag{5.5}$$

Depending on the sign of $2\mu x_0 + 1$, the perturbation either decays to zero or blows up to infinity. Plugging in $x_0 = 0$, we have

$$\epsilon(t) = \epsilon(0)e^t \,. \tag{5.6}$$

Thus regardless of the value of μ the origin is an unstable solution. For $x_0 = -\frac{1}{\mu}$ we get

$$\epsilon(t) = \epsilon(0)e^{-t} \,. \tag{5.7}$$

Again, regardless of the value of μ, the solution $x_0 = -\frac{1}{\mu}$ is a stable steady-state solution. This example illustrates the procedure of stability analysis. Using it, we found that no bifurcation occurs. For the following systems we will see that more interesting behaviour is possible.

Chapter 6

Examples of collective behaviors

1 Flocking behavior and Vicsek model

See this 20min talk by Luca Giomi (starting at 1h 11 min of the video), which discusses this paper on bird flocks [1].

> 🏠 See T6 for details

2 Noisy Kuramoto model

> 🏠 See T6 for details

Glossary

Taken from *The New Physics* edited by Paul Davies, Cambridge University Press.

Correlation length. The correlation length ξ gives a measure of the typical length scale over which fluctuations of one microscopic variable are correlated with the fluctuations of another. In percolation theory, it is the typical cluster diameter of the clusters s_ξ which give the main contribution to the divergence of the second (and higher) moments of the cluster distribution. Close to a critical point $\xi \propto |p - p_c|^{-\mu}$ for $p \to p_c$. 34

Critical exponent. Near a critical point, physical quantities are often proportional to a power of another quantity, such as the distance from the critical point $|p - p_c|$. The power that occurs known as a critical exponent. 34

Critical phenomena. The phenomena which occur in the neighbourhood of a continuous (second order) phase transition, characterised by very long correlation lengths. 7

Critical point. A point in a phase diagram, where the correlation length associated with the physical system is, in principle, infinite. 5

Order parameter. A variable such as the strength of the infinite cluster in percolation theory (or the magnetisation in an Ising model) used to describe the degree of order in a phase above (below) its critical point. In a continuous phase transition (second order phase transition), the order parameter goes continuously to zero as the critical point is approached from above (below). 20

Phase transition. A change of state such as occurs in the boiling or freezing of a liquid, or in the change between ferromagnetic and paramagnetic states of a magnetic solid. An abrupt change, characterised by a jump in an order parameter is known as first order; a change in which the order parameter evolves smoothly to or from zero is called continuous or second order. 4

Scale invariance. A physical system is said to exhibit scale-invariance if it remains unchanged (in a statistical sense) by a coarse-graining operation. 49, 53

Universality. The phenomena whereby many microscopically quite different physical systems exhibits critical point behaviour, with quantitatively identical features, such as critical exponents. In percolation theory e.g. the critical exponents do not depend on the microscopic details of the lattice but only on the Euclidean dimension d. 34

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