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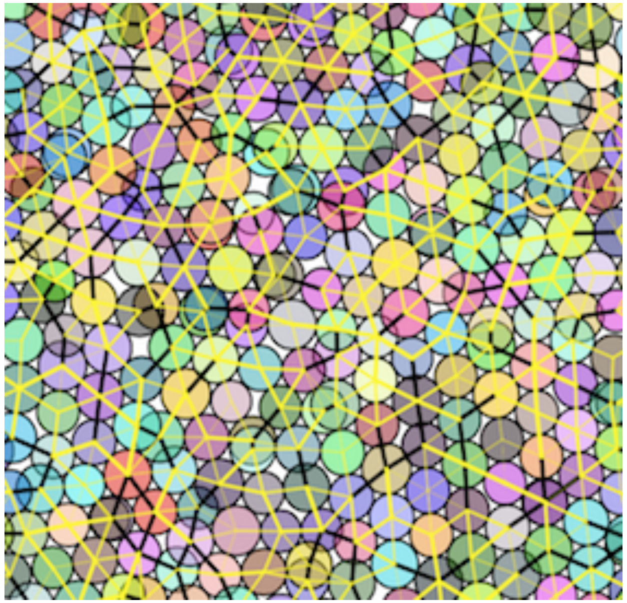
PHYS40071: Complex Disordered Matter

Nigel Wilding, Francesco Turci and Adrian Barnes



Welcome!

Complex Disordered Matter

Course structure

TB 1 | 20 Credits | 3 Lectures per week + Problem Class

📌 **Unifying Concepts** (Weeks 1-5: Nigel Wilding)
- Phase transitions and critical phenomena
- Metastability and dynamics
- Stochastic processes and fluctuations

🧩 **Complex Disordered Systems** (Weeks 7-11: Francesco Turci)
- Colloids and interactions
- Polymers & Surfactants
- Liquid Crystals, Gels, Glasses
- Active Matter

🔬 **Experimental Systems & Techniques** (Weeks 5 and 11: Adrian Barnes)
- Calorimetry
- Microscopy
- Diffraction

Teaching Block 1

Weeks	Commencing	Section	Lecturer	Assessment
1 - 4	22nd Sep	Unifying Concepts	Prof. Nigel Wilding	Coursework 1: Released Monday 13th October (Week 4) 12:30, due Monday 27th October, 09:30 (Week 6). Marks and feedback returned by Fri 14th November.
5	20th Oct	Unifying Concept and Experimental Techniques	Prof. Nigel Wilding and Dr. Adrian Barnes	
6	*27st Oct*	*Consolidation Week*	-	
7 - 10	3rd Nov	Complex Disordered Systems	Dr. Francesco Turci	Coursework 2: Released Thursday 13th Nov 12:30 (Week 8), due Thursday 27th November, 09:30. Marks and feedback returned Friday 12th December.
11	1st Dec	Complex Disordered Systems and Experimental Techniques	Dr. Francesco Turci and Dr. Adrian Barnes	
12	8th *Dec*	*Revision Week*	-	
	15*th Dec*	***Assessment Period (1 week)***	-	**1.5 hour examination**

Each teaching week, we shall meet as follows:

Tuesdays 10:00, Room: 3.34 (Physics)	Lecture
Wednesday 11:00, Room: 3.21 (Berry theatre)	Lecture
Thursdays 12:00, Room: Fry Building G.13	Problems class
Fridays 14:00, Room: 3.21 (Berry theatre)	Lecture

Assessment Breakdown

🖥️ **Computational investigations** - 1 Assignment (30%)
🤔 **Problem set** (20%)
📖 **90 minute exam (Dec)** – Covering all lecture material (50%)

📌 **Total: 100% Assessment** – Equally balanced between coursework and final examination.

As this is a new course, you will be provided with a mock examination paper

Delivery and format (Unifying Concepts)

Complex
Disordered
Matter

- Detailed e-notes (see Blackboard) can be viewed on a variety of devices.

- 'Traditional' lectures (Tues, Wed, Fri) in which I use slides to summarise and explain the lecture content. Questions welcome (within reason…)

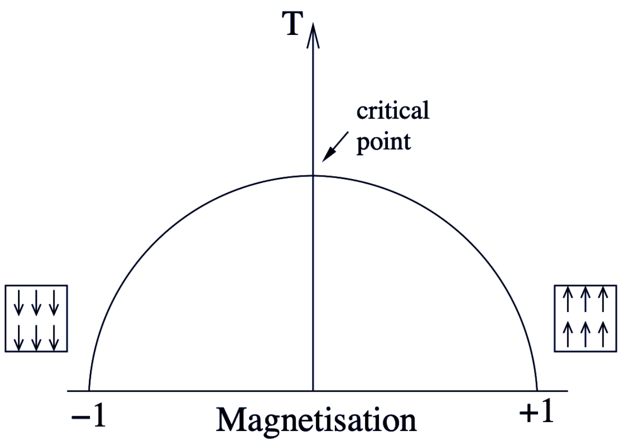
- Try to read ahead in the notes, then come to lectures, listen to my explanations and then reread the notes.

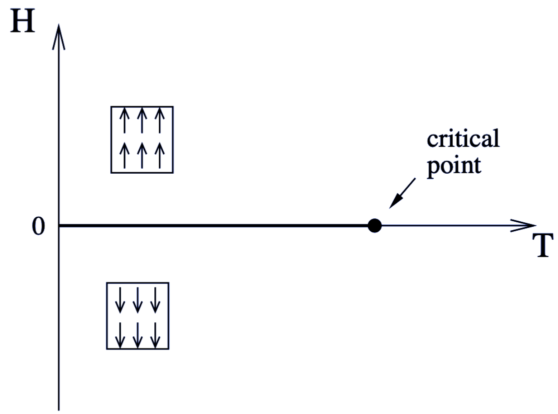
- Rewriting the notes or slides to express your own understanding, or annotating a pdf copy can help wire the material into your own way of thinking.

- Problem class (Thurs) where you can try problem sets and seek help. I will go over some problems with the class. **No classes week 6**.

1. Introduction to phase behaviour

- A wide variety of physical systems undergo rearrangements of their internal constituents in response to changes in thermodynamic conditions.
- Two classic examples of systems displaying such phase transitions are the ferromagnet and fluid systems.

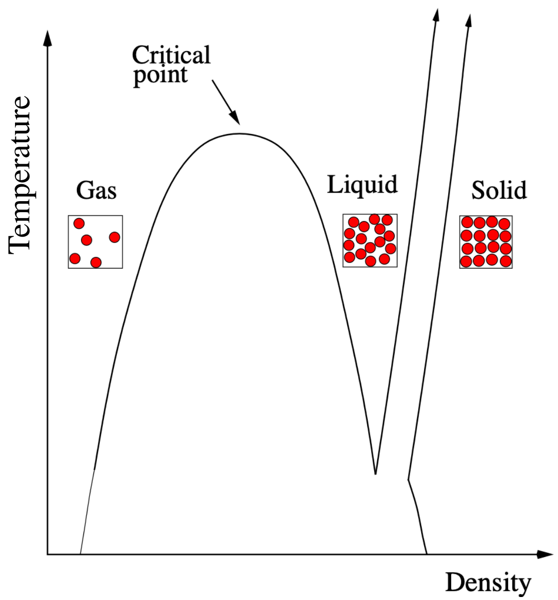


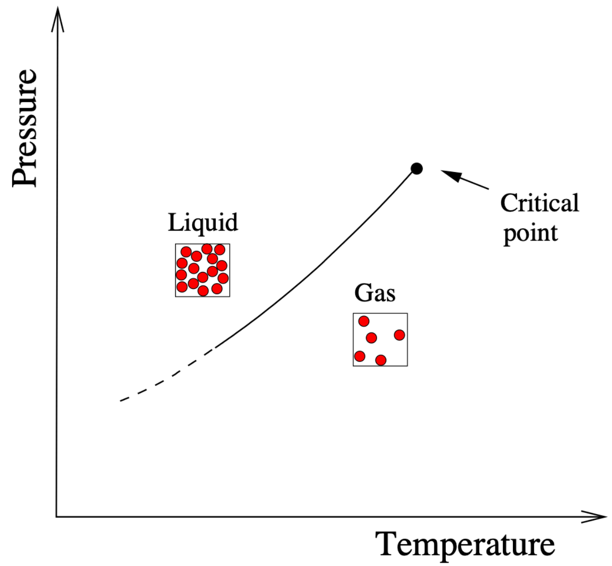


- As the temperature T of a ferromagnet is increased, its magnetic moment is observed to decrease smoothly, until at a certain **critical temperature**, it vanishes altogether

We define the magnetisation to be the **order parameter** of this phase transition.

- Similarly, we can induce a change of state from liquid to gas in a fluid simply by raising the temperature.





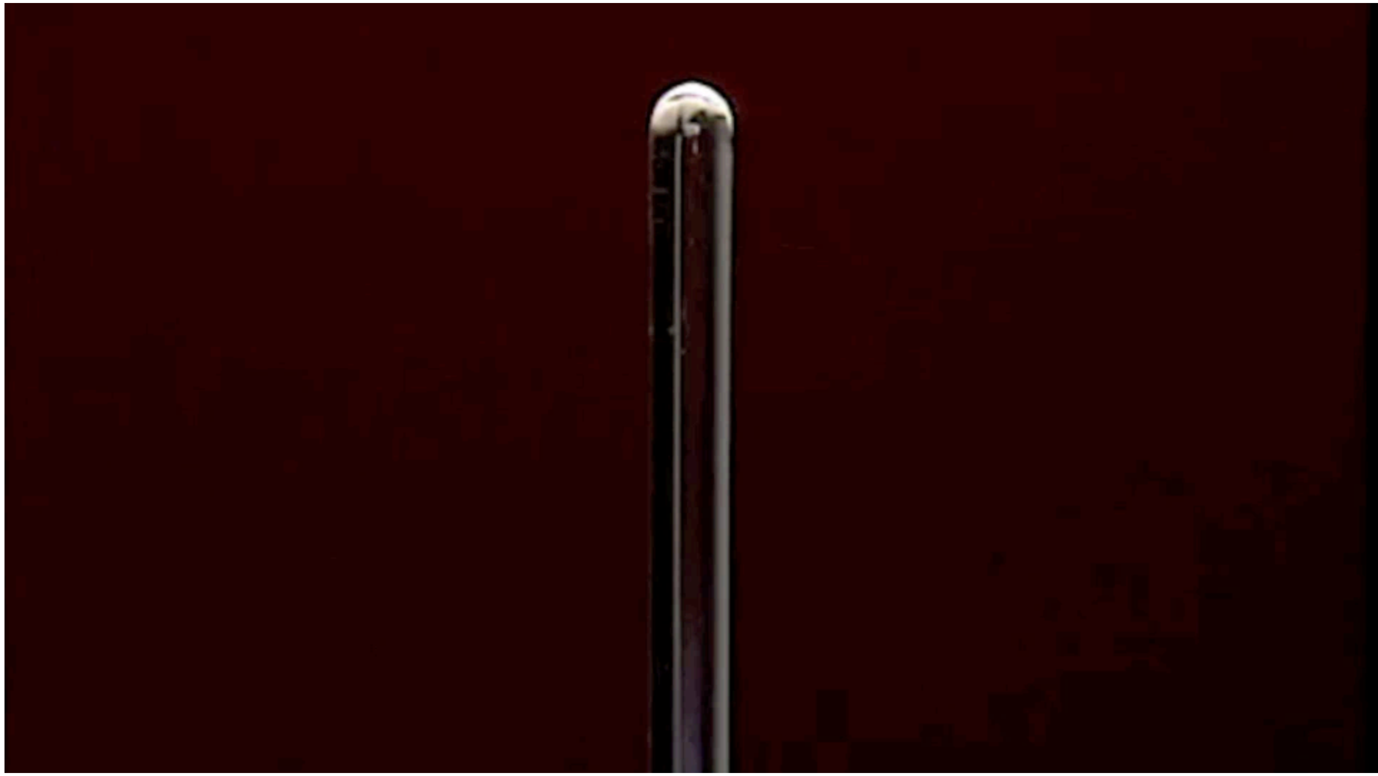
- Typically the liquid-gas transition is abrupt. However, abruptness can be reduced by applying pressure.
- At one particular p, T the jump in density at the transition vanishes. These conditions correspond to the critical point of the fluid.

- For $H_2 0$: $T_c = 374$ K, $P_c = 218$ atm
- For CO_2: $T_c = 304$ K, $P_c = 73$ atm

- Density difference $\rho_{liquid} - \rho_{gas}$ is the order parameter for the liquid-gas phase transition.

- Close to its critical point, a system exhibits a variety of remarkable effects known as **critical phenomena**
- Examples are the divergence (infinite values) of thermal response functions such as the specific heat and the fluid compressibility or magnetic susceptibility
- Origin of the singularities in these quantities tracable to large-length-scale co-operative effects between the microscopic constituents of the system.

- Illustration: CO_2 in a pressurised container at P_c.
- As approach $T_c = 31^{\circ}C$ from above, critical opalescence occurs.
- For $T < T_c$ a liquid-gas meniscus forms



- Understanding the physics of critical points is important because often one observes **quantitatively identical** critical phenomena in a range of apparently quite disparate physical systems.
- This 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 celebrated **universality hypothesis** (see later)

2. Background concepts

- Let us denote the order parameter as Q.
- Q provides a quantitative measure of the difference between the phases coalescing at the critical point:
- Reminder: For the fluid, $Q = \rho_{liq} - \rho_{gas}$. For the ferromagnet $Q = m$, the magnetisation.

- But why should a system exhibit a phase transition at all?
- Statistical Mechanics provides the answer!

- Probability p_a that a physical system at temperature T will have a particular microscopic arrangement ('configuration' or 'state'), labelled a, of energy E_a is

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

- Prefactor Z^{-1} is a T-dependent constant - the partition function (recall year 2 thermal physics). Since the system must always have some specific arrangement, the sum of the probabilities p_a must be unity, implying that

$$Z = \sum_a e^{-E_a/k_B T}$$

where the sum extends over all possible microscopic arrangements.

- Expectation (ie. average) value of an observable O is given by averaging O over all the arrangements a, weighting each contribution by p_a

$$\overline{O} \equiv \langle O \rangle = \frac{1}{Z} \sum_a O_a e^{-E_a/k_B T}$$

- The order parameter is similarly a thermal average over configurations:

$$Q = \frac{1}{Z}\sum_a Q_a e^{-E_a/k_B T} \qquad \dagger$$

- Consider the ferromagnetic case $Q = m$. For T very small, system will be overwhelmingly likely to be in its minimum energy arrangement (ground state) having magnetisation +1, or -1.

- For T large, enhanced prob. of ground state arrangements is insufficient to offset the fact that the sum in eq. $\dagger$ contains a vastly greater number of arrangements in which Q_a has some intermediate value.
- In fact 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 eq. $\dagger$ and $Q \approx 0$.

- Thus T dependence of Q results from a competition between energy-of-arrangements weighting (or simply `energy') and the 'number of arrangements' weighting (or `entropy').

- The critical point is that T at which the system is forced to choose amongst a number of macroscopically different sets of microscopic arrangements i.e. the finite Q arrangements and the zero Q arrangements.

- Partition function provides bridge between stat. mech and thermodynamics via

$$F = -k_B T \ln Z$$

where F is the Helmholtz free energy (see year 2, and preparatory reading).

- All thermodynamic observables, eg. Order parameter Q, specific heat C_H, susceptibility χ and compressibility κ, are obtainable as appropriate derivatives of the free energy. Eg:

$$Z = \sum_a e^{-E_a/k_B T}$$

$$F = -k_B T \ln Z$$

$$\overline{E} = -\left(\frac{\partial(\beta F)}{\partial \beta}\right)_H \qquad \overline{M} = -\left(\frac{\partial F}{\partial H}\right)_T \quad (M = mN)$$

(Here $\beta \equiv (k_B T)^{-1}$)

$$C_H = \left(\frac{\partial \bar{E}}{\partial T}\right)_H \qquad \chi_T = \left(\frac{\partial m}{\partial H}\right)_T$$

Correlations

- Consider first **spatial** correlations.
- Two-point correlation function measures statistical relation between fluctuations at two spatial points
- For scalar field $\phi(\overrightarrow{R})$ eg. local density or local magnetisation, can define

$$C(r) = \langle \phi(\overrightarrow{R})\phi(\overrightarrow{R} + \vec{r})\rangle - \langle \phi(\overrightarrow{R})\rangle^2 \qquad r = |\vec{r}| \text{ is spatial separation}$$

and the average is over configurations

Including this term gives a quantity that decays to zero

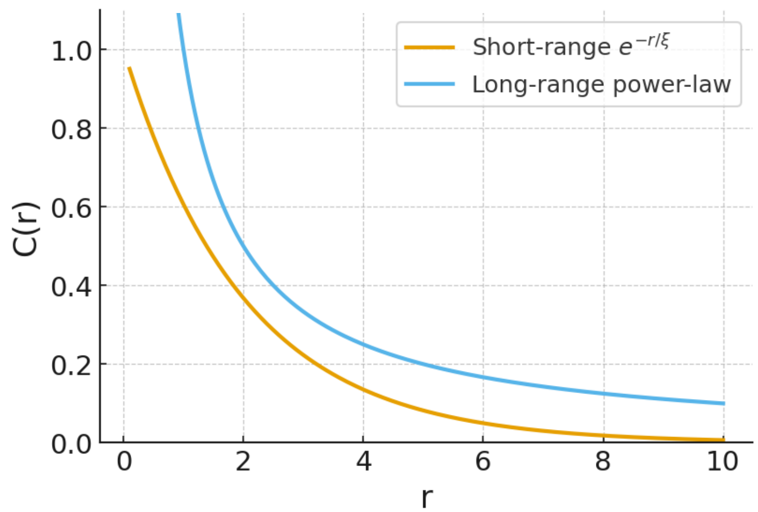
- In homogeneous/isotropic systems, $C(r)$ depends only on r and not the reference point $\overrightarrow{R}$

Behaviour of spatial correlations

- Correlations can be short ranged or long ranged:

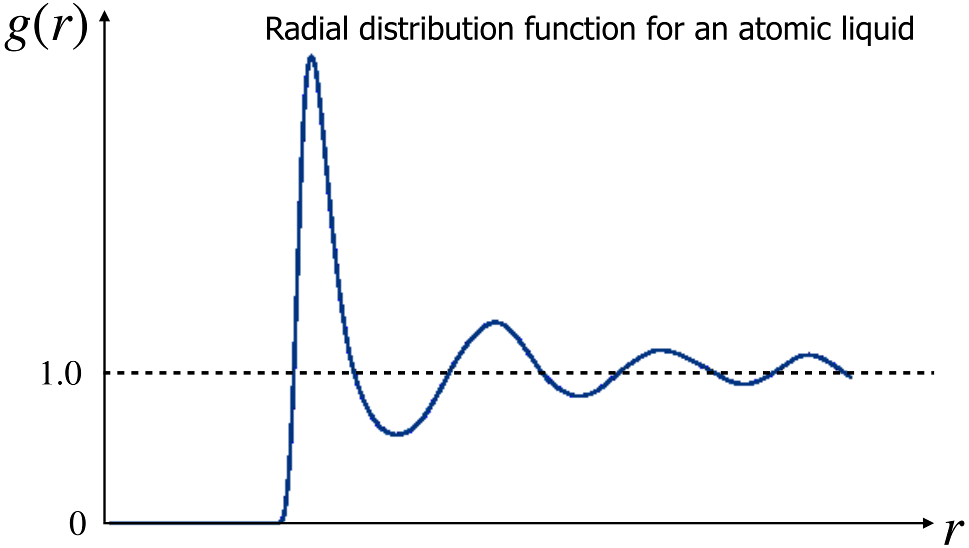
  - Short-range: $C(r) \sim e^{-r/\xi}$, fast decay
  - Long-range (criticality): power-law decay
    $C(r) \sim r^{-x}$

- **Correlation length** ξ sets spatial scale.

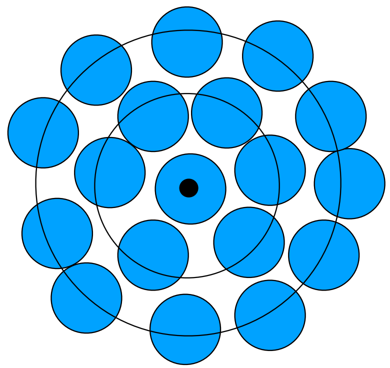


Example: pair correlation function of a fluid (a.k.a radial distribution function)

- For a fluid $\phi(\overrightarrow{R}) = \rho(\overrightarrow{R})$, the local number density
- $g(r)$ = probability of finding particle at distance $r = |\vec{r}|$ relative to ideal gas.
- It is related to density correlations via: $g(r) = \dfrac{1}{\rho^2}\langle\rho(0)\rho(r)\rangle = 1 + C(r)/\rho^2$



- At large r correlation die out, ie.
  $g(r) \to 1$ as $r \to \infty$



- Peaks in $g(r)$ indicate ordering (e.g. shells in liquids).

Structure Factor $S(k)$

- Fourier transform of correlations: $S(k) = \int d^3r\, e^{i\vec{k}\cdot\vec{r}} C(r)$

  $k = \dfrac{2\pi}{\lambda}$ is the scattering wave vector (often also written as q)

- Measured in scattering experiments (see lectures by A. Barnes). Connects real-space correlations with momentum-space

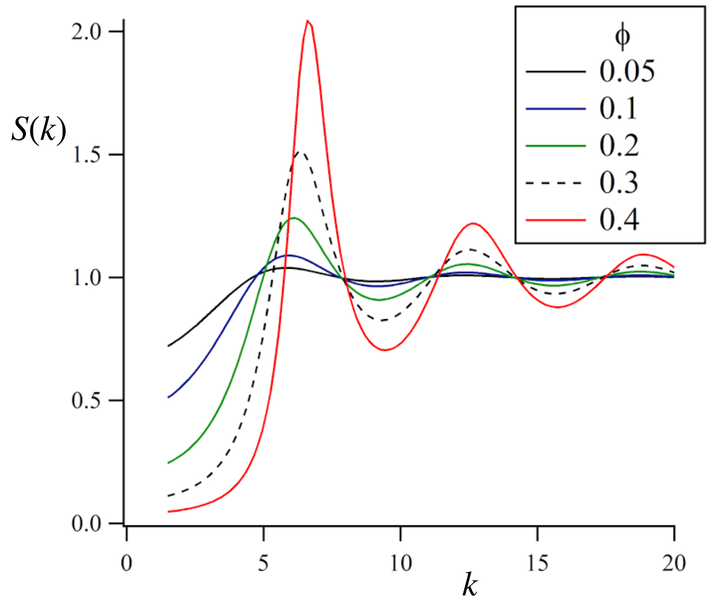
- Peaks in $S(k)$ = characteristic length scales.

- Near criticality: divergence at small k (long-range fluctuations)

- For short ranged correlations, decay of $S(k)$ has a Lorentzian form.

- For long ranged correlations, decay has a power law form (see notes)

Structure factor for an atomic liquid



Temporal correlations

- Consider a thermodynamic variable x with zero mean that fluctuates over time.
- Temporal correlations are characterized by the two-time correlation function:

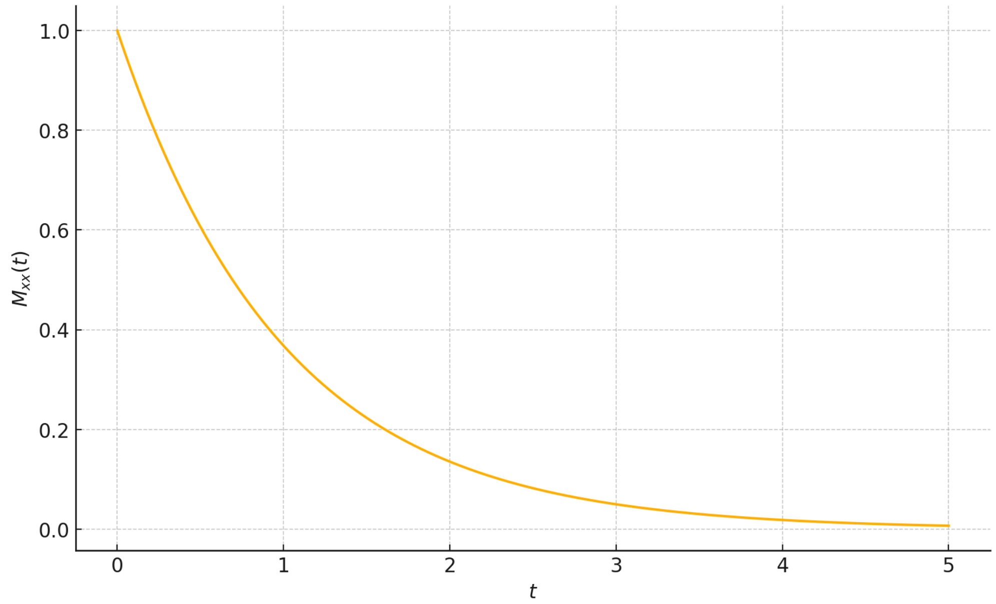
$$\langle x(\tau)x(\tau + t)\rangle$$

- In **equilibrium**: $\langle x(\tau)x(\tau + t)\rangle = M_{xx}(t)$ i.e only depends on t not on τ

- Typically (away from criticality):

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

ie. memory of fluctuations fades exponentially with correlation time t_c



3. The approach to criticality

- Approach to criticality is characterised by the divergence of various thermodynamic observables.

- Eg. in a ferromagnet near T_c, C_H and χ_T are singular functions, diverging as some power of the **reduced temperature** $t \equiv (T - T_c)/T_c$

$$\chi \equiv \frac{\partial m}{\partial h} \propto t^{-\gamma} \qquad C_H \equiv \frac{\partial E}{\partial T} \propto t^{-\alpha}$$

- Recall that the correlation length ξ, measuring the distance over which fluctuations of the magnetic moments are correlated. This diverges with an exponent ν.

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

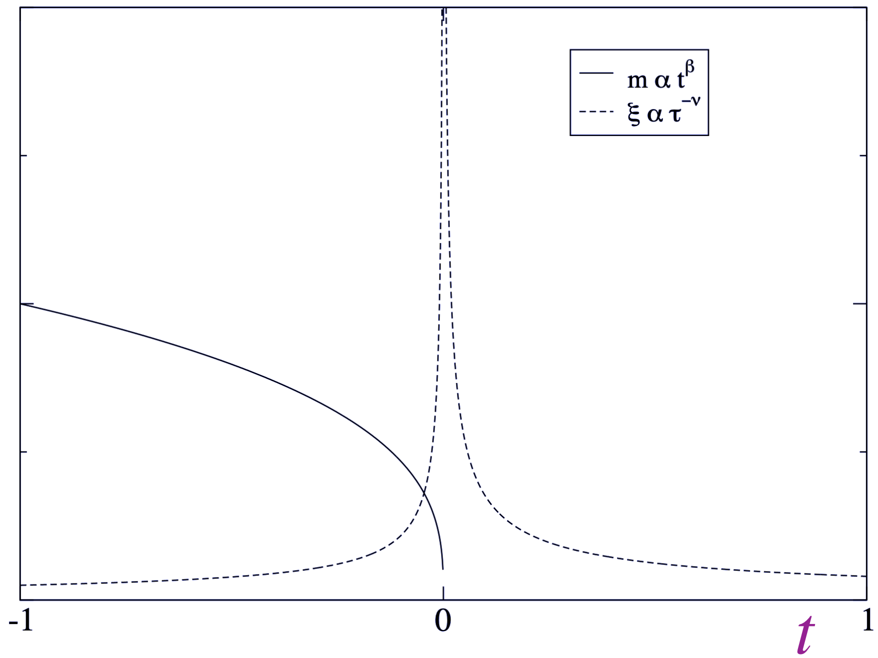
- Similar power law behaviour is found for the order parameter Q which vanishes in a singular fashion (it has infinite gradient) as $T \rightarrow T_c^-$

$$m \propto t^{\beta} \qquad (T < T_c, H = 0)$$

And as a function of magnetic field:

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

with $h \equiv (H - H_c)/H_c$ the reduced magnetic field.



- $\gamma, \alpha, \nu, \beta$ are known as **critical exponents**. They control the rate at which the associated observables change on the approach to criticality.

- Remarkably, similar power laws occurs in many qualitatively distinct systems near their critical point (eg, fluid, polymer solutions, magnets, electrolytes, traffic jams, sandpiles, financial markets).

- To obtain the corresponding power law relationships simply substitute the analogous thermodynamic quantities in to the above equations. eg.

$$\rho_{liq} - \rho_{gas} \sim t^{\beta}; \qquad \kappa \sim t^{-\gamma}$$

- 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 celebrated phenomenon of universality. It implies a deep similarity between systems at their critical points.

4. Ising model

- We can use simple models to probe the properties of the critical region.
- Simplest is the 2d spin-$\frac{1}{2}$ Ising model, which comprises a lattice of N magnetic moments or 'spins' on an infinite plane.

- Each spin can take two values, +1 ('up' spins) or -1 ('down' spins) and interacts with its nearest neighbours via the Hamiltonian

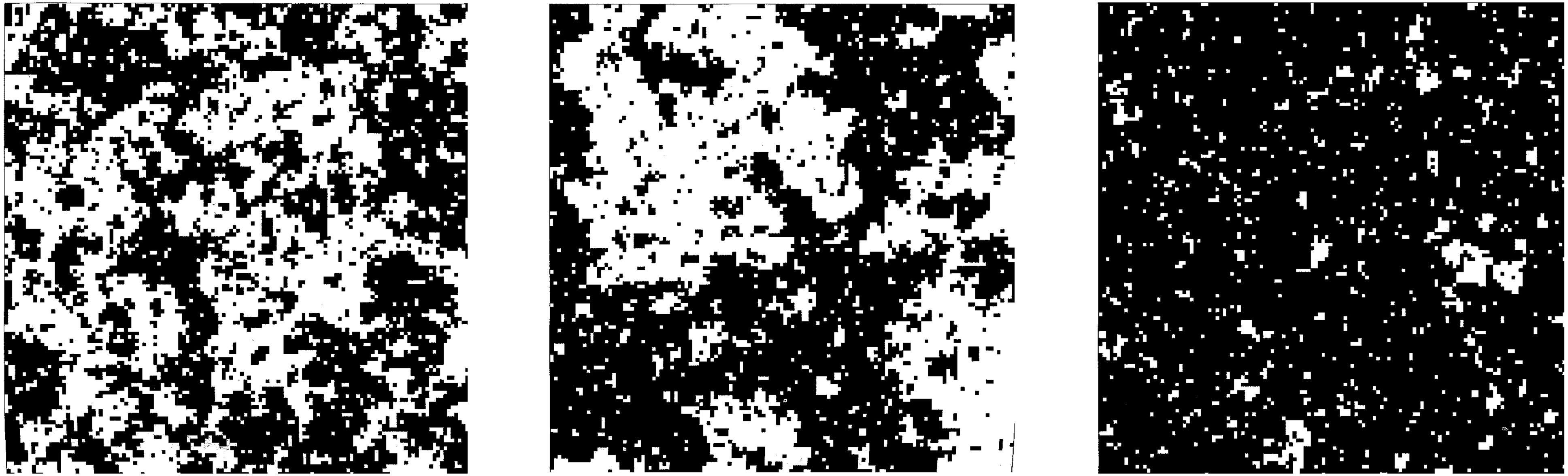
$$\mathscr{H}_I = -J \sum_{<ij>} s_i s_j - H \sum_i s_i \qquad J > 0$$

- The order parameter is simply the average magnetisation: $m = \frac{1}{N} \langle \sum_i s_i \rangle$

- At low temperatures for which there is little thermal disorder, there is a preponderance of aligned spins and hence a net spontaneous magnetic moment $|m| \approx 1$

- As T is raised, thermal disorder increases until at T_c, entropy drives the system through a continuous phase transition to a disordered spin arrangement with $|m| = 0$.

- These trends are visible in configurational snapshots from computer simulations of the 2D Ising model.



$T = 1.2T_c$ $T = T_c$ $T = 0.95T_c$

- 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.

- Despite its simplicity, critical point universality implies that critical exponents of Ising model are same as those of real magnets.

- 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.

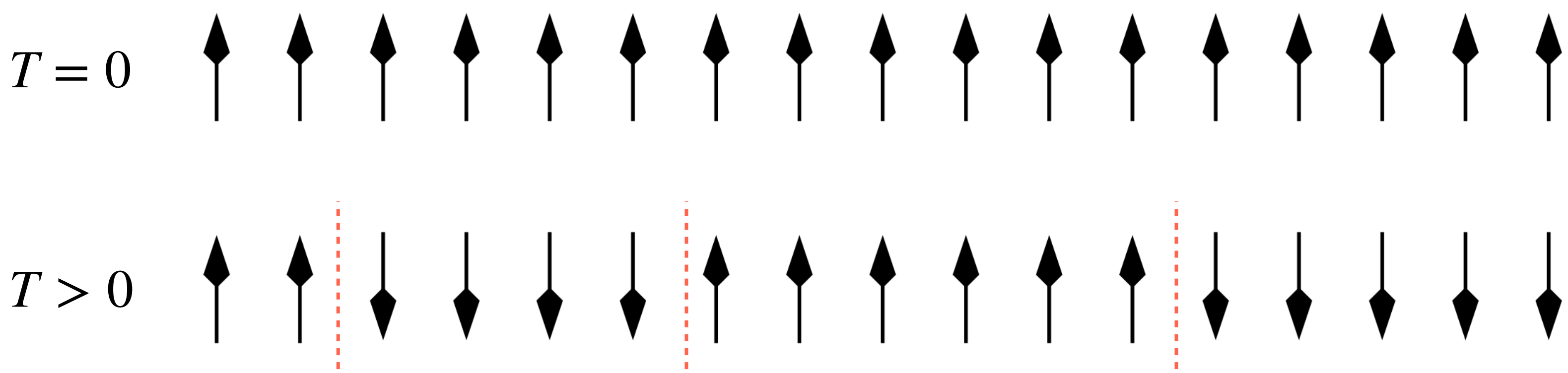
- This universal feature of the model is largely responsible for its ubiquity in the field of critical phenomena.

Exact Solutions: the 1D Ising chain

- Why is the 2D Ising model the simplest to exhibit a phase transition? What happens in 1D?

- In fact there is no phase transition in 1D for $T > 0$.

- Consider the ground state of a 1D Ising chain and a state with various "domain walls" dividing spin-up and spin-down regions



- Transform from a spin representation to a domain wall representation.

- Domain walls can occur on the bonds of the lattice of which there are $N-1$. If a wall is present, the energy cost is $\Delta = 2J$.

- A configuration can be specified by stating whether or not there is a domain wall on each bond.

- Presence of a domain wall on one bond doesn't affect likelihood of domain wall on neighbouring bond (as long as $H = 0$). Thus domain walls are **independent**

- Partition functions from independent contributions multiply.

- Hence the partition function of system is $Z = Z_1^{N-1}$, where for a single domain wall,

$$Z_1 = e^{\beta J} + e^{\beta(J-\Delta)} = e^{\beta J}(1 + e^{-\beta\Delta}) \qquad \beta \equiv \frac{1}{k_B T}$$

So free energy density

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

- Second term arises from the entropy of the domain wall population and since it is negative for all $T > 0$, the free energy is lowered by having domain walls, ie the system is always disordered.

More general 1D spin systems

- For a 1-d assembly of N spins each having m discrete energy states, and in the presence of a magnetic field H, possible to get free energy via the **transfer matrix method**.

- Let us start by assuming that the assembly has cyclic boundary conditions, then the total energy of configuration $\{s\}$ is

$$\begin{aligned}
\mathscr{H}(\{s\}) &= -\sum_{i=1}^{N} (Js_i s_{i+1} + Hs_i) \\
&= -\sum_{i=1}^{N} (Js_i s_{i+1} + H(s_i + s_{i+1})/2) \\
&= \sum_{i=1}^{N} E(s_i, s_{i+1})
\end{aligned}$$

where we have defined $E(s_i, s_{i+1}) = -Js_i s_{i+1} - H(s_i + s_{i+1})/2$.

Partition function may be written

$$
\begin{aligned}
Z_N &= \sum_{\{s\}} \exp\left(-\beta \mathscr{H}(\{s\})\right) \\
&= \sum_{\{s\}} \exp\left(-\beta[E(s_1, s_2) + E(s_2, s_3) + \dots . E(s_N, s_1)]\right) \\
&= \sum_{\{s\}} \exp\left(-\beta E(s_1, s_2)\right) \exp\left(-\beta E(s_2, s_3)\right) \dots . \exp\left(-\beta E(s_N, s_1)\right) \\
&= \sum_{i,j,\dots,l=1}^{m} V_{ij} V_{jk} \dots V_{li} \qquad\qquad \ddagger
\end{aligned}
$$

where the $V_{ij} = \exp(-\beta E_{ij})$ are elements of an $m \times m$ matrix $\mathbf{V}$, known as the transfer matrix.

- Transpires that the sum over the product of matrix elements in $\ddagger$ is the trace of $\mathbf{V}^N$, given by the sum of its eigenvalues:-

$$
Z_N = \lambda_1^N + \lambda_2^N + \dots \lambda_m^N
$$

- As $N \to \infty$, largest eigenvalue λ_1 dominates since $(\lambda_2/\lambda_1)^N$ vanishes. Consequently $Z_N = \lambda_1^N$

- Specializing to the case of the simple Ising model, the transfer matrix takes the form

$$\mathbf{V}(H) = \begin{pmatrix} e^{\beta(J+H)} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta(J-H)} \end{pmatrix}$$

- This matrix has two eigenvalues which can be readily calculated in the usual fashion. They are

$$\lambda_{\pm} = e^{\beta J}\cosh(\beta H) \pm \sqrt{e^{2\beta J}\sinh^2\beta H + e^{-2\beta J}}$$

- Hence the free energy per spin $f = -\,k_B T \ln \lambda_+$ is

$$f = -\,k_B T \ln\left[e^{\beta J}\cosh(\beta H) + \sqrt{e^{2\beta J}\sinh^2\beta H + e^{-2\beta J}}\right]$$

5. Mean field theory

- The critical behaviour of most model systems cannot be found analytically.
- A few exceptions: eg. 2D Ising model (but not the 3D) have been solved $\left(\beta = \frac{1}{8},\, \nu = 1,\, \gamma = \frac{7}{4}.\; T_c = -2J/\ln(\sqrt{2} - 1) \approx 2.269J\right)$
- But such solutions provide little insight into the essential nature of criticality.
- When an exact solution is elusive, can try to make simplifying assumptions to calculate critical behaviour. Mean field theory is such an approximation scheme.

- Look for a mean field expression for the free energy of the Ising model. Write

$$s_i = \langle s_i \rangle + (s_i - \langle s_i \rangle) = m + (s_i - m) = m + \delta s_i$$

- Then

$$\begin{aligned}\mathscr{H}_I &= -J \sum_{<i,j>} [m + (s_i - m)][m + (s_j - m)] - H \sum_i s_i \\ &= -J \sum_{<i,j>} [m^2 + m(s_i - m) + m(s_j - m) + \delta s_i \delta s_j] - H \sum_i s_i \\ &= -J \sum_i (qms_i - qm^2/2) - H \sum_i s_i - J \sum_{<i,j>} \delta s_i \delta s_j\end{aligned}$$

where the sum $\sum_{<i,j>}$ over bonds of a quantity which independent of s_j is just $q/2$ times that quantity, with q the lattice coordination.

- Now the mean field approximation is to ignore the last term giving

$$\mathscr{H}_{mf} = -\sum_i H_{mf} s_i + NqJm^2/2 \qquad \text{where } H_{mf} \equiv Jqm + H$$

- It follows that the partition function is

$$Z = Z(1)^N = e^{-\beta qJm^2N/2}[2\cosh(\beta(qJm + H))]^N$$

so the free energy is

$$F(m) = NJqm^2/2 - Nk_BT\ln[2\cosh(\beta(qJm + H))]$$

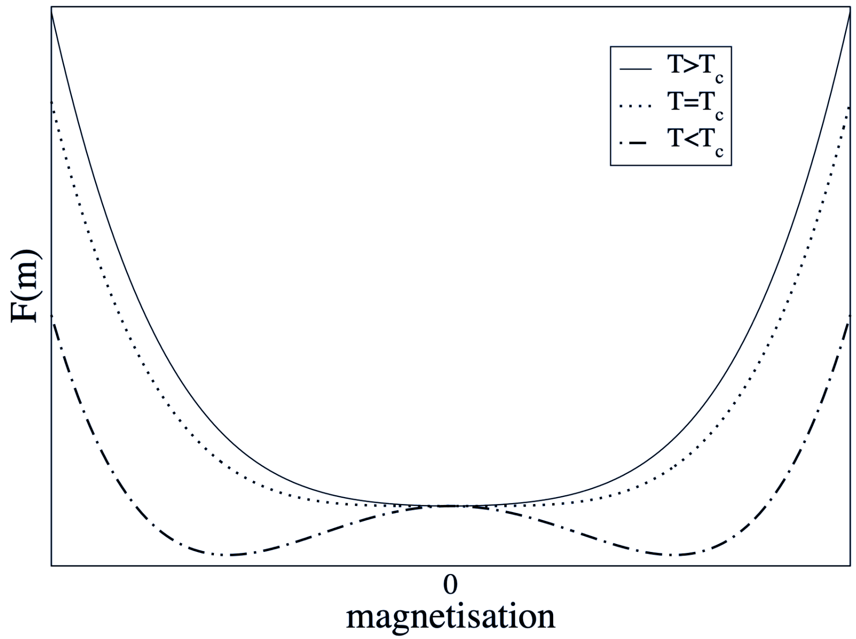
- From which the magnetisation follows as

$$m = -\frac{1}{N}\frac{\partial F}{\partial H} = \tanh(\beta(qJm + H))$$

- To find $m(H, T)$, we must numerically solve this last equation self consistently.

Spontaneous symmetry breaking

- Mean field method reveals what is happening in the Ising model near the critical temperature T_c
- Plot $\beta F(m)/N$ vs T for $H = 0$:
- For $H = 0$, $F(m)$ is symmetric in m. At high T, entropy dominates $\rightarrow$ single minimum in $F(m)$ at $m = 0$.



- As T is lowered, there comes a point ($T = T_c$) where the curvature of $F(m)$ at the origin changes sign; ie.

$$\frac{\partial^2 F}{\partial m^2} = 0$$

- At lower temperature: two minima at nonzero $m = \pm m^\star$, where the equilibrium magnetisation $m^\star$ is the positive root (calculated explicitly below) of

$$m^\star = \tanh(\beta J q m^\star) = \tanh(\frac{m^\star T_c}{T})$$

- $m^\star = 0$ which remains a root of this equation, is clearly an unstable point for $T < T_c$ (since F has a maximum there).

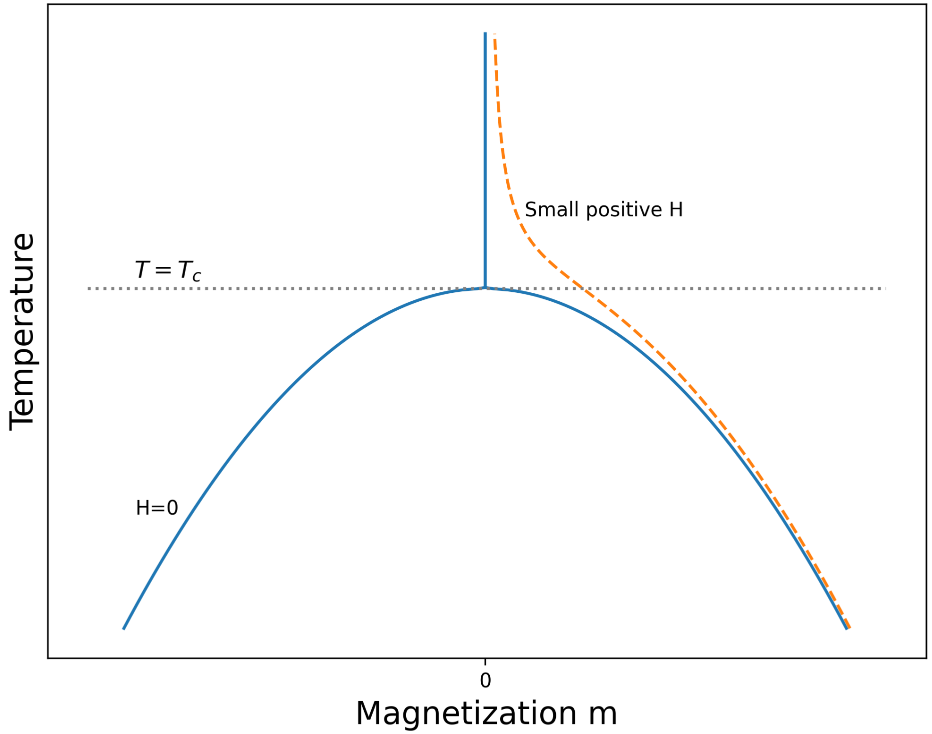
- This is an example of spontaneous symmetry breaking: Pair of ferromagnetic states (spins mostly up, or spins mostly down) which - by symmetry - have the same free energy, lower than the unmagnetized state.

Phase diagram

- The resulting zero-field magnetisation curve:

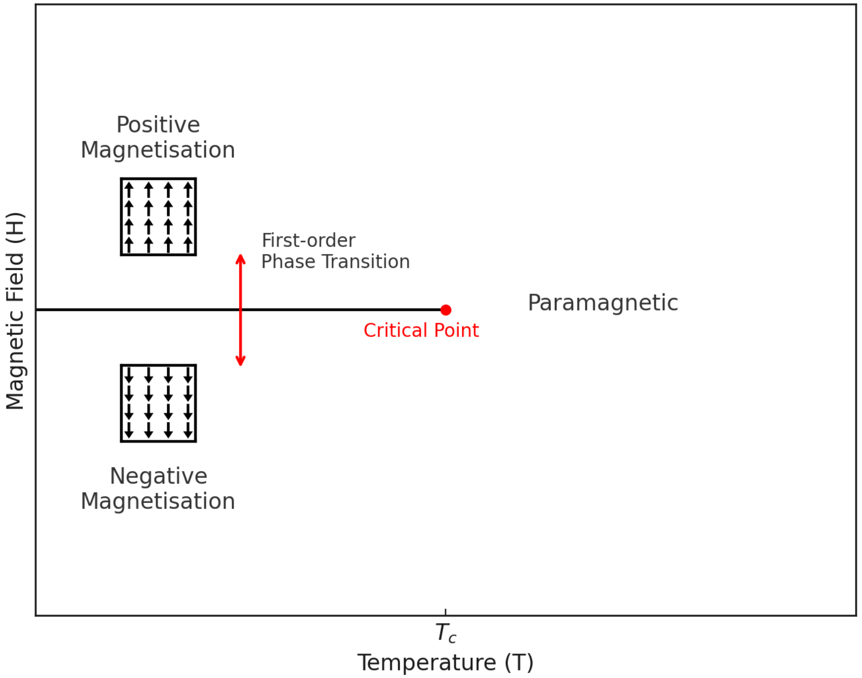
- Sudden change of behaviour at T_c (continuous phase transition).

- For $T < T_c$, arbitrary which of the two roots $\pm m^\star$ is chosen; typically it will be different in different parts of the sample (giving macroscopic ``magnetic domains'').



- Picture is qualitatively modified by a magnetic field H. Then there is always a finite magnetization, even for $T \gg T_c$ (no phase transition).

- Sit below T_c with $H > 0$ and gradually reduce H so that it becomes negative. Obeserve very sudden change of behaviour at $H = 0$: the equilibrium state jumps discontinuously from $m = m^\star$ to $m = -m^\star$.



- This is called a **first order phase transition**.

First order transition: magnetisation (or similar order parameter) depends discontinuously on other variables such as H or T

Continuous transition (criticality): Change of functional form, but no discontinuity in m; typically, however, $(\partial m/\partial T)_H$ (or similar) is either discontinuous, or diverges.

- We say that the phase diagram of the magnet in the H, T plane shows a line of first order phase transitions, terminating at a continuous transition, which is the critical point.

Mean field predictions for critical exponents

- Look for a solution to $m = \tanh(\beta Jqm)$ in zero field ($H = 0$) where m is small ($\ll 1$). Taylor expanding the $\tanh$ function yields

$$m = \frac{mT_c}{T} - \frac{1}{3}\left(\frac{mT_c}{T}\right)^3 + O(m^5)$$

- Then $m = 0$ is one solution. The other solution is given by

$$m^2 = 3\left(\frac{T}{T_c}\right)^3\left(\frac{T_c}{T} - 1\right)$$

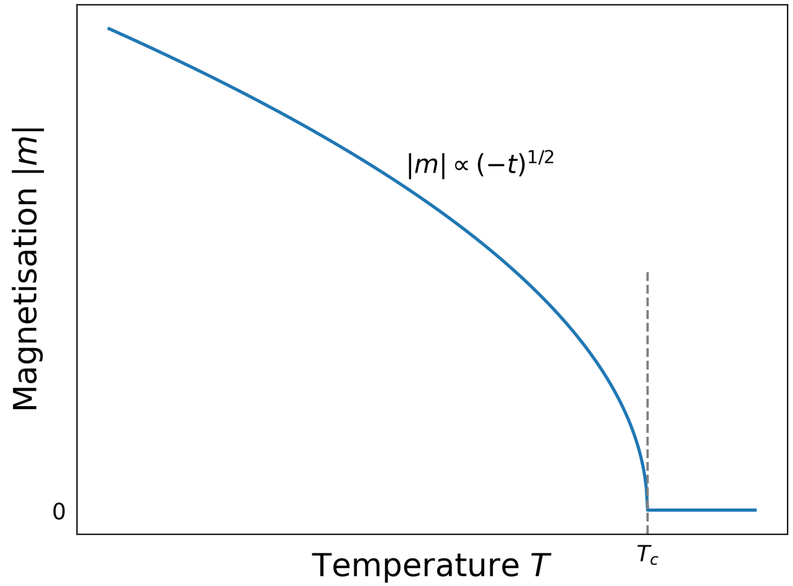
- Now, for T close to T_c (i.e. small m), and writing $t = (T - T_c)/T_c$, one finds

$$m^2 \simeq -3t$$

i.e.

$m = 0$ for $T > T_c$ since otherwise m imaginary

$m = \pm\sqrt{-3t}$ for $T < T_c$ real



- In a small finite field we can make the Taylor expansion

$$m = \frac{mT_c}{T} - \frac{1}{3}\left(\frac{mT_c}{T}\right)^3 + \frac{H}{k_B T}$$

- Consider now the isothermal susceptibility

$$\chi \equiv \left(\frac{\partial m}{\partial H}\right)_T$$

$$= \frac{T_c}{T}\chi - \left(\frac{T_c}{T}\right)^3 \chi m^2 + \frac{1}{k_B T}$$

- Then

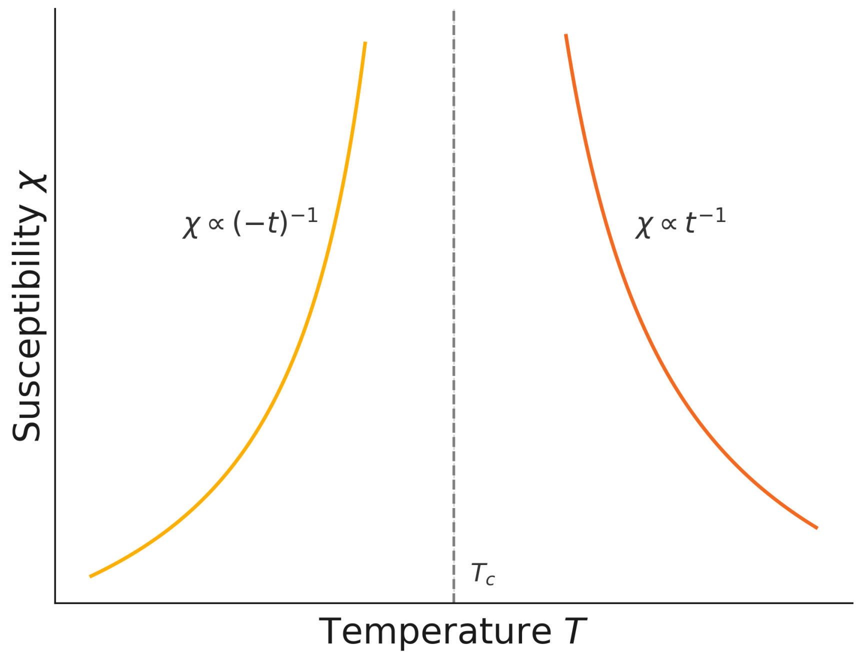
$$\chi\left[1 - \frac{T_c}{T} + \left(\frac{T_c}{T}\right)^3 m^2\right] = \frac{1}{k_B T}$$

- Hence near T_c

$$\chi = \frac{1}{k_B T_c}\left(\frac{1}{t + m^2}\right)$$

And recalling that $m^2 \simeq -3t$ for $T < T_c$

$$\chi = (k_B T_c t)^{-1} \text{ for } \quad T > T_c$$
$$\chi = (-2k_B T_c t)^{-1} \text{ for } \quad T \leq T_c$$



where one has to take the non-zero value for m below T_c to ensure positive χ, i.e. thermodynamic stability.

- This result implies that (within the mean field approximation) the critical exponent $\gamma = 1$.

Landau theory

- Landau theory is more general type of mean field theory. Not based on a particular microscopic model. We say that it is a **coarse-grained** theory.

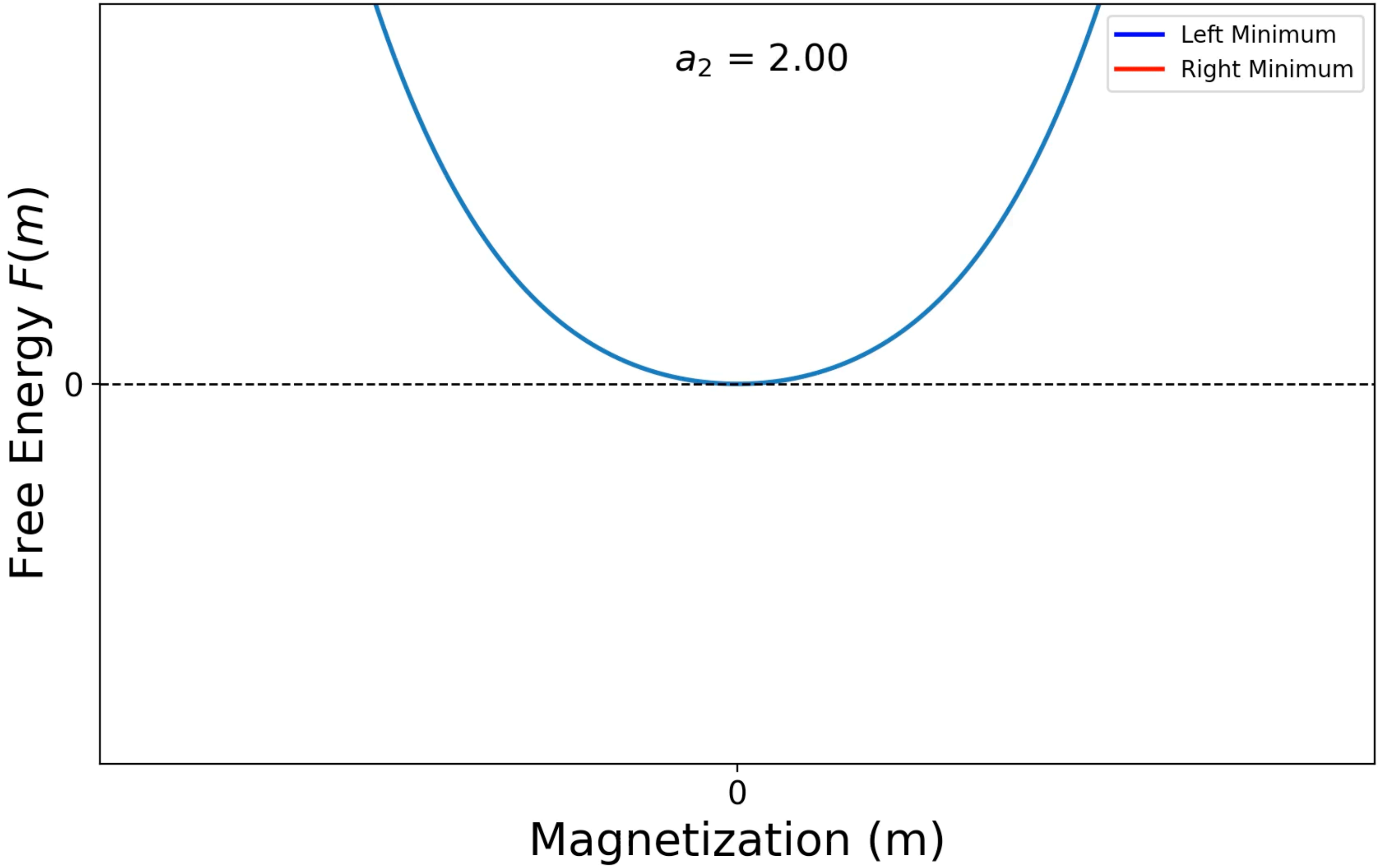
- Starting point is the Helmholtz free energy, which is written as a truncated power series expansion of the order parameter.

- For systems with a symmetrical order parameter (such as a ferromagnet where the energy is invariant under $m \to -m$) this takes the form

$$F(m) = F_0 + a_2 m^2 + a_4 m^4$$

- Equilibrium m is that for which $F(m)$ is minimum.

- Plots of the Landau free energy (for various a_2, with $a_4 > 0$) show how it gives rise to a critical point



a_2 = 2.00
Left Minimum
Right Minimum
Free Energy $F(m)$
0
0
Magnetization (m)

- Thermodynamics tells us that the system adopts the state of lowest free energy.

- Thus for $a_2 > 0$, the system will have $m = 0$, i.e. will be in the disordered (or paramagnetic) phase.

- For $a_2 < 0$, minimum of F occurs at a two symmetric minima at $m = \pm m_0$, i.e., the ordered phase is the stable one.

- $a_2 = 0$ corresponds to the critical point which marks the border between the ordered and disordered phases.

- Thus clearly a_2 controls the deviation from the critical temperature, i.e. $a_2 = \tilde{a}_2 t$

- Can now attempt to calculate critical exponents. First find equilibrium magnetisation, corresponding to the minimum of the Landau free energy:

$$\frac{dF}{dm} = 2\tilde{a}_2 tm + 4a_4 m^3 = 0$$

$$\Rightarrow m \propto (-t)^{1/2}, \qquad \text{so } \beta = 1/2, \text{ (mean field result).}$$

- We can also calculate the effect of a small field H if we sit at T_c. Since $a_2 = 0$, we have

$$F(m) = F_0 + a_4 m^4 - Hm$$

$$\frac{\partial F}{\partial m} = 0 \Rightarrow m(H, T_c) = \left(\frac{H}{4a_4}\right)^{1/3}$$

or $\quad H \sim m^{\delta} \quad ie.\ \delta = 3 \quad$ which defines a second critical exponent.

- Thirdly, magnetic susceptibility at zero field

$$\chi = \left(\frac{\partial m}{\partial H}\right)_{T,V} \sim |T - T_c|^{-\gamma}$$

Exercise: Show that $\gamma = 1$

- Finally heat capacity (per site or per unit volume) C_H, for $H = 0$:

$$C_H \sim |T - T_c|^{-\alpha}$$

Exercise: Show that $\alpha = 0$

Shortcomings of mean field theories

- In real ferromagnets, as well as in more sophisticated theories, the exponents β and γ are not the simple fraction and integers found here.

- This failure of mean field theory to predict the correct exponents is of course traceable to their neglect of correlations.

	Mean Field	$d = 1$	$d = 2$	$d = 3$
Critical temperature $k_B T/qJ$	1	0	0.5673	0.75
Order parameter exponent β	$\frac{1}{2}$	-	$\frac{1}{8}$	0.325 ± 0.001
Susceptibility exponent γ	1	∞	$\frac{7}{4}$	1.24 ± 0.001
Correlation length exponent ν	$\frac{1}{2}$	∞	1	0.63 ± 0.001

6. Static Scaling Hypothesis

- The static scaling hypothesis provides a basis for power law behaviour. Moreover, it predicts the existence of so-called **scaling phenomena** in near-critical systems.

- The hypothesis asserts that: near criticality, the free energy is a so-called generalised homogeneous function of the thermodynamic fields.

- A function of two variables $g(u, v)$ is called a generalised homogeneous function if it has the property

$$g(\lambda^a u, \lambda^b v) = \lambda g(u, v) \quad \text{for } \textbf{all } \lambda$$

where the parameters a and b (known as scaling parameters) are constants

- Example functions:
- $g(u, v) = u^3 + v^2$ with $a = 1/3,\ b = 1/2$
- $g(u, v) = u^4 v^5$ with $a = 1/4,\ b = 1/5$

- For such functions one can always implement a **change of scale**, to reduce the dependence on two variables (e.g. t and h) to dependence on one new variable.

- The arbitrary scale factor λ can be chosen as $\lambda^a = u^{-1}$ giving

$$g(u, v) = u^{1/a} g(1, \frac{v}{u^{b/a}})$$

- Thus $g(u, v)$ satisfies a simple power law in **one** variable, provided $v/u^{b/a} = C$. Note, however, that this relationship specifies neither the function g nor the parameters a and b.

- Scaling hypothesis asserts that in the critical region, the free energy F is a generalised homogeneous function of thermodynamic fields

- Thus for the ferromagnet (fields t and h):

$$F(\lambda^a t, \lambda^b h) = \lambda F(t, h)$$

- Without loss of generality, we can set $\lambda^a = t^{-1}$, implying $\lambda = t^{-1/a}$ and $\lambda^b = t^{-b/a}$.

- Then

$$F(t, h) = t^{1/a}F(1, t^{-b/a}h)$$

where our choice of λ ensures that the r.h.s is now a function of a single variable $t^{-b/a}h$

- An expression for the magnetisation can be obtained simply by taking the field derivative of F

$$m(t, h) = -\,t^{(1-b)/a}m(1, t^{-b/a}h)$$

- In zero applied field $h = 0$, this reduces to

$$m(t, 0) = (-t)^{(1-b)/a}m(1,0)$$

where the r.h.s. is a power law in t

- Can now identify the exponent β in terms of the scaling parameters a and b.

$$\beta = \frac{1-b}{a}$$

- By differentiating the free energy, other relations between scaling parameters and critical exponents may be deduced.

- Such calculations (try as an exercise!) yield the results
$\delta = b/(1-b), \;\; \gamma = (2b-1)/a, \;\; \alpha = (2a-1)/a$

- Relationships between the critical exponents follow by eliminating the scaling parameters from these equations. The principal results (known as ``scaling laws'') are:-

$$\alpha + \beta(\delta + 1) = 2$$
$$\alpha + 2\beta + \gamma = 2$$

- Thus only two critical exponents need be specified, for all others to be deduced.

Experimental Verification of Scaling

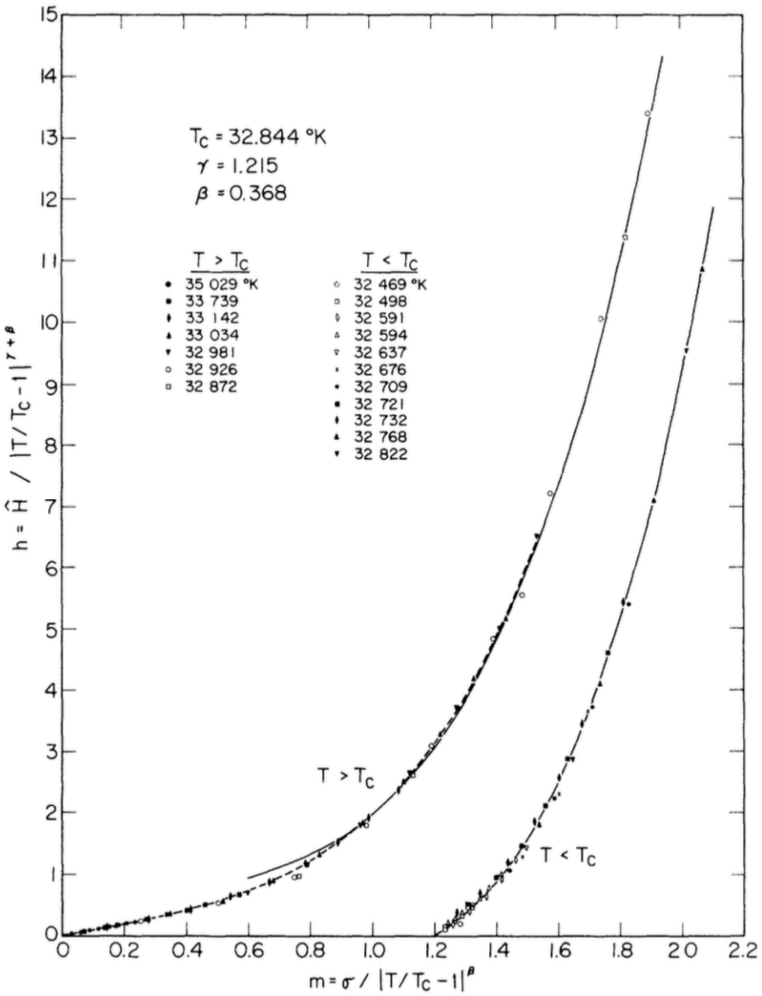
- Experiments confirm the scaling hypothesis.
- Rewriting the above expression for $m(t,h)$ in terms of the exponents β and δ, one finds

$$\frac{m(t,h)}{t^{\beta}} = m(1, \frac{h}{t^{\beta\delta}})$$

where the r.h.s. is a function of the single scaled variable $\tilde{H} \equiv t^{-\beta\delta} h(t,M)$.

- For some magnet, measure m vs h for various fixed temperatures and construct $m-h$ isotherms.
- Plotting the data against the scaling variables $\tilde{M} = t^{-\beta} m(t,h)$ and $\tilde{H} = t^{-\beta\delta} h(t,M)$ one finds scaling, i.e. all isotherms collapse onto a single curve, one for $t > 0$, and another for $t < 0$.

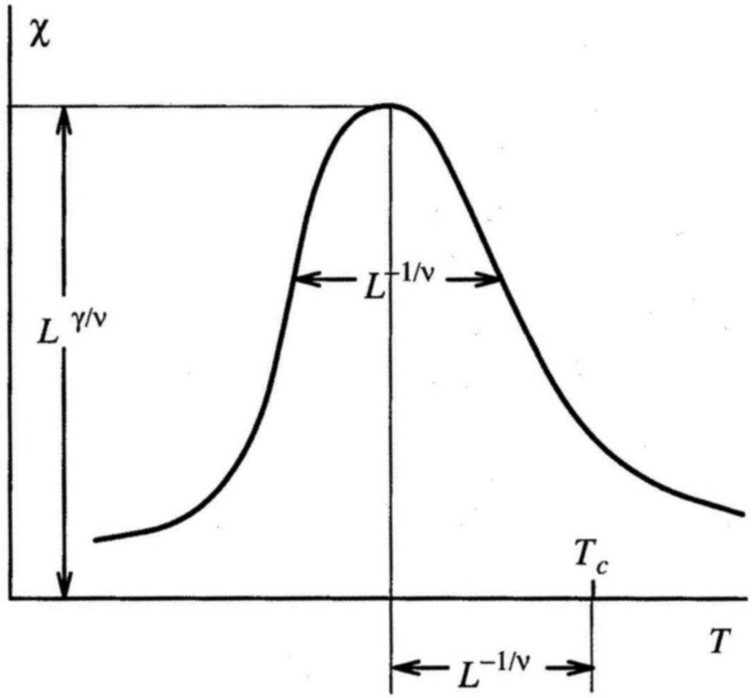
Magnetisation of CrBr3 in the critical region plotted in scaled form



- Similar results are found using the scaled equation of state of simple fluid systems such as He^3 or Xe.

Computer simulation

- Simulation widely used to study critical point phenomena,
- But computational constraints restrict one to dealing with systems of finite-size.
- Cannot access the regime of truly long ranged fluctuations that characterize the near-critical regime.
- As a consequence, the critical singularities in C_V, χ_T, order parameter, etc. appear rounded and shifted in a simulation study of a system of linear extent L.
- The peak position does not provide an accurate estimate of the critical temperature.



- Although the degree of rounding and shifting reduces with system size, it still makes it hard access to the largest system sizes which would provide accurate estimates of critical parameters.

- To deal with this, finite-size scaling methods have been developed.

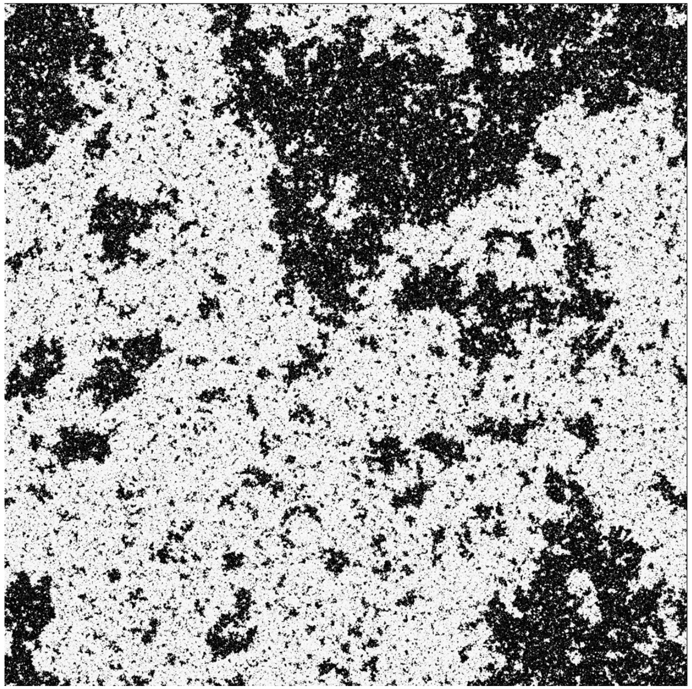
- Finite-size scaling allows extraction of bulk critical properties from simulations of finite size (see later)

7. Universality and Renormalisation Group Theory

- Critical region is characterised by correlated microstructure on **all** length-scales up to and including the correlation length.

- Can only be accurately characterised by a very large number of variables.

- To obtain a fuller understanding of the critical region, must take account of existence of structure on all length-scales.



The critical point: A many length scale problem

- A near critical system can be characterised by three important length scales, namely
  (a) The correlation length, ξ, ie the size of correlated microstructure.
  (b) Minimum length scale L_{min}, i.e. the smallest length in the microscopics of the problem, e.g. lattice spacing of a magnet or the particle size in a fluid.
  (c) Macroscopic size L_{max} eg. size of the system.

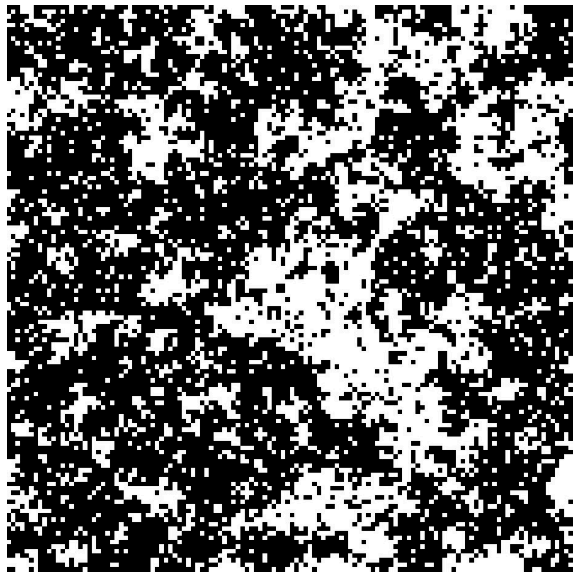
- The authentic critical region is defined by a window condition:

$$L_{\max} \gg \xi \gg L_{\min}$$

- This regime is hard to tackle because it is characterised by configurational structure on all scales between L_{min} and ξ (it is fractal). Moreover structure on different length scales are correlated with one another.

Philosophy and Methodology of the RG

- Central idea: a stepwise elimination of the degrees of freedom of the system on successively larger length-scales.
- Introduce a fourth length scale L, which in contrast to the other three, characterises the **description** of the system.
- L typifies the size of the smallest resolvable detail in a description of the system's microstructure.
- Ising model snapshots contain **all** details of each configuration: the resolution length L coincides with the lattice spacing i.e. $L = L_{min}$.
- But explicit form of the small scale microstructure is irrelevant to the behaviour of ξ. Microstructure is ‘noise'.
- To eliminate it, select a larger value of L, the resolution (or `coarse-graining') length



- There are many ways of implementing this 'coarse-graining' procedure.

- Adopt a simple strategy in which we divide our sample into blocks of side L, each of which contains L^d sites.

- The centres of the blocks define a lattice of points indexed by $I = 1,2,....,N/L^d$. We associate with each block lattice point centre, I, a coarse-grained or block variable $S_I(L)$ defined as the spatial average of the local variables it contains:

$$S_I(L) = L^{-d} \sum_i^I s_i$$

- The set of coarse grained coordinates $\{S(L)\}$ are the basic ingredients of a picture of the system having spatial resolution of order L.

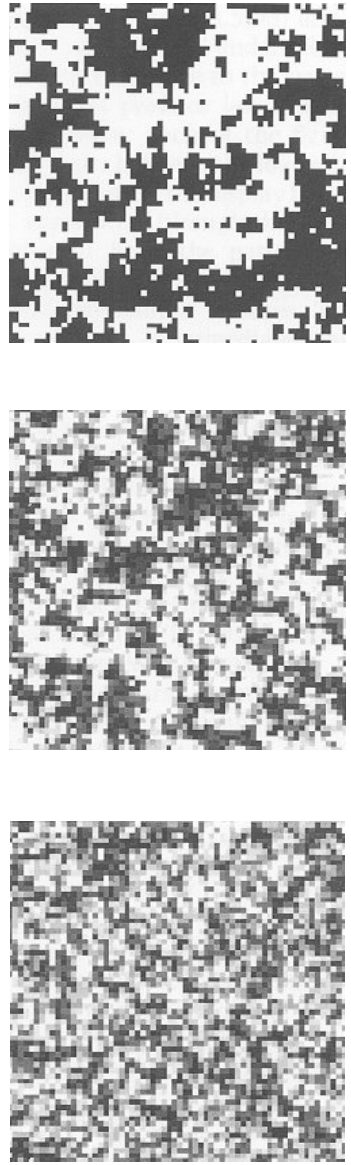
- Such a coarse graining operation is easily implemented on a computer.
- But while the underlying Ising spins can only take two possible values, the block variables $S_I(L)$ have $L^d + 1$ possible values.
- Thus, need a more elaborate colour convention to represent block spins. Adopt a grey scale.
- In presenting results implement:
  - A length scaling: the lattice spacing on each blocked lattice is scaled to that of the original lattice. Can display correspondingly larger portions of the physical system.
  - A variable scaling: adjust the scale (`contrast’) of the block variable so as to match block variable spectrum the full range of grey shades.
- We shall consider the results of coarse-graining configurations typical of three different temperatures: $T > T_c$, $T = T_c$, and $T < T_c$

- Consider first a system marginally above T_c, having $\xi \approx 6$. Apply coarse graining with block sizes $L = 4$ and $L = 8$.

- Coarse-graining amplifies the consequences of the small deviation of T from T_c.

- As L is increased, the ratio of the size of the largest configurational features (ξ) to the size of the smallest (L) is reduced. ξ / L provides a natural measure of how `critical' is a configuration.

$T > T_c$



$L = 1$

$L = 4$

$L = 8$

- Thus coarse-graining generates a representation of the system that is effectively **less critical** the larger the L value.
- Limit is an effectively fully disordered arrangement
- When viewed on length scales L larger than ξ, the correlated microstructure is no longer apparent; each coarse-grained variable is independent.

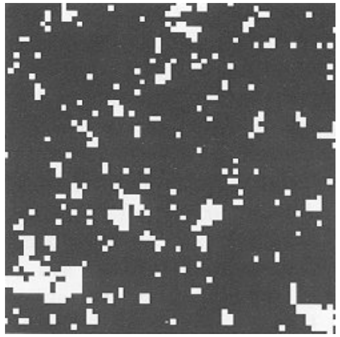
- A similar trend is apparent for $T < T_c$.

- Again, take $\xi \approx 6$. Coarse-graining with $L = 4$ and $L = 8$ again generates representations which are effectively less critical .

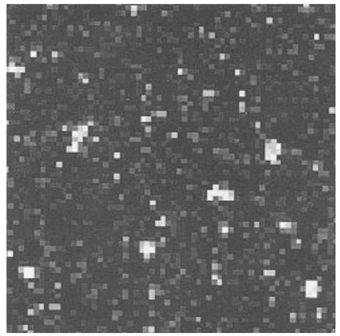
- This time the coarse-graining smoothes out the microstructure which makes the order incomplete.

- The limit point of this procedure is a homogeneously ordered arrangement.

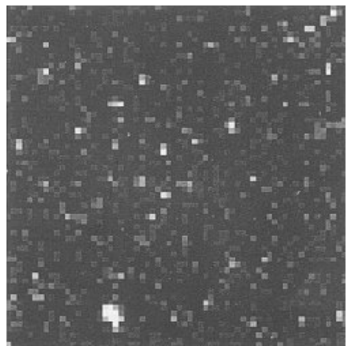
$T < T_c$



$L = 1$



$L = 4$



$L = 8$

- Consider the situation at the critical point.

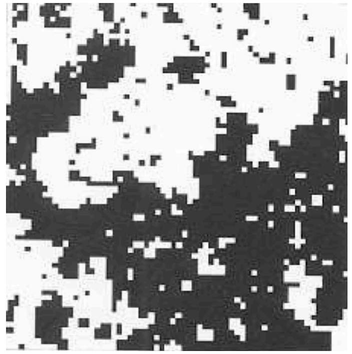
- Since ξ is as large as the system itself, coarse graining does not produce less critical representations.

- In each figure, one sees structure over all length scales between the lower limit set by L and the upper limit set by the display size.

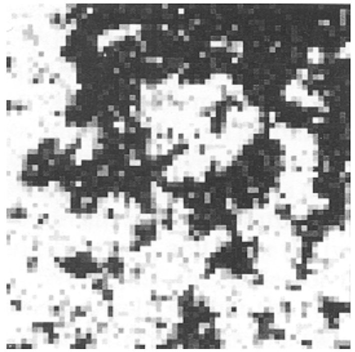
- A limiting trend is nevertheless apparent.

$T = T_c$

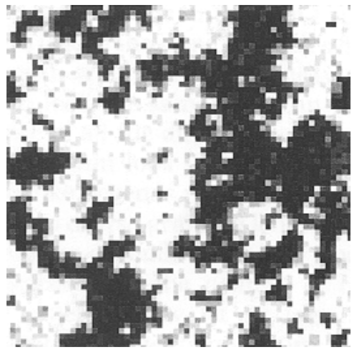
$L = 1$



$L = 4$



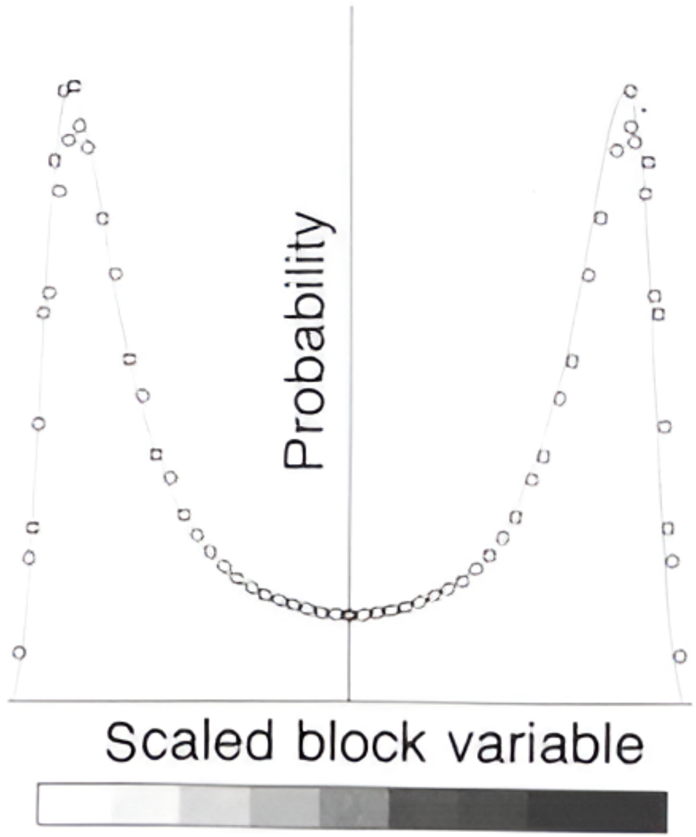
$L = 8$

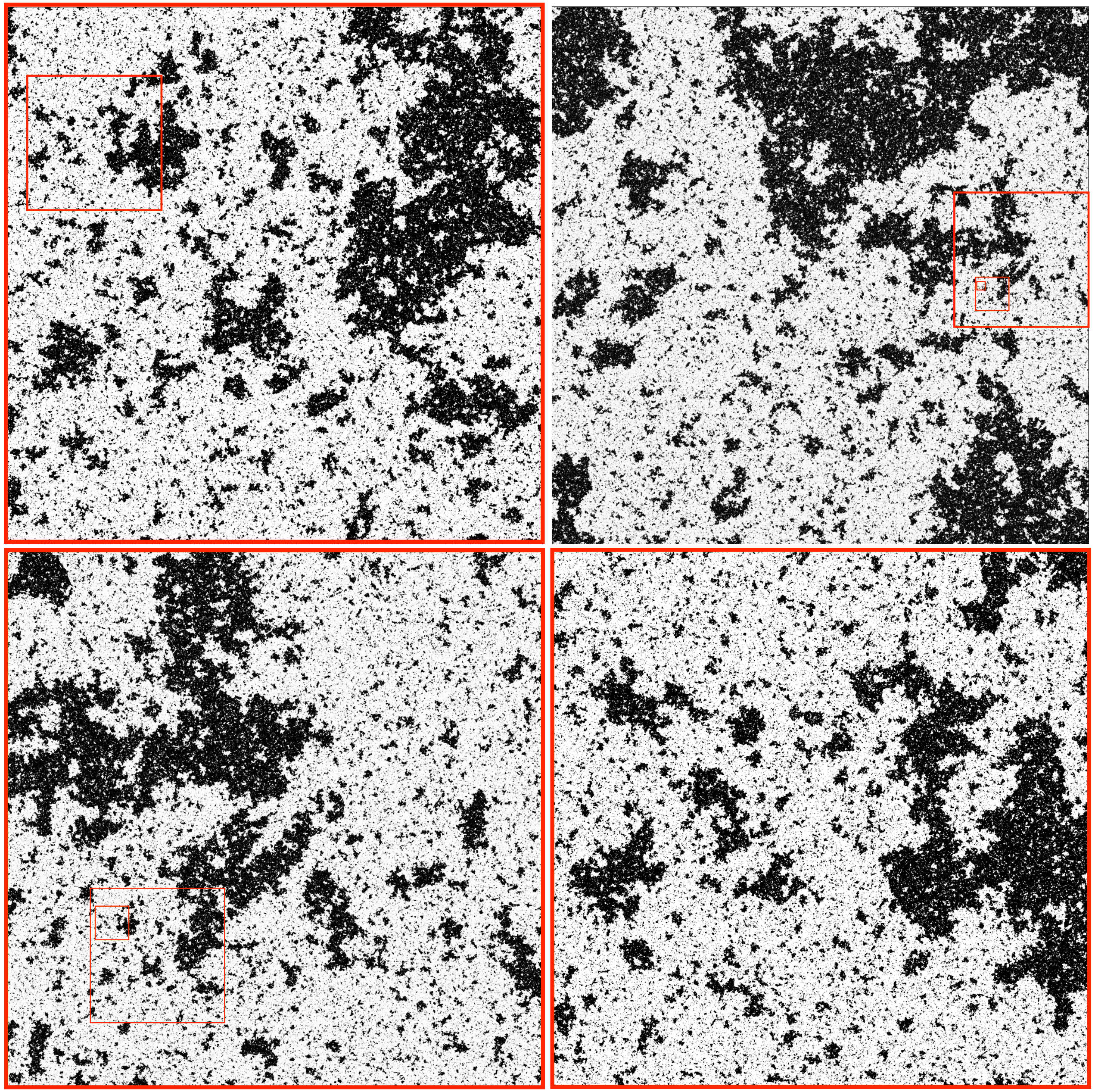


- Although the $L = 4$ pattern differs qualitatively from $L = L_{min}$, the $L = 4$ and $L = 8$ patterns display qualitatively similar features.

- Thus patterns formed by the ordering variable at criticality look statistically the same when viewed on all sufficiently large length scales (fractal like).

- A statistical analysis of the spectrum of $L = 4$ configurations shows that it is almost identical to that of the $L = 8$ configurations.





- **Summary**: Under the coarse-graining operation there is an evolution or flow of the system's configuration spectrum.

- The flow tends to a limit, or **fixed point**, such that the pattern spectrum does not change under further coarse-graining.

- These scale-invariant limits have a trivial character for $T > T_c$, (a perfectly disordered arrangement) and $T < T_c$, (a perfectly ordered arrangement).

- The hallmark of the critical point is the existence of a scale-invariant limit which is neither fully ordered nor fully disordered but which possesses structure on **all** length scales.