Department of Physics

PH40073

Phase Transitions

11 lectures, Spring Semester 2018

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Timetable

- Mondays 10:15, room 1E2.4
- Wednesdays 11:15, room 1E2.4
- Thursdays 14.15, room 1E2.4

Recommended text books

- Best book: *Statistical Mechanics of Phase Transitions*, by J.M. Yeomans (Oxford). There are 5 copies in the library, shelfmark 536.71 Yeo.

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

- *The Critical Point* C. Domb, (Taylor and Francis). Shelfmark 536.71
- *Lectures on Phase Transitions and the Renormalization Group*, N. Goldenfeld (Addison Wesley) Shelfmark 536.71 Gol.
- *The Theory of Critical Phenomena,* J.J. Binney, N.J. Dowrick, A.J. Fisher and M.E.J. Newman; (Oxford).

Introduction

- A wide variety of physical systems undergo rearrangements of their internal constituents in response to the thermodynamic conditions to which they are subject.

- 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 T (the critical temperature), it vanishes altogether:

- 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 jump in density at the transition vanishes. These conditions correspond to the *critical point* of the fluid.

- In the vicinity of a critical point a system will exhibit a variety of remarkable effects known collectively 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.

- It transpires that the origin of the singularities in these quantities can be traced to large-length-scale co-operative effects between the microscopic constituents of the system.

- Understanding the physics of critical points is important because often one observes *quantitatively identical* critical phenomena in a whole range of apparently quite disparate physical systems.

- 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 some 35 years ago, has enjoyed considerable success.

Background concepts

- Let us define the *order parameter*, Q.
- Q provides a quantitative measure of the difference between the phases coalescing at the critical point:
- In the case of the fluid, the order parameter is density difference $Q = \rho_{liq} - \rho_{gas}$.
- In the ferromagnet $Q = m$, the magnetisation.
- But why should a system exhibit a phase transition at all?
- Statistical Mechanics provides the answer!

- The probability p_a that a physical system at temperature T will have a particular microscopic arrangement (configuration), labelled a, of energy E_a is

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

- 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

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

where the sum extends over all possible microscopic arrangements.

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

$$\bar{O} = \frac{1}{Z} \sum_a O_a e^{-E_a/k_B T}$$

- It follows that the order parameter is:

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

- Now consider the ferromagnetic case $Q = m$.

- For T very small, system will be overwhelmingly likely to be in its minimum energy arrangements (ground states) having magnetisation $+1$, or -1.

- For T large, enhanced prob. of ground state arrangements in eq. † is insufficient to offset the fact that the sum 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. † 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 (in the course of the competition) 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".

- All thermodynamic observables, eg. Q, C_H, χ_R and κ_T are obtainable as appropriate derivatives of the free energy:

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 $t \equiv (T - T_c)/T_c$:-

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

$$C_H \equiv \frac{\partial E}{\partial T} \propto t^{-\alpha} \quad (H = 0)$$

- Another key quantity is the *correlation length* ξ, measuring the distance over which fluctuations of the magnetic moments are correlated, which 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_c approached:

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

and as a function of magnetic field:

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

with $h = (H - H_c)/H_c$, 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.

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

- 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.

The Ising model

- Can use simple models to probe the properties of the critical region.

- Simplest is the 2d spin spin-$\frac{1}{2}$ Ising model, which comprises a lattice of 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

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

- $J > 0$ measures the strength of the coupling between spins. Sum extends over nearest neighbour spins s_i and s_j. H is a magnetic field term.

- 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 a certain temperature T_c, entropy drives the system through a continuous phase transition to a disordered spin arrangement with $|m| \approx 0$.

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

- 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 $\Delta = 2J$ independent of position (ie domain walls don't interact).

- The partition function of system is

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

where for a single domain wall,

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

so

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

- The second term arises from the free energy 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, 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

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

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

Now the partition function may be written

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

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 matrix elements in equation (1) is simply just the trace of $\mathbf{V}^N$, given by the sum of its eigenvalues:-

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

- 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 in the presence of an applied field H, 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

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

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 ($\beta = \frac{1}{8}, \nu = 1, \gamma = \frac{7}{4}$. $T_c = -2J/\ln(\sqrt{2}-1) \approx 2.269J$)

- 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.

Mean field theory

- 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

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

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

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

$$\mathcal{H}_{mf} = -\sum_i H_{mf} s_i + NqJm^2/2$$

with $H_{mf} \equiv Jqm + H$.

- It follows that the partition function is

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

- 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 (calculate explicitly below) of

$$m^\star = \tanh(\beta J q m^\star) = \tanh(\frac{m^\star T_c}{T}) \qquad (2)$$

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

- 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: like:

- 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 field $H \to$ always a magnetization, even $T \gg T_c$ (no phase transition).

- Sit below T_c with $H > 0$ and gradually reduce H so that it becomes negative. $\Rightarrow$ *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 variable (such as h or T).

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

- 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:

Zero H solution

$$m = \tanh(\frac{mT_c}{T})$$

- We look for a solution 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.

$$\begin{aligned} m &= \quad 0 \quad && \text{for } T > T_c \\ m &= \pm\sqrt{-3t} && \text{for } T < T_c \end{aligned}$$

Finite (but small) field solution

- In a small field we can make the Taylor expansion

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

- Consider now the isothermal susceptibility

$$\begin{aligned} \chi &\equiv \left(\frac{\partial m}{\partial H}\right)_T \\ &= \frac{T_c}{T}\chi - \left(\frac{T_c}{T}\right)^3 \chi m^2 + \frac{1}{k_B T} \end{aligned}$$

- 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

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

Then

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

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

Landau theory

- Landau theory is more general type of mean field theory. Not based on a particular microscopic model.

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

- For a ferromagnet (up-down spin symmetry) 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

- 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.

$$a_2 = \tilde{a_2} t$$

where t is the reduced temperature.

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

$$\frac{dF}{dm} = 2\tilde{a_2} t m + 4 a_4 m^3 = 0$$

i.e.

$$m \propto (-t)^{1/2},$$

so $\beta = 1/2$, (mean field result).

- We can calculate the effect of a small field H if we sit at the critical temperature 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

$$H \sim m^\delta \qquad \delta = 3$$

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 $H = 0$:

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

with $\alpha = 0$.

- 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

Lattice Gas model

- A crude representation of a fluid.
- Particles can occupy the sites of a hypercubic lattice.
- Occupancy variables $c_i = 1$ (occupied) or $c_i = 0$ (vacant).
- The average particle number density is given $c = L^{-d} \sum_i c_i$
- Hamiltonian:

$$\mathcal{H}_{LG} = -\epsilon \sum_{<i,j>} c_i c_j - \mu \sum_i c_i$$

- Particle density fluctuates around a mean value controlled by μ.

- The lattice gas model maps onto (is *isomorphic* to) the Ising model, extending its applicability to fluids.

- Write the partition function of the lattice gas:

$$\Xi = \sum_{\{c\}} \exp\left[\beta\epsilon \sum_{<i,j>} c_i c_j + \beta\mu \sum_i c_i\right]$$

- Now change variables to

$$c_i = (1 + s_i)/2; \qquad J = \frac{\epsilon}{4} \qquad h = \frac{\epsilon q + 2\mu}{4}$$

Hence

$$\mathcal{H}_{LG} = \mathcal{H}_{\mathrm{I}} + \text{constant}$$

- Since the last term does not depend on the configuration, it has no physical implications.

- **Phase diagram** Using the translation rules we can plot the phase diagram of the lattice gas in the $\mu - T$ plane.

- Again there is a line of first order phase transitions terminating at a critical point.

- First order line means that if $T < T_c$ we smoothly increase the chemical potential through coexistence, density of particles c jumps discontinuously:

$$c_{\text{gas}} = \frac{1 - m^\star}{2} \rightarrow c_{\text{liquid}} = \frac{1 + m^\star}{2}$$

  These values merge at T_c, the gas-liquid critical point. At higher temperatures, the distinction between the phases disappears.

- **Real Fluids**. Compare this with a real fluid. Main difference is that the lattice gas has "Particle-hole" symmetry, $c \to 1 - c$. $\Rightarrow$ Phase diagram in a real fluid looks lopsided.

Series expansion

- Perturbation theory, going beyond mean field approximation.

- Seeks to deduce results for the critical region using known results obtained away from criticality.

- Simple example is the high-T series, which expresses Boltzmann factor as expansion in $1/T$ (assumed small).

$$\exp(-\mathcal{H}/k_BT) = 1 - \mathcal{H}/k_BT + \frac{1}{2!}(\mathcal{H}/k_BT)^2 + ...$$

- Successively higher terms characterise correlations over successively larger distances.

- Known results for the high-T fully disordered phase permit the calculation of Z using the significant terms in this expansion.

- Method breaks down close to T_c, due to divergent correlation length.

The 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 functions* of the thermodynamic fields.

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

$$g(\lambda^a u, \lambda^b v) = \lambda g(u, v)$$

for all λ, where the parameters a and b (known as scaling parameters) are constants.

- 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 rhs 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 yield the results $\delta = b/(1-b)$,$\gamma = (2b-1)/a$, and $\alpha = (2a-1)/a$. Try it as an exercise!

- 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 the exponents β and δ, one finds

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

  where the RHS 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 $M = t^{-\beta} m(t,h)$ 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 ($t < 0$).

- 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 restict 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, order parameter, etc. appear rounded and shifted in a simulation study.

- 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 estaimates of critical parameters.

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

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

Renormalisation Group Theory

- Critical region is characterised by correlated microstructure on $\underline{all}$ length-scales up to and including the correlation length.

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

- MFT and series expansion fail because they at best incorporate interactions among only a few nearby spins.

- The scaling hypothesis fails to provide more than qualitative insight because it focuses on only one length-scale, effectively ξ.

- 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:

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

- 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 in coincides with the lattice spacing i.e. $L = L_{\text{min}}$.

- But explicit form of the small scale microstructure is irrelevant to the behaviour of ξ. The small scale 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.

- 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.

- Consider the results of coarse-graining configurations typical of three different temperatures: $T > T_c$, $T < T_c$ and $T = T_c$.

- Two auxiliary operations are implicit in these results.

  1. First is 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.

  2. Second is a *variable scaling*: adjust the scale ('contrast') of the block variable so as to match block variable spectrum the full range of grey shades.

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

- Find that the 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.

- 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 lengthscales L larger than ξ, the correlated microstructure is no longerapparent; 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.

- Consider now 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.

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

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

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

- 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.

Universality and scaling

- Introduce a three state (spin-1) variant of the Ising model. ($s_i = 1, 0, -1$).

- 2-state and 3-state model have properties which are clearly different: eg. T_c for the 3-state model is some 30% lower than that of the 2-state model.

- However, the two models have the same universal properties. Let us explore the differences and similarities in the configurations.

- Raw spin configurations are different.

- As with 2-state model, coarse-graining operation bears the configuration spectrum to a non-trivial scale-invariant limit.

- Remarkably, the limit is the same for both models! Coarse-graining erases the local differences apparent in configs, and exposes a profound configurational similarity.

- Similarity of the configurations of the different systems is not restricted to T_c itself.

- Suppose we have a 2-state model and a 3-state model each as some $t > 0$.

- Systems will have different correlation lengths, $\xi_1 = a_1 t^{-\nu}$ and $\xi_2 = a_2 t^{-\nu}$.

- Although this difference survives the coarse-graining itself, it can be suppressed by the combined coarse graining and the auxiliary *length-scale* operations.

- Specifically, we choose lengths L_1 for L_2 for the two models such that $\xi_1/L_1 = \xi_2/L_2$.

- We adjust the snapshot sizes so that the sizes of the minimum-length-scale structure (set by L_1 and L_2) looks the same for each system

- Then the configurations again look (statistically) identical. Precisely what they look like depends upon our choice if ξ/L.

Fluid-magnet universality

- The similarities in the critical behaviour of fluids and magnets can be traced to the underlying similarity in their coarse-grained configurations

- In a magnet, the relevant configurations are those formed by the coarse-grained magnetisation (the magnetic moment averaged over a block of side L).

- In a fluid, the relevant configurations are those of the coarse-grained density (the mass averaged over a block if side L)

- Patterns of bubbles of liquid or vapour may be matched to pattern in the former (microdomains of the magnetisation), given appropriate scaling operations to camouflage the differences between the length scales and the differences between the variable scales

Universality classes

- Coarse graining does not erase all differences between the physical properties of critical systems.

- Differences in the space dimension d of two critical systems will lead to different universal properties such as critical exponents.

- Eg. critical exponents of the 2D magnet, match those of the 2d fluid, but they are different to those of 3d magnets and fluids.

	$d=2$	$d=3$
Critical temperature	0.5673	0.75
Order parameter exponent β	$\frac{1}{8}$	0.325 ± 0.001
Susceptibility exponent γ	$\frac{7}{4}$	1.24 ± 0.001
Correlation length exponent ν	1	0.63 ± 0.001

- d is one of a small set of qualitative features which survive coarse graining and which together serve to define the system's universal behaviour, or *universality class*.

- Set includes the number of components n of the order parameter. For the fluid and magnet the order parameter is a scalar, for which $n = 1$.

- In some ferromagnets, the order parameter may be a vector ($n = 2$ or $n = 3$).

- A third important feature which can change the universality class of a critical system is the range of the interaction potential between its constituent particles.

- For the Ising model, interactions are inherently nearest neighbour in range.

- Most fluids interact via short ranged dispersion forces.

- However some systems (such as charged systems) have much longer ranged interactions and thus different critical exponents to the Ising model and fluid.

Critical exponents

- How can the critical exponents, be computed from the properties of the coarse-grained configuration spectrum?

- Consider one typical coarse-grained variable of our Ising system, which we shall denote $S(L)$.

- Suppose that t is sufficiently small that the important observables are dominated by large-scale microstructure: $\xi \gg L_{\text{min}}$.

- Configurational universality is expressed in the claim that, for *any* L and t, scale factors $a(L)$ and $b(L)$ may be found such that the probability distribution $p(S(L))$ of the coarse-grained variable can be written in the form

$$p(S(L), t) = b(L)\tilde{p}(b(L)S(L), a(L)t)$$

where $\tilde{p}$ is a function unique to a universality class.

- The role of the scale factors a and b is to absorb the basic non-universal scales identified before.

- Values of exponents are implicit in the L dependence of these scale factors. The key results are

$$\begin{aligned} a(L) &= a_0 L^{1/\nu} \\ b(L) &= b_0 L^{\beta/\nu} \end{aligned}$$

  The amplitudes a_0 and b_0 are system specific (non-universal) constants.

- Thus the basic critical exponents ($1/\nu$, β/ν) serve to characterise the ways in which the configuration spectrum evolves under coarse-graining.

- Consider first β/L.

- Precisely at criticality, the overall scale of the coarse-grained variable $S(L)$ is eroded with increasing L.

- Need to amplify scale of $S(L)$ to match configurations of coarse-graining length L_1 to those of a larger length L_2.

- Required amplification is $b(L_2)/b(L_1) = (L_2/L_1)^{\beta/\nu}$.

- The index β/ν thus controls the rate at which the scale of the ordering variable decays with increasing coarse-graining length.

- Consider now $1/\nu$.

- For small but finite t (large but finite ξ) there is second way in which the configuration spectrum evolves with L.

- As noted previously, coarse graining reduces the ratio of ξ to L, and results in configurations with a less critical appearence.

- More precisely, increasing L from L_1 to L_2 at constant t has the same effect as keeping L constant while amplifying the reduced temperature t by a factor $a(L_2)/a(L_1) = (L_2/L_1)^{1/\nu}$.

- One may think of the combination $a(L)t$ as a measure of the effective reduced temperature of the physical system viewed with resolution length L.

Finite-size scaling

- Consider the average of the block variable $S(L)$.

- This is non other than the value of the order parameter Q, measured over a block of side L.

- Now the block variable average $\bar{S}(L)$ is defined by the first moment of the probability distribution p, i.e.

$$Q(L,t) = \bar{S}(L,t) = \int S(L) p(S(L),t) dS(L)$$

substituting for $p(S(L),t)$ gives

$$\begin{aligned} Q(L,t) &= \int S(L) b(L) \tilde{p}(S(L)b(L), a(L)t) dS(L) \\ &= b^{-1}(L) \int S(L) b(L) \tilde{p}(S(L)b(L), a(L)t) d(S(L)b(L)) \\ &= b^{-1}(L) f(a(L)t) \\ &= b_0 L^{-\beta/\nu} f(a_0 L^{1/\nu} t) \end{aligned}$$

where f is a universal function (defined by the first moment of $\tilde{p}$).

- FSS provides us with a prescription for measuring critical exponent ratios β/ν and $1/\nu$ via computer simulations of near critical systems.

- For instance, at criticality ($t = 0$) and for finite L $Q(L, 0)$ will not be zero (the T at which Q vanishes for finite L is above the true T_c).

- However, we know that its value must vanish in the limit of infinite L; it does so like

$$Q(L, 0) = b_0 L^{-\beta/\nu} f(0) \equiv Q_0 L^{-\beta/\nu}$$

- Thus by studying the critical point L dependence of Q we can estimate β/ν.

- A similar approach in which we study two block sizes L, and tune t separately in each case so that the results for $QL^{\beta/\nu}$ are identical provides information on the value of $1/\nu$.

The renormalisation group: effective coupling viewpoint

- Return to our fundamental equation

$$p = Z^{-1} e^{-\mathcal{H}}$$

  where $\mathcal{H} \equiv E/k_B T$.

- Imagine that we generate, via simulation procedure, a sequence of configurations with relative probability $\exp(-\mathcal{H})$.

- Use these to produce a set of coarse-grained configurations.

- Q: What is the energy function $\mathcal{H}'$ of the coarse-grained variables which would produce these coarse-grained configurations with the correct relative probability $\exp(-\mathcal{H}')$?

- Clearly the form of $\mathcal{H}'$ depends on the form of $\mathcal{H}$, thus

$$\mathcal{H}' = R(\mathcal{H})$$

- The operation R, defines the RG transformation linking the coarse-grained configurational energy to the microscopic Hamiltonian.

- Suppose our system is near criticality and that we wish to calculate its large-distance properties.

- Structure on all length-scales renders basic Stat Mech problem difficult.

- Make it easier by tackling the not-quite-so-many-length-scale problem, described by the energy $\mathcal{H}'$.

- Large-distance properties of this coarse-grained system are the same as the large-distance properties of the physical system.

- Stat. Mech. of $\mathcal{H}'$ poses a a problem which is easier (less critical).

- The benefits accruing from this procedure may be amplified by repeating it.

- Repeated application of the RGT will eventually result in a coarse-grained $\mathcal{H}$ describing configurations in which ξ is no bigger than the minimum length scale.

- The associated coarse-grained system is far from criticality. Its properties may be reliably computed by mean field or series expansion methods.

- These properties are the desired large-distance properties of the physical system.

- Let us return to the Ising model.

- Generalise it to include other kinds of interactions. eg. products of 2nd neighbour spins with strength J_2 or, 3rd nearest neighbours with strength J_3.

- Can allow a family of exchange couplings J_1,J_2,J_3,..., or $J_a, a = 1, 2, \ldots$ In reduced units, the equivalent coupling strengths are $K_a = J_a/k_BT$. Their values determine uniquely the energy for any given configuration.

- Under the coarse-graining procedure, $\mathcal{H}'$ will be expressible in terms of some new coupling strengths K' describing the interactions amongst the block spin variables

- The RGT states that K'_1 is some function f_1 of all the original couplings:

$$K'_a = f_a(K_1, K_2, \ldots) = f_a(\mathbf{K}),\ a = 1, 2, \ldots$$

where $\mathbf{K} = K_1, K_2, \ldots$

- NB It necessary to allow for other types of interactions because even if we start with only the nearest neighbour coupling in $\mathcal{H}$ the transformation will in general produce others in $\mathcal{H}'$.

Example

- Consider a simple 2D Ising model.

- Simple coarse graining scheme – 'decimation': Divide spins into two sets: $\{s'\}$ form a square lattice of spacing 2, others denoted by $\{\tilde{s}\}$.

- Define an effective energy function $\mathcal{H}'$ for the s' spins by averaging over all possible arrangements of $\tilde{s}$ spins

$$\exp(-\mathcal{H}') = \sum_{\{\tilde{s}\}} \exp(-\mathcal{H}).$$

- The new energy function realizes two basic aims of the renormalisation group method:
  - Long-distance physics still contained in system described by $\mathcal{H}'$ (partition functions are the same)
  - New system is 'further' from criticality because the ratio of correlation length to lattice spacing has been reduced by 1/2

- But how to perform the partial configuration sum?

- This cannot in general be done exactly (except in 1D–see problem set 2).

- Resort to approximations, eg high temperature expansion:

$$\exp(-\mathcal{H}/k_BT) = 1 - \mathcal{H}/k_BT + \frac{1}{2!}(\mathcal{H}/k_BT)^2 + ...$$

- Substitute this into RHS of RG transformation and look for terms which depend on the s' spins after partial summation.

- Find (see notes)

$$K' = K^2 \qquad \dagger$$

- Many other terms and couplings are generated by the higher orders of the high temperature expansion.

- Need to include these to produce reliable values for the T_c and exponents.

- But qualitative picture already emerges from above

- First point is that eq.† has the unstable fixed point $K^* = 1$: the flow of couplings under repeated iteration of eq. † is away from the fixed point,

- At criticality, we must identify $K' = K$ since coarse graining a critical system leaves it critical. Thus $K^* = 1$ is a candidate for the critical point K_c,

$$K_c = J/k_B T_c = 1$$

(In poor agreement with accepted values due to neglect of higher order terms in series expansion)

- Can also get information on critical exponents. Expanding eq. † about $K = K^\star$ we find

$$K' - K^* = 2(K - K^*) + (K - K^*)^2$$

- Close to criticality, can neglect final term.

- Thus deviation of coupling from its fixed point (critical) value is bigger for the new system than it is for the old by a factor of two $\Rightarrow$ reduced temperature is also bigger by a factor of two:

$$t' = 2t$$

- But correlation length is smaller by a factor of 1/2 (by construction):

$$\xi' = \xi/2$$

  Thus, when we double t, we halve ξ, implying that

$$\xi \propto t^{-1}$$

  i.e $\nu = 1$.

Universality

- In order to expose universality, should allow for several different kinds of coupling J_a, and show how systems with *different* J_a can have the *same* critical behaviour.

- Can form a representation of the space of all coupling strengths K_a in the energy function $\mathcal{H}/k_BT$.

- Each "ray" from the origin represents the temperature behaviour of a given model. Points on a ray close to the origin represent the high T behaviour.

- Points far from the origin represent the low T behaviour.

- The critical point is represented by a specific point on this ray, $K_a = J_a/k_B T, a = 1, 2, \ldots$.

- The set of critical points on all of the possible rays forms a *surface*, the critical surface.

- Our immediate goal then is to understand how the RGT can explain why different physical systems near this critical surface have the same behaviour.

- Suppose we start with a physical system, with coupling strengths $K_a, a = 1, 2, \ldots$.

- RGT generate a new point in the figure, at the coupling strengths $K_a^{(1)} = f_a(\mathbf{K})$; these are the couplings appearing in the effective energy function describing the coarse-grained system.

- Repeating the transformation, gives a new $\mathcal{H}'$ with coupling strengths $K_a^{(2)} = f_a(\mathbf{K})$.

  Repeated RGTs $\rightarrow$ a flow of points in the figure: $\mathbf{K} \rightarrow \mathbf{K^{(1)}} \rightarrow \ldots \rightarrow \mathbf{K^{(n)}}$

- Consider the coupling flow for the Ising model at its critical point. L/ξ remains infinite after any finite number of steps.

  The behaviour of the coupling flows tends to a limit, K^*, i.e.

$$K_a^* = f_a(K^*) \quad a = 1, 2.....$$

- This point $\mathbf{K}^* \equiv K_1^*, K_2^*, \ldots$ is therefore a *fixed point* which lies in the critical surface.

- Now consider the Ising model at temperature $T > T_c$;

- New flow appears initially to follow towards the same fixed point.

- However, the flow must eventually move away from the fixed point because each coarse-graining now produces a model further from criticality.

- The resulting flow is represented schematically by one set of black dots and tends to the high temperature fixed point.

- Similarly for $T < T_c$, the flow ultimately converges on the low temeprature fixed point.

- We are now in a position to understand universality within this framework.

- We will suppose that there exists a single fixed point in the critical surface which sucks in all flows starting from a point in that surface.

- Any system at its critical point will exhibit large-length scale physics (large-block spin behaviour) described by the single set of fixed point coupling constants.

- The uniqueness of this limiting set of coupling constants is the essence of critical point universality.