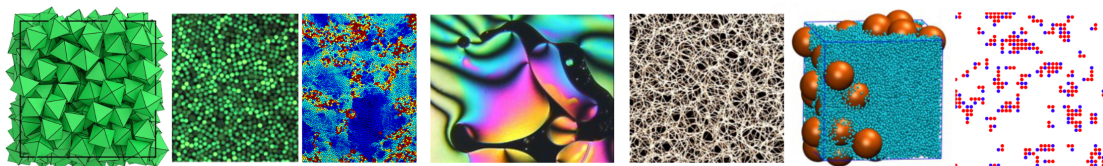


# **Table of contents**

# Welcome to the Complex Disordered Matter Course!



## Overview

This course introduces you to the theoretical, computational and experimental aspects of the physics of complex disordered matter.

Complex disordered matter is the study of a wide range of systems like **polymers**, **colloids**, **glasses**, **gels**, and **emulsions**, which lack long-range order but exhibit intricate behaviour. Colloids, suspensions of microscopic particles in a fluid, are useful for studying disordered structures due to their observable dynamics. Similarly, polymer systems can form amorphous solids or glasses when densely packed or cooled, showing solid-like rigidity despite their disordered structure. These materials often undergo phase transitions, such as demixing and crystallisation, and near these transitions, they can display critical phenomena with extensive fluctuations and correlations.

These various are examples of **soft matter** systems. In soft matter systems, the interplay between disorder, softness, and phase behavior leads to rich physical phenomena, particularly near critical points where even small changes in external conditions can trigger large-scale reorganizations and universal behaviour. Glasses, for instance, exhibit slow relaxation and memory effects, while colloidal systems may crystallize, phase separate, or become jammed depending on particle interactions and concentration. Understanding such behaviors involves studying how microscopic interactions and thermal fluctuations influence macroscopic properties, especially in non-equilibrium conditions. Through techniques like scattering, microscopy, rheology, and simulation, one can explore how disordered soft materials respond to stress, age, or undergo transitions—insights that are vital for applications in materials design, biotechnology, and beyond.

This course is organized into three interconnected parts, each offering a distinct perspective on the study of complex disordered matter.

- **Part 1: Unifying concepts** (Nigel Wilding) introduces the theoretical framework for rationalising complex disordered matter which is grounded in statistical mechanics and thermodynamics. We emphasize the theory of phase transitions, thermal fluctuations, critical phenomena, and stochastic dynamics—providing the essential theoretical tools

needed to describe and predict the behavior of soft and disordered systems.

- **Part 2: Complex disordered matter** (Francesco Turci) explores the phenomenology of key examples of complex disordered soft matter systems, including colloids, polymers, liquid crystals, glasses, gels, and active matter. These systems will be analyzed using the theoretical concepts introduced in Part 1, highlighting how disorder, interactions, and fluctuations shape their macroscopic behavior.
- **Part 3: Experimental techniques** (Adrian Barnes) focuses on the methods of microscopy, and scattering via x-rays, neutrons and light that are used to study complex disordered matter, offering insight into how their properties are measured and understood in real-world contexts.

In addition to theory and experiment, computer simulation plays a central role in soft matter research. This course includes a substantial coursework component consisting of two computational projects. These exercises will allow you to apply state-of-the-art simulation techniques to investigate the complex behavior of disordered systems, bridging theory and observation through hands-on exploration.

## Delivery and format

- Detailed e-notes (accessible via Blackboard) can be viewed on a variety of devices. Pdf is also available.
- We will give ‘traditional’ lectures (Tuesdays, Wednesdays, Fridays) in which we use slides to summarise and explain the lecture content. Questions are welcome (within reason...)
- Try to read ahead in the notes, then come to lectures, listen to the explanations and then reread the notes.
- Rewriting the notes or slides to express your own thoughts and understanding, or annotating a pdf copy can help wire the material into your own way of thinking.
- There are problem classes (Thursdays) where you can try problem sheets and seek help. Lecturers may go over some problems with the class.
- The navigation bar on the left will allow you to access the lecture notes and problem sets.

## Intended learning outcomes

The course will

- Introduce you to the qualitative features of a range of complex and disordered systems and the experimental techniques used to study them.
- Introduce you to a range of model systems and theoretical techniques used to elucidate the physics of complex disordered matter.
- Provide you with elementary computational tools to model complex disordered systems numerically and predict their properties.
- Allow you to apply your physics background to understand a variety of systems of interdisciplinary relevance.
- Connect with the most recent advances in the research on complex disordered matter.

## Contact details

The course will be taught by

- Prof Nigel B. Wilding (unit director): [nigel.wilding@bristol.ac.uk](mailto:nigel.wilding@bristol.ac.uk)
- Dr Francesco Turci: [F.Turci@bristol.ac.uk](mailto:F.Turci@bristol.ac.uk)
- Dr Adrian Barnes: [a.c.barnes@bristol.ac.uk](mailto:a.c.barnes@bristol.ac.uk)

## Questions and comments

If you have any questions about the course, please don't hesitate to contact the relevant lecturer, either by email (see above) or in a problems class.

Finally, this is a new course for 2025/26. If you find any errors or mistakes or something which isn't clear, please let us know by email, or fill in this anonymous form:

[Submit an error/mistake/query](#)

# Recommended texts and literature

*Needs to be tidied and unified.*

*Experimental textbooks?*

One motivation for supplying you with detailed notes for this course is the absence of a wholly ideal text book. However, it should be stressed that while these notes approach (in places) the detail of a book, the notes are not fully comprehensive and should be regarded as the 'bare bones' of the course, to be fleshed out via your own reading and supplementary note taking. To this end perhaps the most appropriate textbooks are:

A good book at the right level for the phase transitions and critical phenomena part of the course is

- **J.M. Yeomans: Statistical Mechanics of Phase Transitions**

A good book covering all aspects of this part of the course including non-equilibrium systems is

- **D. Chandler: Introduction to Modern Statistical Mechanics**

You might also wish to dip into the introductory chapters of the following more advanced texts

- **N Goldenfeld: Lectures on Phase Transitions and the Renormalization Group**
- **J.J. Binney, N.J. Dowrick, A.J.Fisher and M.E.J. Newman: The Theory of Critical Phenomena**

For revision on thermodynamics and statistical mechanics

- **F. Mandl: Statistical Physics.**

For Stochastic dynamics

- **N.G. van Kampen: Stochastic processes in Physics and Chemistry**

The best overall text for part 2 of the course is: R.A.L Jones, Soft Condensed Matter, Oxford University Press.

Additionally, the following more specialised texts should also be useful. They can be found in the University Library under the stated shelfmark.

## Colloids

- (1) D.F.Evans, H.Wennerström: The Colloidal Domain - Where Physics, Chemistry, Biology, and Technology Meet. VCH Publishers (1994).
- (2) R.J.Hunter: Introduction to Modern Colloid Science. Oxford University Press (1993).
- (3) W.B.Russel, D.A.Saville, W.R.Schowalter: Colloidal Dispersions Cambridge University Press (1989).
- (4) D.H.Everett: Basic Principles of Colloid Science.

Royal Society of Chemistry Paperbacks (1988)

### **Polymers and surfactants**

- (1) R.J. Young and P.A. Lovell: Introduction to polymers .
- (2) M. Doi: Introduction to polymer physics
- (3) J.Israelachvili, Intermolecular and Surface Forces, Academic Press (1992), Chs. 16 and 17

### **Glasses**

- (1) J. Zarzycki; Glasses and the vitreous state. Cambridge University Press (1991).

## **Part I**

# **Unifying concepts**

# Chapter 1

## Introduction to phase behaviour and enhanced fluctuations

A phase transition can be defined as a macroscopic rearrangement of the internal constituents of a system in response to a change in the thermodynamic conditions to which they are subject. A wide variety of physical systems undergo such transitions. Understanding the properties of phase transitions is fundamental to the study of soft and complex matter, as these systems often exhibit rich and subtle transformations between different states of organization. Whether in colloidal suspensions, polymer blends, liquid crystals, or biological materials, phase transitions underpin a wide range of physical behaviours, from self-assembly and pattern formation to critical phenomena and dynamical arrest. By analysing how macroscopic phases emerge from microscopic interactions and external conditions, one gains crucial insight into the principles that govern structure, stability, and functionality in these intricate systems. As such, an understanding of phase transitions not only enriches theoretical understanding but also informs practical applications across materials science, biophysics, and nanotechnology. For these reasons we will devote a large proportion of this course to the study of phase transitions.

Two classic examples of systems displaying phase transitions are the ferromagnet and fluid systems. For the magnet, a key observable is the magnetisation defined as the magnetic moment per spin, given by  $m = M/N$ , with  $N$  the number of spins.  $m$  can be positive or negative, dependent on whether the spins are aligned ‘up’ or ‘down’. As the temperature of a ferromagnet is increased, its net magnetisation  $|m|$  is observed to decrease smoothly, until at a certain temperature known as the critical temperature,  $T_c$ , it vanishes altogether (see left part of Figure ??). We define the magnetisation to be the *order parameter* of this phase transition.

One can also envisage applying a magnetic field  $H$  to the system which, depending on its sign (i.e. whether it is aligned (positive) or anti-aligned (negative) relative to the magnetisation axis), favours up or down spin states respectively, as shown schematically in Figure ?? (right part). Changing the sign of the magnetic field  $H$  for  $T < T_c$  leads to a phase transition characterised by a discontinuous jump in  $m$ . We shall explore this behaviour in more detail in section 6.

Similarly, a change of state from liquid to gas can be induced in a fluid system (though not in an ideal gas) simply by raising the temperature. Typically the liquid-vapour transition is abrupt, reflecting the large number density difference between the states either side of the transition. However the abruptness of this transition can be reduced by applying pressure. At one particular pressure and temperature the discontinuity in the density difference between the two states vanishes and the two phases coalesce. These conditions of pressure and temperature serve to locate the critical point for the fluid. We define the density difference  $\rho_{liq} - \rho_{vap}$  to be the order parameter for the liquid-gas phase transition. We shall meet order parameters for other,



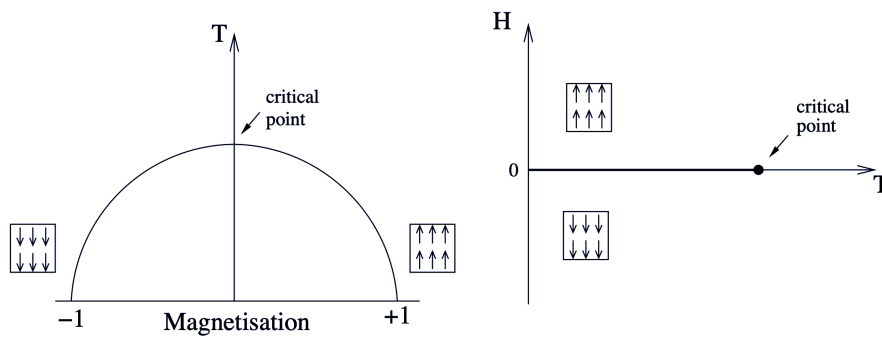


Figure 1.1: Phase diagram of a simple magnet (schematic). Left: magnetisation as a function of temperature for zero applied magnetic field,  $H = 0$ . Right: Applying a magnetic field that is aligned or antialigned with the direction of the magnetisation leads to a phase transition. The  $H = 0$  axis at  $T < T_c$  is the coexistence curve for which positive and negative magnetisations are equally likely.

more complex, systems in Section ??,

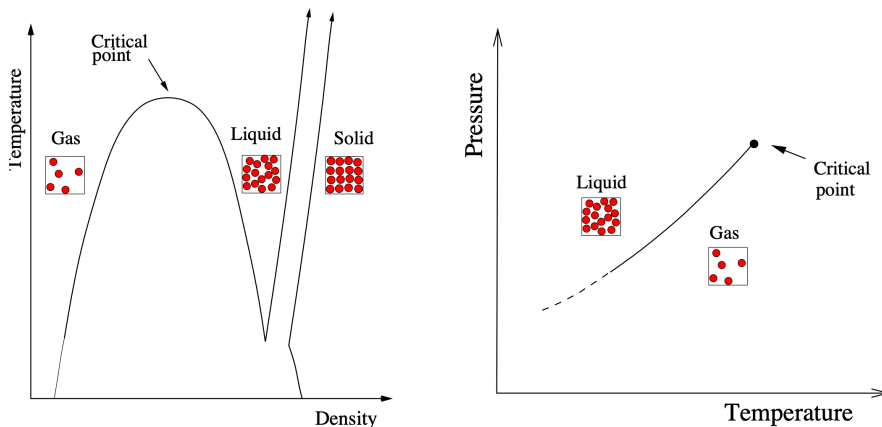


Figure 1.2: Phase diagram of a simple fluid (schematic)

In the vicinity of a critical point, a system displays a host of remarkable behaviors known as *critical phenomena*. Chief among these is the divergence of thermal response functions—such as specific heat, compressibility, or magnetic susceptibility—which signal an enhanced sensitivity to external perturbations. These singularities arise from the emergence of large-scale cooperative interactions among the system's microscopic constituents, as measured by a diverging *correlation length* (see Chapter ??). One visually striking manifestation of this is *critical opalescence*, particularly observed in fluids like  $\text{CO}_2$ . As carbon dioxide nears its critical temperature and pressure, the distinction between its liquid and gas phases vanishes, giving rise to huge fluctuations in density. These fluctuations scatter visible light, rendering the fluid milky or opalescent. This scattering effect directly reflects the long-range correlations developing within the fluid. The movie below illustrates the effect as the critical temperature of  $\text{CO}_2$  is approached from above. Note the appearance of a liquid-vapour interface (meniscus) as the system enters the two-phase region.

[Movies/critical\\_point\\_1.mp4](#)

The recalcitrant problem posed by the critical region is how best to incorporate such collective effects within the framework of a rigorous mathematical theory that affords both physical insight and quantitative explanation of the observed phenomena. This matter has been (and still is!)

the subject of intense theoretical activity.

The importance of the critical point stems largely from the fact that many of the phenomena observed in its vicinity are believed to be common to a whole range of apparently quite disparate physical systems. Systems such as liquid mixtures, superconductors, liquid crystals, ferromagnets, antiferromagnets and molecular crystals may display identical behaviour near criticality. This observation implies a profound underlying similarity among physical systems at criticality, regardless of many aspects of their distinctive microscopic nature. These ideas have found formal expression in the so-called 'universality hypothesis' which, since its inception in the 1970s, has enjoyed considerable success.

In the next few lectures, principal aspects of the contemporary theoretical viewpoint of phase transitions and critical phenomena will be reviewed. Mean field theories of phase transitions will be discussed and their inadequacies in the critical region will be exposed. The phenomenology of the critical region will be described including power laws, critical exponents and their relationship to scaling phenomena. These will be set within the context of the powerful renormalisation group technique. The notion of universality as a phenomenological hypothesis will be introduced and its implications for real and model systems will be explored. Finally, the utility of finite-size scaling methods for computer studies of critical phenomena will be discussed, culminating in the introduction of a specific technique suitable for exposing universality in model systems. Thereafter we will consider some foundational concepts in the dynamics of complex disordered matters. We shall look at the processes by which one phase transform into another and introduce differential equations that allow us to deal with the inherent stochasticity of thermal systems. The wider applicability of these unifying concepts to complex disordered systems such as colloids, polymers, liquid crystals and glasses will be covered in part 2 of the course.

## Chapter 2

# Key concepts for phase transitions

### 2.1 Observables and expectation values

In seeking to describe phase transition and critical phenomena, it is useful to have a quantitative measure of the difference between the phases: this is the role of the *order parameter*,  $Q$ . In the case of the fluid, the order parameter is taken as the difference between the densities of the liquid and vapour phases. In the ferromagnet it is taken as the magnetisation. As its name suggest, the order parameter serves as a measure of the kind of orderliness that sets in when the temperature is cooled below a critical temperature.

Our first task is to give some feeling for the principles which underlie the ordering process. Referring back to **sec-canonical**, the probability  $p_a$  that a physical system at temperature  $T$  will have a particular microscopic arrangement (alternatively referred to as a ‘configuration’ or ‘state’), labelled  $a$ , of energy  $E_a$  is

$$p_a = \frac{1}{Z} e^{-E_a/k_B T} \quad (2.1)$$

The prefactor  $Z^{-1}$  is the *partition function*: since the system must always have *some* specific arrangement, the sum of the probabilities  $p_a$  must be unity, implying that

$$Z = \sum_a e^{-E_a/k_B T} \quad (2.2)$$

where the sum extends over all possible microscopic arrangements.

These equations assume that physical system evolves rapidly (on the timescale of typical observations) amongst all its allowed arrangements, sampling them with the probabilities Equation ?? the expectation value of any physical observable  $O$  will thus be given by averaging  $O$  over all the arrangements  $a$ , weighting each contribution by the appropriate probability:

$$\overline{O} = \frac{1}{Z} \sum_a O_a e^{-E_a/k_B T} \quad (2.3)$$

Sums like Equation ?? are not easily evaluated. Nevertheless, some important insights follow painlessly. Consider the case where the observable of interest is the order parameter, or more specifically the magnetisation of a ferromagnet.

$$Q = \frac{1}{Z} \sum_a Q_a e^{-E_a/k_B T} \quad (2.4)$$

It is clear from Equation ?? that at very low temperature the system will be overwhelmingly likely to be found in its minimum energy arrangements (ground states). For the ferromagnet, these are the fully ordered spin arrangements having magnetisation  $+1$ , or  $-1$ .

Now consider the high temperature limit. The enhanced weight that the fully ordered arrangement carries in the sum of Equation ?? by virtue of its low energy, is now no longer sufficient to offset the fact that arrangements in which  $Q_a$  has some intermediate value, though each carry a smaller weight, are vastly greater in number. A little thought shows that the arrangements which have essentially zero magnetisation (equal populations of up and down spins) are by far the most numerous. At high temperature, these disordered arrangements dominate the sum in Equation ?? and the order parameter is zero.

The competition between energy-of-arrangements weighting (or simply ‘energy’) and the ‘number of arrangements’ weighting (or ‘entropy’) is then the key principle at work here. The distinctive feature of a system with a critical point is that, in the course of this competition, the system is forced to choose amongst a number of macroscopically different sets of microscopic arrangements.

Finally in this section, we note that the probabilistic (statistical mechanics) approach to thermal systems outlined above is completely compatible with classical thermodynamics. Specifically, the bridge between the two disciplines is provided by the following equation

$$F = -k_B T \ln Z \quad (2.5)$$

where  $F$  is the “Helmholtz free energy”. All thermodynamic observables, for example the order parameter  $Q$ , and response functions such as the specific heat or magnetic susceptibility are obtainable as appropriate derivatives of the free energy. For instance, utilizing Equation ??, one can readily verify (try it as an exercise!) that the average internal energy is given by

$$\overline{E} = -\frac{\partial \ln Z}{\partial \beta},$$

where  $\beta = (k_B T)^{-1}$ .

The relationship between other thermodynamic quantities and derivatives of the free energy are given in fig. Figure ??

## 2.2 Correlations

### 2.2.1 Spatial correlations

The two-point connected correlation function measures how fluctuations at two spatial points are statistically related. For a scalar field  $\phi(\vec{R})$ , which could represent eg. the local magnetisation  $m$  in a magnet at position vector  $\vec{R}$ , or the local particle number density  $\rho$  in a fluid, it is defined as:

$$C(r) = \langle \phi(\vec{R}) \phi(\vec{R} + \vec{r}) \rangle - \langle \phi(\vec{R}) \rangle^2,$$

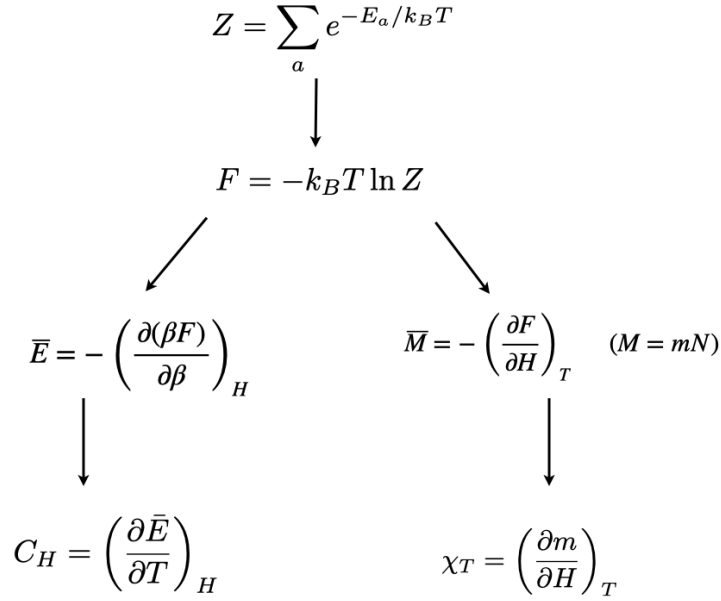


Figure 2.1: Relationships between the partition function and thermodynamic observables

where  $\langle \cdot \rangle$  denotes an ensemble or spatial average over all  $\vec{R}$ , and  $r = |\vec{r}|$  is the spatial separation between the two points.

$C(r)$  quantifies the spatial extent over which field values are correlated and in homogeneous and isotropic systems, it depends only on the separation  $r$ .

If  $C(r)$  decays quickly, we say that correlations are short-ranged. Typically this occurs well away from criticality and takes the form of exponential decay

$$C(r) \sim e^{-r/\xi}$$

where the correlation length  $\xi$  is the characteristic scale over which correlations decay.

Near a critical point  $C(r)$  decays more slowly - in a power-law fashion - and correlations are long-ranged.

$$C(r) \sim r^{-(d-2+\eta)}$$

where  $d$  is the spatial dimension and  $\eta$  is a critical exponent.

In isotropic fluids and particle systems, a closely related and more directly measurable quantity (particularly in simulations) is the **radial distribution function**  $g(r)$ , which describes how particle density varies as a function of distance from a reference particle. For such systems, the two-point correlation function of the number density field  $\rho(\vec{r})$  is related to  $g(r)$  as follows:

$$g(r) = 1 + \frac{C(r)}{\rho^2},$$

where  $\rho$  is the average number density. This relation shows that  $g(r)$  encodes the same spatial correlations as  $C(r)$ , but in a form that is more natural for discrete particle systems. Note that

by definition  $g(r) \rightarrow 1$  in the absence of correlations ie. when  $C(r) = 0$ . This is typically the case for  $r \gg \xi$ .

Experimentally one doesn't typically have direct access to  $C(r)$ , but rather its Fourier transform known as the **structure factor**

$$S(k) = \int d^d r e^{-i\vec{k} \cdot \vec{r}} C(r),$$

where  $k$  is the scattering wavevector.

In equilibrium:

- For short-range correlations (finite  $\xi$ ),  $S(k)$  typically has a Lorentzian form:

$$S(k) \sim \frac{1}{k^2 + \xi^{-2}}.$$

- At criticality (where  $\xi \rightarrow \infty$ ),  $S(k)$  follows a power law:

$$S(k) \sim k^{-2+\eta}.$$

This relation enables the extraction of  $\xi$  from experimental or simulation data, especially via scattering techniques.

## 2.2.2 Temporal correlations

Consider a thermodynamic variable  $x$  with zero mean that fluctuates over time. Examples include the local magnetization in a magnetic system or the local density in a fluid. Here,  $x$  represents a deviation from the average value — a fluctuation.

We're interested in how such fluctuations are correlated over time when the system is in thermal equilibrium. For instance, if  $x$  is positive at some time  $t$ , it's more likely to remain positive shortly after.

These temporal correlations are characterized by the two-time correlation function (also known as an auto-correlation function):

$$\langle x(\tau)x(\tau + t) \rangle$$

In equilibrium, the correlation function must be independent of the starting time  $\tau$ . Therefore, we define:

$$\langle x(\tau)x(\tau + t) \rangle = M_{xx}(t)$$

That is,  $M_{xx}(t)$  depends only on the time difference  $t$ .

We typically expect  $M_{xx}(t)$  to decay exponentially over a characteristic correlation time  $t_c$ :

$$M_{xx}(t) \sim \exp(-t/t_c)$$

This exponential decay reflects how the memory of fluctuations fades with time.

Now consider two different fluctuating variables,  $x$  and  $y$  (e.g., local magnetizations at different positions). Their cross-correlation function is defined as:

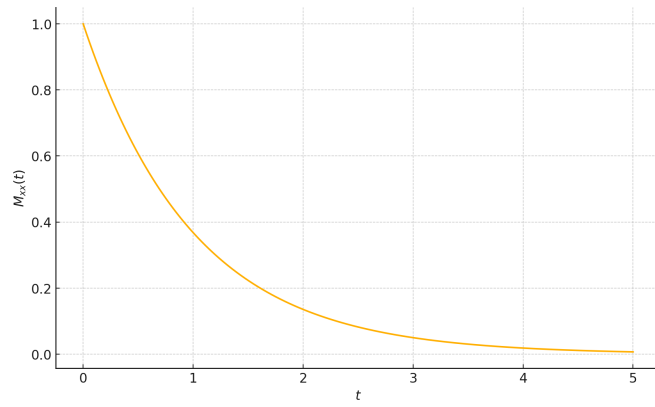


Figure 2.2: Sketch of  $M_{xx}(t)$  against  $t$

$$\langle x(\tau)y(\tau + t) \rangle = M_{xy}(t)$$

This defines the elements of a dynamic correlation matrix, of which  $M_{xx}(t)$  is the diagonal.

## Chapter 3

# The Approach to Criticality

It is a matter of experimental fact that the approach to criticality in a given system is characterized by the divergence of various thermodynamic observables. Let us remain with the archetypal example of a critical system, the ferromagnet, whose critical temperature will be denoted as  $T_c$ . For temperatures close to  $T_c$ , the magnetic response functions (the magnetic susceptibility  $\chi$  and the specific heat) are found to be singular functions, diverging as a *power* of the reduced (dimensionless) temperature  $t \equiv (T - T_c)/T_c$ :

$$\chi \equiv \frac{\partial M}{\partial H} \propto t^{-\gamma} \quad (H = 0) \quad (3.1)$$

(where  $M = mN$ ),

$$C_H \equiv \frac{\partial E}{\partial T} \propto t^{-\alpha} \quad (H = \text{constant}) \quad (3.2)$$

Another key quantity is the correlation length  $\xi$ , which measures the distance over which fluctuations of the magnetic moments are correlated. This is observed to diverge near the critical point with an exponent  $\nu$ .

$$\xi \propto t^{-\nu} \quad (T > T_c, H = 0) \quad (3.3)$$

Similar power law behaviour is found for the order parameter  $Q$  (in this case the magnetisation) which vanishes in a singular fashion (it has infinite gradient) as the critical point is approached as a function of temperature:

$$m \propto t^\beta \quad (T < T_c, H = 0) \quad (3.4)$$

(here the symbol  $\beta$ , is not to be confused with  $\beta = 1/k_B T$ —this unfortunately is the standard notation.)

Finally, as a function of magnetic field:

$$m \propto h^{1/\delta} \quad (T = T_c, H > 0). \quad (3.5)$$

with  $h = (H - H_c)/H_c$ , the reduced magnetic field.

As examples, the behaviour of the magnetisation and correlation length are plotted in Figure ?? as a function of  $t$ .



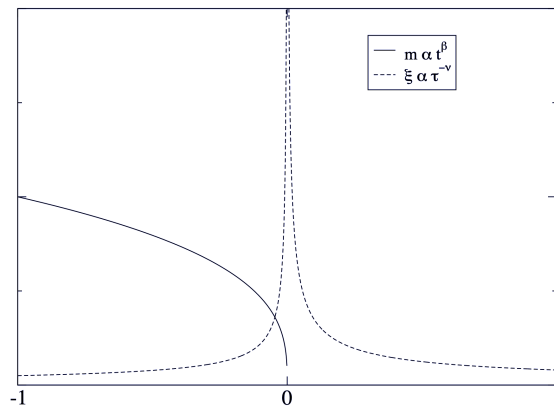


Figure 3.1: Singular behaviour of the correlation length and order parameter in the vicinity of the critical point as a function of the reduced temperature  $t$ .

The quantities  $\gamma, \alpha, \nu, \beta$  in the above equations are known as critical exponents. They serve to control the rate at which the various thermodynamic quantities change on the approach to criticality.

Remarkably, the form of singular behaviour observed at criticality for the example ferromagnet also occurs in qualitatively quite different systems such as the fluid. All that is required to obtain the corresponding power law relationships for the fluid is to substitute the analogous thermodynamic quantities in to the above equations. Accordingly the magnetisation order parameter is replaced by the density difference  $\rho_{liq} - \rho_{gas}$  while the susceptibility is replaced by the isothermal compressibility and the specific heat capacity at constant field is replaced by the specific heat capacity at constant volume. The approach to criticality in a variety of qualitatively quite different systems can therefore be expressed in terms of a set of critical exponents describing the power law behaviour for that system (see the book by Yeomans for examples).

Even more remarkable is the experimental observation that the values of the critical exponents for a whole range of fluids and magnets (and indeed many other systems with critical points) are *identical*. This is the phenomenon of *universality*. It implies a deep underlying physical similarity between ostensibly disparate critical systems. The principal aim of theories of critical point phenomena is to provide a sound theoretical basis for the existence of power law behaviour, the factors governing the observed values of critical exponents and the universality phenomenon. Ultimately this basis is provided by the Renormalisation Group (RG) theory, for which K.G. Wilson was awarded the Nobel Prize in Physics in 1982.

More about the scientists mentioned in this chapter:

[Kenneth Wilson](#)

## Chapter 4

# The Ising model: the prototype model for a phase transition

In order to probe the properties of the critical region, it is common to appeal to simplified model systems whose behaviour parallels that of real materials. The sophistication of any particular model depends on the properties of the system it is supposed to represent. The simplest model to exhibit critical phenomena is the two-dimensional Ising model of a ferromagnet. Actual physical realizations of 2-d magnetic systems do exist in the form of layered ferromagnets such as  $\text{K}_2\text{CoF}_4$ , so the 2-d Ising model is of more than just technical relevance.

### 4.1 The 2D Ising model

The 2-d spin- $\frac{1}{2}$  Ising model envisages a regular arrangement of magnetic moments or ‘spins’ on an infinite plane. Each spin can take two values,  $+1$  (‘up’ spins) or  $-1$  (‘down’ spins) and is assumed to interact with its nearest neighbours according to the Hamiltonian

$$H_I = -J \sum_{\langle ij \rangle} s_i s_j - H \sum_i s_i \quad (4.1)$$

where  $J > 0$  measures the strength of the coupling between spins and the sum extends over nearest neighbour spins  $s_i$  and  $s_j$ , i.e it is a sum of the bonds of the lattice.  $H$  is a magnetic field term which can be positive or negative (although for the time being we will set it equal to zero). The order parameter is simply the average magnetisation:

$$m = \frac{1}{N} \langle \sum_i s_i \rangle,$$

where  $\langle \cdot \rangle$  means an average over configurations.

The fact that the Ising model displays a phase transition was argued in Chapter ???. Thus at low temperatures for which there is little thermal disorder, there is a preponderance of aligned spins and hence a net spontaneous magnetic moment (ie. the system is ferromagnetic). As the temperature is raised, thermal disorder increases until at a certain temperature  $T_c$ , entropy drives the system through a continuous phase transition to a disordered spin arrangement with zero net magnetisation (ie. the system is paramagnetic). These trends are visible in configurational snapshots from computer simulations of the 2D Ising model (see Figure ??). Although

each spin interacts only with its nearest neighbours, the phase transition occurs due to cooperative effects among a large number of spins. In the neighbourhood of the transition temperature these cooperative effects engender fluctuations that can extend over all length-scales from the lattice spacing up to the correlation length.

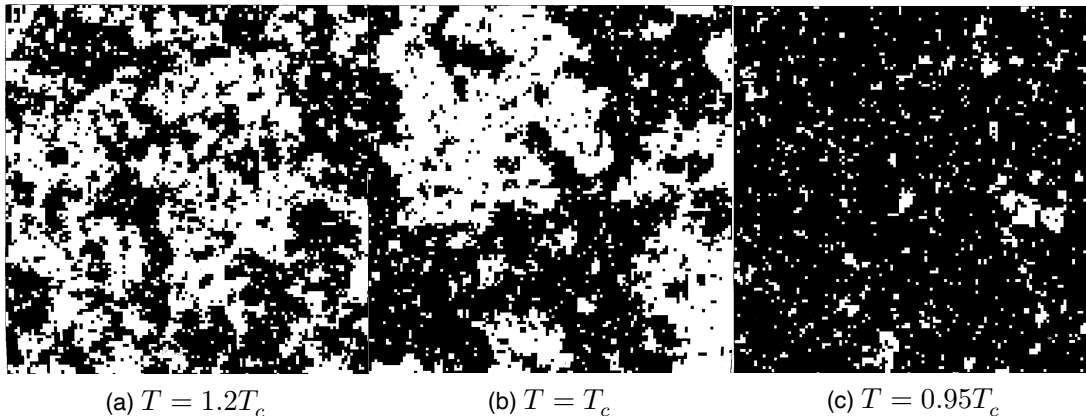


Figure 4.1: Configurations of the 2d Ising model. The patterns depict typical arrangements of the spins (white= $+1$ , black= $-1$ ) generated in a computer simulation of the Ising model on a square lattice of  $N = 512$  sites, at temperatures (from left to right) of  $T = 1.2T_c$ ,  $T = T_c$ , and  $T = 0.95T_c$ . In each case only a portion of the system containing 128 sites is shown. The typical island size is a measure of the correlation length  $\xi$ : the excess of black over white (below  $T_c$  is a measure of the order parameter).

[An interactive Monte Carlo simulation of the Ising model](#) demonstrates the phenomenology. By altering the temperature you will be able to observe for yourself how the spin arrangements change as one traverses the critical region. Pay particular attention to the configurations near the critical point. They have very interesting properties. We will return to them later!

Although the 2-d Ising model may appear at first sight to be an excessively simplistic portrayal of a real magnetic system, critical point universality implies that many physical observables such as critical exponents are not materially influenced by the actual nature of the microscopic interactions. The Ising model therefore provides a simple, yet *quantitatively* accurate representation of the critical properties of a whole range of real magnetic (and indeed fluid) systems. This universal feature of the model is largely responsible for its ubiquity in the field of critical phenomena. We shall explore these ideas in more detail later in the course.

## 4.2 Exact solutions: the one dimensional Ising chain

One might well ask why the 2D Ising model is the simplest model to exhibit a phase transition. What about the one-dimensional Ising model (ie. spins on a line)? In fact in one dimension, the Ising model can be solved exactly. It turns out that the system is paramagnetic for all  $T > 0$ , so there is no phase transition at any finite temperature. To see this, consider the ground state of the system in zero external field. This will have all spins aligned the same way (say up), and hence be ferromagnetic. Now consider a configuration with a various “domain walls” dividing spin up and spin down regions:

Instead of considering the underlying spin configurations, we shall describe the system in terms of the statistics of its domain walls. The energy cost of a wall is  $\Delta = 2J$ , independent of position. Domain walls can occupy the bonds of the lattice, of which there are  $N - 1$ . Moreover, the walls are noninteracting, except that you cannot have two of them on the same bond. (Check through these ideas if you are unsure.)

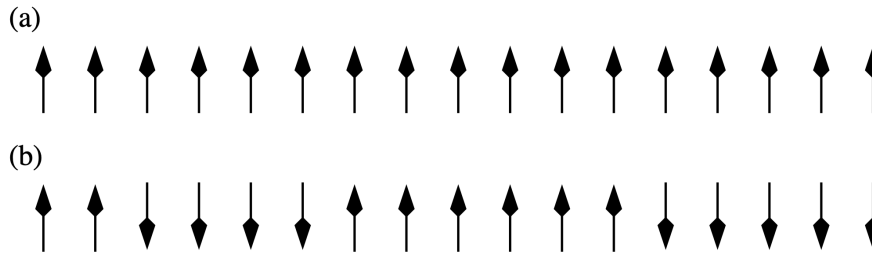


Figure 4.2: (a) Schematic of an Ising chain at  $T = 0$ . (b) At a small finite temperature the chain is split into domains of spins ordered in the same direction. Domains are separated by notional domain “walls”, which cost energy  $\Delta = 2J$ . Periodic boundary conditions are assumed.

In this representation, the partition function involves a count over all possible domain wall arrangements. Since the domain walls are non interacting (eg it doesn’t cost energy for one to move along the chain) we can calculate  $Z$  by considering the partition function associated with a single domain wall being present or absent on some given bond, and then simply raise to the power of the number of bonds:

$$Z = Z_1^{N-1}$$

where

$$Z_1 = e^{\beta J} + e^{\beta(J-\Delta)} = e^{\beta J}(1 + e^{-\beta\Delta})$$

is the domain wall partition function for a single bond and represent the sum over the two possible states: domain wall absent or present. Then the free energy per bond of the system is

$$\beta f \equiv \beta F/(N - 1) = -\ln Z_1 = -\beta J - \ln(1 + e^{-\beta\Delta})$$

The first term on the RHS is simply the energy per spin of the ferromagnetic (ordered) phase, while the second term arises from the free energy of domain walls. Clearly for any finite temperature (ie. for  $\beta < \infty$ ), this second term is finite and negative. Hence the free energy will always be lowered by having a finite concentration of domain walls in the system. Since these domain walls disorder the system, leading to a zero average magnetisation, the 1D system is paramagnetic for all finite temperatures. *Exercise:* Explain why this argument works only in 1D.

The animation below lets you see qualitatively how the typical number of domain walls varies with temperature. If you’d like to explore more quantitatively, a python code performing a Monte Carlo simulation is available. You will learn about Monte Carlo simulation in the coursework and in later parts of the course.

```
#Monte Carlo simulation of the 1d Ising chain with periodic boundary conditions
import numpy as np
import matplotlib.pyplot as plt
from matplotlib.animation import FuncAnimation
from matplotlib.widgets import Slider

# Number of spins
N = 20

# Initialize spins (+1 or -1)
spins = np.random.choice([-1, 1], size=N)
```

```

# Initial temperature
T = 2.0

# Set up figure and axis for the spins
fig, ax = plt.subplots(figsize=(10, 2))
plt.subplots_adjust(bottom=0.25) # make room for slider
ax.set_xlim(-0.5, N - 0.5)
ax.set_ylim(-1, 1)
ax.axis('off')

# Create text objects for each spin
texts = []
for i in range(N):
    arrow = '↑' if spins[i] == 1 else '↓'
    t = ax.text(i, 0, arrow, fontsize=24, ha='center', va='center')
    texts.append(t)

def update(frame):
    """Perform Metropolis updates over all spins, then refresh display."""
    global spins, T
    for _ in range(N):
        i = np.random.randint(N)
        left = spins[(i - 1) % N]
        right = spins[(i + 1) % N]
        deltaE = 2 * spins[i] * (left + right)
        # Metropolis criterion ensures configurations appear with the correct Boltzmann probability
        if deltaE < 0 or np.random.rand() < np.exp(-deltaE / T):
            spins[i] *= -1
    # Update arrows on screen
    for idx, t in enumerate(texts):
        t.set_text('↑' if spins[idx] == 1 else '↓')
    return texts

# Create the animation with caching disabled and blit turned off
ani = FuncAnimation(
    fig,
    update,
    interval=200,
    blit=False,
    cache_frame_data=False
)

# Add a temperature slider
ax_T = plt.axes([0.2, 0.1, 0.6, 0.03], facecolor='lightgray')
slider_T = Slider(ax_T, 'Temperature T', 0.1, 5.0, valinit=T)

def on_T_change(val):
    """Callback to update T when the slider changes."""
    global T
    T = val

slider_T.on_changed(on_T_change)

```