Phase Transitions and Collective Phenomena

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Preface

The fundamental goal of **statistical mechanics** is to provide a framework in which the **microscopic** probabilistic description of systems with large numbers of degrees of freedom (such as the particles which constitute a gas) can be reconciled with the description at the **macroscopic** level (using equilibrium state variables such as pressure, volume and temperature). When we first meet these ideas they are usually developed in parallel with simple examples involving collections of weakly or non-interacting particles. However, strong interactions frequently induce transitions and lead to new equilibrium phases of matter. These phases exhibit their own characteristic fluctuations or elementary excitations known as **collective modes**. Although a description of these phenomena at the microscopic level can be quite complicated, the important large scale, or long-time "hydrodynamic" behaviour is often simple to describe. Phenomenological approaches based on this concept have led to certain **quantum** as well as **classical field theories** that over recent years have played a major role in shaping our understanding of condensed matter and high energy physics.

The goal of this course is to motivate this type of description; to establish and begin to develop a framework in which to describe critical properties associated with classical and quantum phase transitions; and, at the same time, to emphasise the importance and role played by **symmetry** and **topology**. Inevitably there is insufficient time to study such a wide field in any great depth. Instead, the aim will always be to develop fundamental concepts.

The phenomenological **Ginzburg-Landau theory** has played a pivotal rôle in the development of our understanding *critical phenomena* in both classical and quantum statistical mechanics, and much of our discussion will be based on it. The majority of the course will be involved in developing the important concept of **universality** in statistical mechanics and establish a general framework to describe critical phenomena — the **scaling theory** and the **renormalisation group**.

Synopsis

- ▷ INTRODUCTION TO CRITICAL PHENOMENA: Concept of Phase Transitions; Order Parameters; Response Functions; Universality. [1]
- ▷ GINZBURG-LANDAU THEORY: Mean-Field Theory; Critical Exponents; Symmetry Breaking, Goldstone Modes, and the Lower Critical Dimension; Fluctuations and the Upper Critical Dimension; Importance of Correlation Functions; Ginzburg Criterion. [3]
- ▷ SCALING: Self-Similarity; The Scaling Hypothesis; Kadanoff's Heuristic Renormalisation Group (RG); Gaussian Model; Fixed Points and Critical Exponent Identities; Wilson's Momentum Space RG; Relevant, Irrelevant and Marginal Parameters; $^\dagger\epsilon$-expansions. [4]
- ▷ TOPOLOGICAL PHASE TRANSITIONS: Continuous Spins and the Non-linear σ-model; XY-model; Algebraic Order; Topological defects, Confinement, the Kosterlitz-Thouless Transition and †Superfluidity in Thin Films. [2]
- ▷ QUANTUM PHASE TRANSITIONS: Classical/Quantum Mapping; the Dynamical Exponent; Quantum Rotors; †Haldane Gap; †Asymptotic Freedom; †Quantum Criticality. [2]

Material indicated by a † will be included if time allows.

Bibliography

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[10] J. Zinn-Justin, **Phase Transitions and Renormalization Group**, (Oxford Graduate Texts) 2013. *Exceptionally complete mathematical and physical treatment, but perhaps less introductory than the above texts.*

This course follows no particular text but a number of books may be useful. Those which are particularly useful are marked by a "*" in the list. I wish to thank Prof. Simons and Dr Kwasigroch for earlier versions of these notes.

Contents

Chapter 1

Critical Phenomena

The aim of this introductory chapter is to introduce the concept of a phase transition and to motivate the subject of statistical field theory. Here we introduce the concept of universality as applied to critical phenomena and define some of the notation used throughout these lectures.

1.1 Collective Phenomena: from Particles to Fields

It is rare in physics to find examples of *interacting* many-particle systems which admit to a full and accessible microscopic description. More useful is a *hydrodynamic* description of the **collective** long-wavelength behaviour which surrenders information at the microscopic scale. A familiar example is the Navier-Stokes equation of fluid dynamics. The averaged variables appropriate to these length and time scales are no longer the discrete set of particle degrees of freedom but rather slowly varying continuous fields describing the collective motion of a macroscopic set of particles. Familiar examples include magnetic spin-waves, and vibrational or phonon modes of an atomic lattice.

The most striking consequence of interactions among particles is the appearance of new phases of matter whose collective behaviour bears little resemblance to that of a few particles. How do the particles then transform from one macroscopic state to another? Formally, all macroscopic properties can be deduced from the free energy or the partition function. However, since phase transitions typically involve dramatic changes in response functions, they must correspond to singularities in the free energy. Since the canonical partition function of a finite collection of particles is always analytic, phase transitions can only be associated with infinitely many particles, i.e. the **thermodynamic limit**. The study of phase transitions is thus related to finding the origin of various singularities in the free energy and characterising them.

Consider the classical equilibrium statistical mechanics of a regular lattice of an **Ising ferromagnet** (i.e. spin degrees of freedom which can take only two values, ± 1, with short range interactions that favour the spins to be aligned). When viewed microscopically, the development of magnetic moments on the atomic lattice sites of a crystal and the subsequent ordering of the moments is a complex process involving the cooperative phenomena of many interacting electrons. However, remarkably, the thermodynamic properties of different macroscopic ferromagnetic systems are observed to be the same — e.g. temperature dependence of the specific heat, susceptibility, etc. Moreover, the thermodynamic critical properties of completely different physical systems, such as an Ising ferromagnet and a liquid at its boiling point, show the same dependence on, say, temperature. What is the physical origin of this **Universality**?

Suppose we take a ferromagnetic material and measure some of its material properties such as magnetisation. Dividing the sample into two roughly equal halves, keeping the internal variables like temperature and magnetic field the same, the macroscopic properties of each piece will then be the same as the whole. The same holds true if the process is repeated. But eventually, after many iterations, something different must happen because we know that the magnet is made up of electrons and ions. The characteristic length scale at which the overall properties of the pieces begins to differ markedly from those of the original system defines a **correlation length**. It is the typical length scale over which the fluctuations of the microscopic degrees of freedom are correlated.

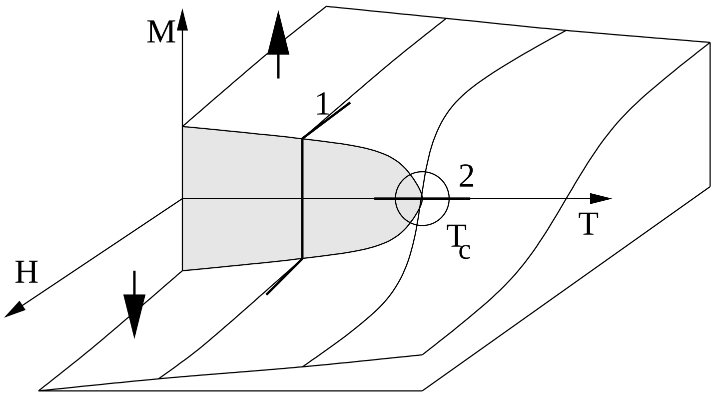


Figure 1.1: Phase diagram of the Ising ferromagnet showing the average magnetisation M as a function of magnetic field H and temperature T. Following trajectory 1 by changing the magnetic field at constant temperature $T < T_c$, the sample undergoes a first order phase transition from a phase in which the average magnetisation is positive (i.e. 'spin-up') to a phase in which the average is negative (i.e. 'spin-down'). Secondly, by changing the temperature at fixed zero magnetic field, the system undergoes a second order phase transition at $T = T_c$ whereupon the average magnetisation grows continuously from zero. This second order transition is accompanied by a **spontaneous symmetry breaking** in which the system chooses to be in either an up or down-spin phase. (Contrast this phase diagram with that of the liquid-gas transition — magnetisation $M \to$ density ρ, and magnetic field $H \to$ pressure.) The circle marks the region in the vicinity of the critical point where the correlation length is large as compared to the microscopic scales of the system, and 'Ginzburg-Landau theory' applies.

Now experience tells us that a ferromagnet may abruptly change its macroscopic behaviour when the external conditions such as the temperature or magnetic field are varied. The points at which this happens are called **critical points**, and they mark a

phase transition from one state to another. In the ferromagnet, there are essentially two ways in which the transition can occur (see Fig. 1.1). In the first case, the two states on either side of the critical point (spin up) and (spin down) coexist at the critical point. Such transitions, involve **discontinuous** behaviour of thermodynamic properties and are termed **first-order** (cf. melting of a three-dimensional solid). The correlation length at such a first-order transition is generally finite.

In the second case, the transition is **continuous**, and the correlation length becomes effectively infinite. Fluctuations become correlated over all distances, which forces the whole system to be in a unique, critical, phase. The two phases on either side of the transition (paramagnetic and ferromagnetic) must become identical as the critical point is approached. Therefore, as the correlation length diverges, the magnetisation goes smoothly to zero. The transition is said to be **second-order**.

The divergence of the correlation length in the vicinity of a second order phase transition suggests that properties near the critical point can be accurately described within an effective theory involving only long-range collective fluctuations of the system. This invites the construction of a phenomenological Hamiltonian or Free energy which is constrained only by the fundamental symmetries of the system. Such a description goes under the name of **Ginzburg-Landau theory**. Although the detailed manner in which the material properties and microscopic couplings of the ferromagnet influence the parameters of the effective theory might be unknown, qualitative properties such as the **scaling** behaviour are completely defined.

From this observation, we can draw important conclusions: critical properties in the vicinity of classical and quantum second order phase transitions fall into a limited number of **universality classes** defined not by detailed material parameters, but by the fundamental symmetries of the system. When we study the critical properties of the transition in an Ising ferromagnet, we learn about the nature of the liquid-gas transition! (See below.) Similarly, in the jargon of statistical field theory, a superconductor, with its complex order parameter, is in the same universality class as the two-component or 'XY Heisenberg' ferromagnet. The analysis of critical properties associated with different universality classes is the subject of **Statistical field theory**.

1.2 Phase Transitions

With these introductory remarks in mind, let us consider more carefully the classic example of a phase transition involving the condensation of a gas into a liquid. The phase diagram represented in Fig. 1.2a exhibits several important and generic features of a second order phase transition:

1. In the (T, P) plane, the phase transition occurs along a line that terminates at a **critical point** (T_c, P_c).

2. In the $(P, v \equiv V/N)$ plane, the transition appears as a **coexistence interval**, corresponding to a mixture of gas and liquid of densities $\rho_g = 1/v_g$ and $\rho_l = 1/v_l$ at temperatures $T < T_c$.

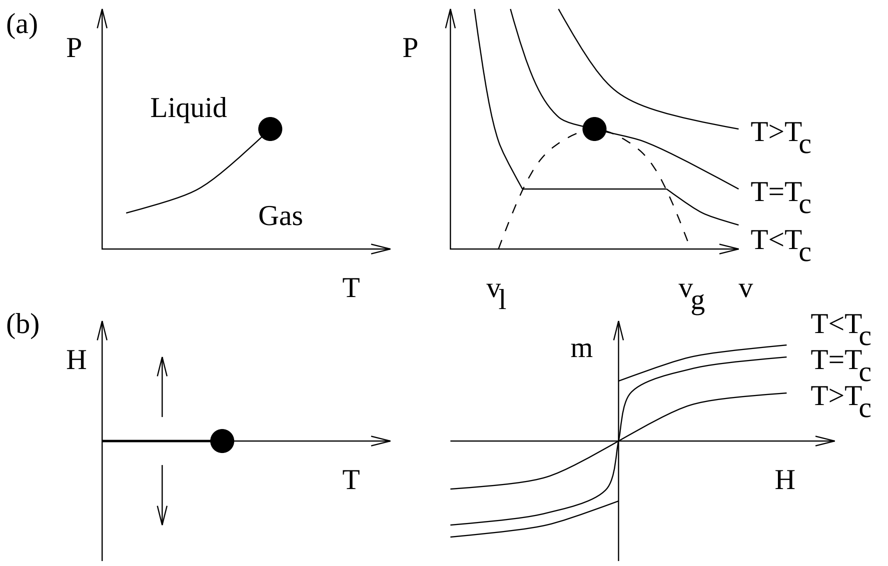


Figure 1.2: Phase diagrams of (a) the liquid-gas transition, and (b) the ferromagnetic transition. In each case the phase diagrams are drawn in two different planes. Notice the similarity between the two ($1/v \leftrightarrow m$, $P \leftrightarrow H$). Isotherms above, below, and at T_c are sketched.

3. Due to the termination of the coexistence line, it is possible to go from the gas phase to the liquid phase continuously (without a phase transition) by going around the critical point. Thus there are no fundamental differences between the liquid and gas phases (i.e. there is no change of fundamental symmetry).

   From a mathematical perspective, the free energy of this system is an analytic function in the (P, T) plane except for some form of branch cut along the phase boundary. Observations in the vicinity of the critical point further indicate that:

4. The difference between the densities of the coexisting liquid and gas phases vanishes on approaching T_c, i.e. $\rho_l \to \rho_g$ as $T \to T_c^-$.

5. The pressure versus volume isotherms become progressively more flat on approaching T_c from the high temperature side. This implies that the **isothermal compressibility**, the rate of change of density with pressure, $\kappa_T = -(1/V)\partial V/\partial P|_T$ diverges as $T \to T_c^+$.

6. The fluid appears "milky" close to criticality. This phenomenon, known as **critical opalescence**, suggests the existence of collective fluctuations in the gas at long enough wavelengths to scatter visible light. These fluctuations must necessarily involve many particles, and a coarse-graining procedure must be appropriate to their description.

How does this phase diagram compare with the phase transition that occurs between paramagnetic and ferromagnetic phases of certain substances such as iron or nickel? These materials become spontaneously magnetised below a Curie temperature, T_c. Redrawn in cross-section, the phase diagram of Fig. 1.1 is shown in Fig. 1.2b. There is a discontinuity in magnetisation as the magnetic field, H goes through zero, and the magnetisation isotherms, $M(H)$ have much in common with the condensation problem. In both cases, a line of discontinuous transitions terminates at a critical point, and the isotherms exhibit singular behaviour in the vicinity of this point. The phase diagram is simpler in appearance because the symmetry $H \to -H$ ensures that the critical point occurs at $H_c = M_c = 0$.

In spite of the apparent similarities between the magnetic and liquid-gas transition, our intuition would suggest that they are quite different. Magnetic transitions are usually observed to be **second-order** — that is, the magnetisation m, which plays the role of an **order parameter**, rises continuously from zero below the transition. On the other hand, our everyday experience of boiling a kettle of water shows the liquid-gas transition to be **first-order** — that is, the order parameter, corresponding to the difference between the actual density and the density at the critical point, $\rho - \rho_c$, jumps discontinuously at the critical point with an accompanying absorption of latent heat of vapourisation (implying a discontinuous jump in the entropy of the system: $Q_L = T_c \Delta S$).

However, the perceived difference in behaviour simply reflects different paths through the transition in the two cases. In a ferromagnet, the natural experimental path ($b \to c \to d$ in Fig. 1.3a) is one in which the external magnetic field takes the value $H = 0$. For $T > T_c$, the average magnetisation is zero, while for $T < T_c$ the magnetisation grows continuously from zero. In a liquid, the natural path is one in which temperature is varied at constant pressure ($b' \to c' \to d'$ in Fig. 1.3b). Along this path, there is a discontinuous change in the density. This is the first-order boiling transition.

A path in the ferromagnetic (H, T) plane analogous to the constant pressure path in a fluid is shown in Fig. 1.3c. Along this path m is negative from $b' \to c'$ and then jumps discontinuously to a positive value as the coexistence line is crossed and remains positive from $c' \to d'$. It is clear that the path in a fluid that most closely resembles the $H = 0$ path in a magnet, which shows a second-order transition, is the one with density fixed at its critical value ρ_c, i.e. the **critical isochore** ($b \to c \to d$ in Fig. 1.3d).

†**The Lattice-Gas model**: We can directly show the equivalence between the Ising ferromagnet and a lattice gas model. Consider a classical three dimensional gas of N particles in a volume V and subject to the Hamiltonian

$$H = \sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{2m} + \frac{1}{2} \sum_{ij} u(\mathbf{r}_i - \mathbf{r}_j).$$

By integrating over the phase space configurations of the particles, the grand partition function $\Theta = \mathrm{tr}\, e^{-\beta(H - \mu N)}$ can be written as

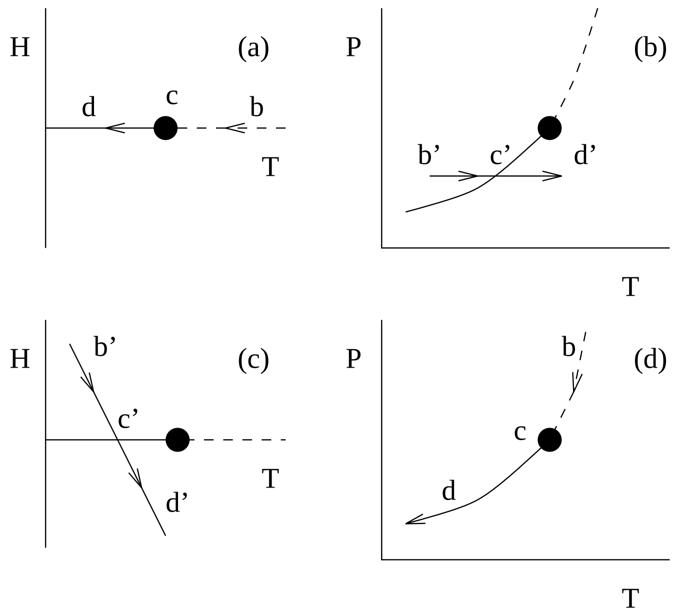


Figure 1.3: Comparison of the ferromagnetic phase transition with the liquid-gas transition. The different paths identified in the figure are discussed in the text.

$$\Theta = \sum_{N=0}^{\infty} \frac{1}{N!} \left(\frac{e^{\beta\mu}}{\lambda^3}\right)^N \int \prod_{i=1}^{N} d^3\mathbf{r}_i \exp\left[-\frac{\beta}{2}\sum_{ij} u(\mathbf{r}_i - \mathbf{r}_j)\right],$$

where μ denotes the chemical potential, and $\lambda = h/(2\pi mkT)^{1/2}$.

The volume V is now subdivided into $N_s = V/a^3$ cells of volume a^3 (N_s is not to be confused with N), with spacing a chosen small enough so that each cell α is either empty or occupied by *one* particle; i.e., the cell occupation number n_α is restricted to 0 or 1 ($\alpha = 1, 2, \cdots N$). After approximating the integrals $\int d^3\mathbf{r}$ by sums $a^3 \sum_{\alpha=1}^{N_s}$, the grand canonical partition function becomes

$$\Theta \approx \sum_{\{n_\alpha=0,1\}} \left(\frac{a^3 e^{\beta\mu}}{\lambda^3}\right)^{\sum_\alpha n_\alpha} \exp\left[-\frac{\beta}{2}\sum_{\alpha,\beta}^{N_s} n_\alpha n_\beta u(\mathbf{r}_\alpha - \mathbf{r}_\beta)\right].$$

By setting $n_\alpha = (1 + \sigma_\alpha)/2$ and approximating the potential by $u(\mathbf{r}_\alpha - \mathbf{r}_\beta) = -J$ for nearest-neighbours only, the model becomes identical to the Ising ferromagnet with discrete spins $\sigma_\alpha \pm 1$.

$$\Theta = \sum_{\sigma_\alpha \pm} \exp\left[h \sum_{\alpha} \sigma_\alpha - \frac{\beta J}{4} \sum_{<\alpha\beta>} \sigma_\alpha \sigma_\beta\right], \tag{1.1}$$

where $h = \ln\left(\frac{a^3}{\lambda^3}\right) + \beta\mu - \frac{3}{2}J\beta$ is the effective magnetic field. Using Maxwell's relation

$$\left(\frac{\partial\mu}{\partial V}\right)_{N,T} = -\left(\frac{\partial p}{\partial N}\right)_{V,T}, \tag{1.2}$$

and from the fact that in the thermodynamic limit the variables are only functions of the particle density $\rho = \frac{N}{V}$, we can relate the isothermal compressibility to the ferromagnetic susceptibility

$$\rho\left(\frac{\partial\rho}{\partial p}\right)_T = \left(\frac{\partial\rho}{\partial\mu}\right)_T = \frac{2V}{T}\left(\frac{\partial m}{\partial h}\right)_T \sim (T-T_c)^{-\gamma}, \tag{1.3}$$

which has a power law divergence at the critical temperature $T = T_c$. The magnetisation m is given by $m = 2\rho V - N_s$. Note that the left and right hand sides of the above equation are evaluated at $h = 0$. In fact, since the chemical potential $\mu(T,p)$ can be expressed as a function of temperature and pressure, the following relation serves to define p_c at each temperature T

$$h = \ln\left(\frac{a^3}{\lambda^3}\right) + \beta\mu(T,p_c) - \frac{3}{2}J\beta = 0. \tag{1.4}$$

Using the relation $\left(\frac{\partial\mu}{\partial p}\right)_T = \frac{1}{\rho}$, we can expand h around $p = p_c$

$$h = \frac{\beta}{\rho_c}\left(p - p_c\right). \tag{1.5}$$

Further, note that the spontaneous magnetisation can be related to the shape of the *coexistence curve*

$$\rho_g - \rho_l = \frac{m}{V} \sim (T_c - T)^{\beta}, \tag{1.6}$$

which rises with a power law below the critical temperature.

Comment: This type of manifest equivalence is usually quite straightforward. The equivalence premised on the Universality Principle, with respect to quantitative critical properties, connects systems which cannot be straightforwardly mapped onto each other.

1.3 Critical Behaviour

The singular behaviour in the vicinity of the critical point is characterised by a set of **critical exponents**. These exponents describe the non-analyticity of various thermodynamic functions. Remarkably transitions as different as the liquid/gas and ferromagnetic transition can be described by the same set of critical exponents and are said to belong to the same **Universality class**.

1.3.1 Significance of Power laws

▷ INFO: Prior to defining physically relevant critical exponents, we take a mathematical digression in probability theory. First consider an exponential probability density function

$$p(x) = ae^{-ax}$$

for $x > 0$. The mean $\langle x\rangle = 1/a$ and mean squared $\langle x^2\rangle = 2/a$. So, for this distribution the *typical* scale is $1/a$ with typical fluctuations of $1/a$. Now, consider a power law distribution

$$p(x) \sim \frac{1}{x^{1+\mu}}.$$

For $\mu \leq 1$ the mean diverges $\langle x\rangle \to \infty$, which implies that there is no typical size. Also for $\mu \leq 2$, $\langle x^2\rangle \to \infty$ so flucluations are also unbounded. Such power laws distributions have no typical size and are thus scale invariant. They also have fluctuations or structure at all length scales.

Those critical exponents most commonly encountered are defined below.

1.3.2 Order Parameter

By definition, there is more than one equilibrium phase on a coexistence line. As mentioned above, the **order parameter** is a thermodynamic function that is different in each phase, and hence can be used to distinguish between them. For a (uniaxial) magnet, the order parameter is provided by the total magnetisation $M(H, T)$, or magnetisation density,

$$\boxed{m(H, T) = \frac{M(H, T)}{V}.}$$

In zero field, m vanishes for a paramagnet and is non-zero in a ferromagnet (see Fig. 1.4), i.e.

$$\boxed{m(T, H \to 0^+) \propto \begin{cases} 0 & T > T_c, \\ |t|^\beta & T < T_c, \end{cases}}$$

where $t = (T - T_c)/T_c$ denotes the **reduced temperature**. The singular behaviour of the order parameter along the coexistence line is therefore characterised by a critical exponent β. The singular behaviour of m along the critical isotherm is governed by another exponent, δ (see Fig. 1.2)

$$\boxed{m(T = T_c, H) \propto H^{1/\delta}.}$$

The two phases along the liquid-gas coexistence line are distinguished by their density allowing one to define $\rho - \rho_c$, where ρ_c denotes the critical density, as the order parameter.

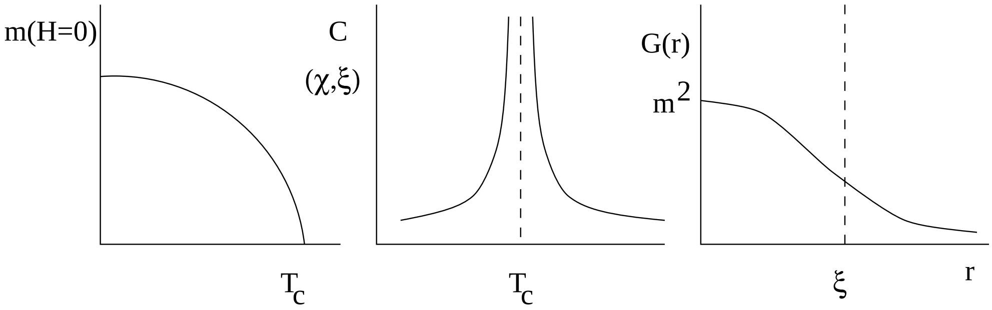


Figure 1.4: Critical behaviour of the magnetisation and response functions close to the ferromagnetic transition.

1.3.3 Response Functions

The critical system is highly sensitive to external perturbations: for example, at the liquid-gas critical point, the compressibility $\kappa_T = -(1/V)\partial V/\partial P|_T$ becomes infinite. The divergence of the compressibility or, more generally, the **susceptibility** of the system (i.e. the response of the order parameter to a field conjugate to it) is characterised by another critical exponent γ. For example, in a magnet, the analogous quantity is the zero-field **susceptibility**

$$\boxed{\chi_\pm(T, H \to 0^+) = \frac{\partial m}{\partial H}\bigg|_{H=0^+} \propto |t|^{-\gamma_\pm},}$$

where, in principle, two exponents γ_+ and γ_- are necessary to describe the divergences on the two sides of the phase transition. Actually, in almost all cases, the same singularity governs both sides, and $\gamma_+ = \gamma_- = \gamma$.

Similarly, the **heat capacity** represents the thermal response function, and its singularities at zero field are described by the exponent α,

$$\boxed{C_\pm = \frac{\partial E}{\partial T} \propto |t|^{-\alpha_\pm},}$$

where E denotes the internal energy and, again, the exponents usually coincide $\alpha_+ = \alpha_- = \alpha$.

1.3.4 Long-range Correlations

Since the response functions are related to equilibrium fluctuations, their divergence in fact implies that fluctuations are correlated over long distances. To see this let us consider the magnetic susceptibility of, say, the **Ising ferromagnet**. The latter describes a lattice of scalar or two-valued spins which interact ferromagnetically with their neighbours. Starting with the microscopic Ising Hamiltonian

$$H_{\text{Ising}} = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j,$$

where $\{\sigma_i = \pm 1\}$ denotes the set of Ising spins, $M = \sum_i \sigma_i$ represents the total magnetisation, and the sum $\sum_{\langle ij\rangle}$ runs over neighbouring lattice sites. The total partition function takes the form[1]

$$\boxed{\mathcal{Z}(T,h) = \sum_{\{\sigma_i\}} e^{-\beta(H_{\text{Ising}} - hM)}.}$$

Here we have included an external magnetic field h, and the sum extends over the complete set of microstates $\{\sigma_i\}$. From $\mathcal{Z}$, the thermal average magnetisation can be obtained from the equation

$$\boxed{\langle M\rangle \equiv \frac{\partial \ln \mathcal{Z}}{\partial(\beta h)} = \frac{1}{\mathcal{Z}} \sum_{\{\sigma_i\}} M e^{-\beta(H_{\text{Ising}} - hM)}}.$$

Taking another derivative one obtains the susceptibility

$$\chi(T,h) = \frac{1}{V}\frac{\partial \langle M\rangle}{\partial h} = \frac{\beta}{V}\left\{\frac{1}{\mathcal{Z}}\sum_{\{\sigma_i\}} M^2 e^{-\beta(H_{\text{Ising}} - hM)} - \left(\frac{1}{\mathcal{Z}}\sum_{\{\sigma_i\}} M e^{-\beta(H_{\text{Ising}} - hM)}\right)^2\right\}$$

which gives the relation

$$\boxed{\frac{V\chi}{\beta} = \text{var}(M) \equiv \langle M^2\rangle - \langle M\rangle^2.}$$

Now the overall magnetisation can be thought of as arising from separate contributions from different parts of the system, i.e. taking a continuum limit

$$M = \int d\mathbf{x}\; m(\mathbf{x}),$$

where $m(\mathbf{x})$ represents the "local" magnetisation. Substituting this definition into the equation above we obtain

$$k_B T\chi = \frac{1}{V}\int d\mathbf{x} \int d\mathbf{x}' \left[\langle m(\mathbf{x}) m(\mathbf{x}')\rangle - \langle m(\mathbf{x})\rangle \langle m(\mathbf{x}')\rangle\right].$$

Since the system is symmetric under spatial translation, $\langle m(\mathbf{x})\rangle$ is a constant m independent of position, while $\langle m(\mathbf{x})m(\mathbf{x}')\rangle = G(\mathbf{x}-\mathbf{x}')$ depends only on the spatial separation. Thus, in terms of the '**connected**' correlation function defined as $G_c(\mathbf{x}) \equiv \langle m(\mathbf{x})m(0)\rangle_c \equiv \langle m(\mathbf{x})m(0)\rangle - m^2$, the susceptibility is given by

$$\boxed{k_B T\chi = \int d\mathbf{x}\; \langle m(\mathbf{x})m(0)\rangle_c.}$$

[1] Throughout these notes $1/k_BT$ and the symbol β (not to be mistaken for the order parameter exponent) will be used interchangeably.

The connected correlation function is a measure of how the local fluctuations in one part of the system affect those in another. Typically such influences occur over a characteristic distance ξ known as the **correlation length** (see Fig. 1.4). (In many cases, the connected correlation function $G_c(\mathbf{x})$ decays exponentially $\exp[-|\mathbf{x}|/\xi]$ at separations $|\mathbf{x}| > \xi$.) If $g \sim m^2$ denotes a typical value of the correlation function for $|\mathbf{x}| < \xi$, it follows that $k_B T\chi < g\xi^d$ where d denotes the dimensionality of the system; the divergence of χ necessarily implies the divergence of ξ. This divergence of the correlation length also explains the observation of **critical opalescence**. The correlation function can be measured by scattering probes, and its divergence

$$\boxed{\xi_\pm(T, H=0) \propto |t|^{-\nu_\pm}}$$

is controlled by exponents $\nu_+ = \nu_- = \nu$.

This completes our preliminary survey of phase transitions and critical phenomena. We found that the singular behaviour of thermodynamic functions at a critical point (the termination of a coexistence line) can be characterised by a set of critical exponents. Experimental observations indicate that these exponents are **universal**, independent of the material, and to some extent of the nature of the transition. Moreover the divergence of the response functions, as well as fluctuations, indicate that correlations become long-ranged in the vicinity of this point. The fluctuations responsible for the correlations involve many particles, and their description calls for a "coarse-graining" approach. In the next chapter we will exploit this idea to construct a **statistical field theory** which reveals the origin of the universality. To do so it will be convenient to frame our discussion in the language of magnetic systems whose symmetry properties are transparent. The results, however, have a much wider range of validity.

Chapter 2

Ginzburg-Landau Phenomenology

The divergence of the correlation length in the vicinity of a second-order phase transition indicates that the properties of the critical point are insensitive to microscopic details of the system. This redundancy of information motivates the search for a phenomenological description of critical phenomena which is capable of describing a wide range of model systems. In this chapter we introduce and investigate such a phenomenology known as the Ginzburg-Landau theory. Here we will explore the 'mean-field' properties of the equilibrium theory and investigate the influence of spatial fluctuations.

2.1 Ginzburg-Landau Theory

Consider the magnetic properties of a metal, say iron, close to its Curie point. The microscopic origin of magnetism is quantum mechanical, involving such ingredients as itinerant electrons, their spin, and the exclusion principle. Clearly a microscopic description is complicated, and material dependent. Such a theory would be necessary if we are to establish which elements are likely to produce ferromagnetism. However, if we accept that such behaviour exists, a microscopic theory is not necessarily the most useful way to describe its disappearance as a result of thermal fluctuations. This is because the (quantum) statistical mechanics of a collection of interacting electrons is excessively complicated. However, the degrees of freedom which describe the transition are long-wavelength collective excitations of spins. We can therefore "coarse-grain" the magnet to a scale much larger than the lattice spacing, and define a magnetisation vector field $\mathbf{m}(\mathbf{x})$, which represents the *average* of the elemental spins in the vicinity of a point $\mathbf{x}$. It is important to emphasise that, while $\mathbf{x}$ is treated as a continuous variable, the functions $\mathbf{m}$ do not exhibit any variations at distances of the order of the lattice spacing a, i.e. their Fourier transforms involve wavevectors with magnitude less than some upper cut-off $\Lambda \sim 1/a$.

In describing other types of phase transitions, the role of $\mathbf{m}(\mathbf{x})$ is played by the appropriate order parameter. For this reason it is useful to examine a generalised magnetisation vector field involving n-component magnetic moments existing in a d-dimensional space, i.e.

$$\mathbf{x} \equiv (x_1, \cdots x_d) \in \mathbb{R}^d \quad \text{(space)}, \qquad \mathbf{m} \equiv (m_1, \cdots m_n) \in \mathbb{R}^n \quad \text{(spin)}.$$

Some specific problems covered in this framework include:

$n = 1$: Liquid-gas transitions; binary mixtures; and uniaxial magnets;

$n = 2$: Superfluidity; superconductivity; and planar magnets;

$n = 3$: Classical isotropic magnets.

While most applications occur in three-dimensions, there are also important phenomena on surfaces ($d = 2$), and in wires ($d = 1$). (Relativistic field theory is described by a similar structure, but in $d = 4$.)

A general coarse-grained Hamiltonian can be constructed on the basis of appropriate symmetries:

1. **Locality**: The Hamiltonian should depend on the local magnetisation and short range interactions expressed through gradient expansions:

$$\beta H = \int d\mathbf{x}\; f[\mathbf{m}(\mathbf{x}), \nabla\mathbf{m}, \cdots]$$

2. **Rotational Symmetry**: Without magnetic field, the Hamiltonian should be isotropic in space and therefore invariant under rotations, $\mathbf{m} \mapsto \mathbf{R}_n\mathbf{m}$.

$$\beta H[\mathbf{m}] = \beta H[\mathbf{R}_n\mathbf{m}].$$

3. **Translational and Rotational Symmetry in x**: This last constraint finally leads to a Hamiltonian of the form

$$\beta H = \int d\mathbf{x}\; \Big[\tfrac{t}{2}\mathbf{m}^2 + u\mathbf{m}^4 + \cdots + \tfrac{K}{2}(\nabla\mathbf{m})^2 + \tfrac{L}{2}(\nabla^2\mathbf{m})^2 + \tfrac{N}{2}\mathbf{m}^2(\nabla\mathbf{m})^2 + \cdots - \mathbf{h}\cdot\mathbf{m}\Big]. \quad (2.1)$$

(Recall that, as we are primarily interested in transitions between different phases and the fields are the order parameters of these transitions, we can work close enough to the critical point to be able to assume that the magnitude of the fields and of their derivatatives are small and can be expanded upon.) Equation (2.1) is known as the **Ginzburg-Landau Hamiltonian**. It depends on a set of *phenomenological* parameters t, u, K, etc. which are *non-universal* functions of microscopic interactions, *as well as external parameters such as temperature, and pressure.*[1]

[1]It is essential to appreciate the latter point, which is usually the source of much confusion. The probability for a particular configuration of the field is given by the Boltzmann weight $\exp\{-\beta H[\mathbf{m}(\mathbf{x})]\}$. This does NOT imply that all terms in the exponent are proportional to $(k_BT)^{-1}$. Such dependence

2.2 Landau Mean-Field Theory

The original problem has been simplified considerably by focusing on the coarse-grained magnetisation field described by the Ginzburg-Landau Hamiltonian. The various thermodynamic functions (and their singular behaviour) can now be obtained from the corresponding partition function

$$\boxed{\mathcal{Z}[T,\mathbf{h}] = \int D\mathbf{m}(\mathbf{x})\ e^{-\beta H[\mathbf{m},\mathbf{h}]}} \tag{2.2}$$

Since the degrees of freedom appearing in the Hamiltonian are functions of $\mathbf{x}$, the symbol $\int D\mathbf{m}(\mathbf{x})$ refers to the **functional integral**. As such, it should be regarded as a limit of discrete integrals, i.e., for a one-dimensional Hamiltonian,

$$\int D\mathbf{m}(\mathbf{x})\ z[\mathbf{m}(\mathbf{x}), \partial\mathbf{m}, \cdots] \equiv \lim_{a\to 0, N\to\infty} \int \prod_{i=1}^{N} d\mathbf{m}_i\ z[\mathbf{m}_i, (\mathbf{m}_{i+1} - \mathbf{m}_i)/a, \cdots].$$

In general, evaluating the functional integral is not straightforward. However, we can obtain an estimate of $\mathcal{Z}$ by applying a saddle-point or mean-field approximation to the functional integral

$$\boxed{\mathcal{Z}[T,\mathbf{h}] \equiv e^{-\beta F[T,\mathbf{h}]}, \qquad \beta F[T,\mathbf{h}] \simeq \min_{\mathbf{m}} \left[\beta H\left[\mathbf{m},\mathbf{h}\right]\right],}$$

where $\min_{\mathbf{m}}[\beta H[\mathbf{m},\mathbf{h}]]$ represents the minimum of the function with respect to variations in $\mathbf{m}$. Such an approach is known as **Landau mean-field theory**. For $K > 0$, the minimum free energy occurs for a uniform vector field $\mathbf{m}(\mathbf{x}) \equiv \bar{m}\hat{\mathbf{e}}_h$, where $\hat{\mathbf{e}}_h$ points along the direction of the magnetic field, and $\bar{m}$ is obtained by minimizing the **Landau free energy density**

$$f(m,h) \equiv \frac{\beta F}{V} = \tfrac{t}{2}m^2 + um^4 - hm$$

In the vicinity of the critical point $\bar{m}$ is small, and we are justified in keeping only the lowest powers in the expansion of $f(m,h)$. The behaviour of $f(m,h)$ depends sensitively on the sign of t (see Fig. 2.1).

1. For $t > 0$ the quartic term can be ignored, and the minimum occurs for $\bar{m} \simeq h/t$. The vanishing of the magnetisation as $h \to 0$ signals paramagnetic behaviour, and the zero-field susceptibility $\chi \sim 1/t$ diverges as $t \to 0$.

holds only for the true microscopic Hamiltonian. The Ginzburg-Landau Hamiltonian is more accurately regarded as an effective free energy obtained by integrating over the microscopic degrees of freedom (coarse-graining), while constraining their average to $\mathbf{m}(\mathbf{x})$. It is precisely because of the difficultly of carrying out such a first principles program that we postulate the form of the resulting effective free energy on the basis of symmetries alone. The price we pay is that the phenomenological parameters have an unknown functional dependence on the original microscopic parameters, as well as on external constraints such as temperature (since we have to account for the entropy of the short distance fluctuations lost in the coarse-graining procedure).

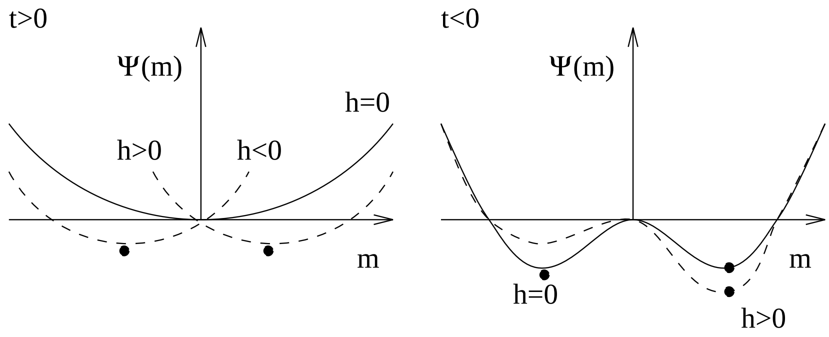


Figure 2.1: Schematic diagram of the mean-field Landau free energy.

2. For $t < 0$ a quartic term with a positive value of u is required to ensure stability (i.e. to keep the magnetisation finite). The function $f(m, h)$ now has degenerate minima at a non-zero value of $\bar{m}$. At $h = 0$ there is a *spontaneous breaking of rotational symmetry in spin space* indicating ordered or ferromagnetic behaviour. Switching on an infinitesimal field h leads to a realignment of the magnetisation along the field direction and breaks the degeneracy of the ground state.

Thus a saddle-point evaluation of the Ginzburg-Landau Hamiltonian suggests paramagnetic behaviour for $t > 0$, and ferromagnetic behaviour for $t < 0$. Without loss of generality (i.e. by adjusting the scale of the order parameter), we can identify the parameter t with the reduced temperature $t = (T - T_c)/T_c$. More generally, we can map the phase diagram of the Ginzburg-Landau Hamiltonian to that of a magnet by setting

$$\begin{aligned} t(T, \cdots) &= (T - T_c)/T_c + O(T - T_c)^2, \\ u(T, \cdots) &= u_0 + u_1(T - T_c) + O(T - T_c)^2, \\ K(T, \cdots) &= K_0 + K_1(T - T_c) + O(T - T_c)^2, \end{aligned}$$

where u_0, K_0 are unknown positive constants depending on material properties of the system. With this identification, let us determine some of the thermodynamical properties implied by the mean-field analysis.

▷ **Magnetisation**: An explicit expression for the average magnetisation $\bar{m}$ can be found from the stationary condition

$$\left.\frac{\partial f}{\partial m}\right|_{m=\bar{m}} = 0 = t\bar{m} + 4u\bar{m}^3 - h.$$

In zero magnetic field we find

$$\boxed{\bar{m} = \begin{cases} 0 & t > 0, \\ \sqrt{-t/4u} & t < 0, \end{cases}}$$

which implies a universal exponent of $\beta = 1/2$, while the amplitude is material dependent.

▷ **Heat Capacity**: For $h = 0$, the free energy density is given by

$$\boxed{f(m, h = 0) \equiv \frac{\beta F}{V}\bigg|_{h=0} = \begin{cases} 0 & t > 0, \\ -t^2/16u & t < 0. \end{cases}}$$

Thus, by making use of the identities

$$E = -\frac{\partial \ln \mathcal{Z}}{\partial \beta}, \qquad \frac{\partial}{\partial \beta} = -k_B T^2 \frac{\partial}{\partial T} \simeq -k_B T_c \frac{\partial}{\partial t},$$

the singular contribution to the heat capacity is found to be

$$\boxed{C_{\text{sing.}} = \frac{\partial E}{\partial T} = \begin{cases} 0, & t > 0, \\ k_B/8u & t < 0. \end{cases}}$$

This implies that the specific heat exponents $\alpha_+ = \alpha_- = 0$. In this case we observe only a discontinuity in the singular part of the specific heat. However, notice that by including higher order terms, we can in principle obtain non-zero critical exponents.

▷ **Susceptibility**: The magnetic response is characterised by the (longitudinal) susceptibility

$$\boxed{\chi_l \equiv \frac{\partial \bar{m}}{\partial h}\bigg|_{h=0}, \qquad \chi_l^{-1} = \frac{\partial h}{\partial \bar{m}}\bigg|_{h=0} = t + 12u\bar{m}^2\Big|_{h=0} = \begin{cases} t & t > 0, \\ -2t & t < 0, \end{cases}}$$

which, as a measure of the variance of the magnetisation, must be positive. From this expression, we can deduce the critical exponents $\gamma_+ = \gamma_- = 1$. Although the amplitudes are parameter dependent, their ratio $\chi_l^+/\chi_l^- = 2$ is also universal.

▷ **Equation of State**: Finally, on the critical isotherm, $t = 0$, the magnetisation behaves as

$$\boxed{\bar{m} = \left(\frac{h}{4u}\right)^{1/3} \sim h^{1/\delta}.}$$

giving the exponent $\delta = 3$.

This completes our survey of the critical properties of the Ginzburg-Landau theory in the Landau mean-field approximation. To cement these ideas one should attempt to find the mean-field critical exponents associated with a **tricritical point** (see, for example, the first problem set).To complement these notes it is also useful to refer to Section 4.2 (p151–154) of Chaikin and Lubensky on Landau theory.

Landau mean-field theory accommodates only the minimum energy configuration. To test the validity of this approximation scheme, and to determine spatial correlations it is necessary to take into account configurations of the field $\mathbf{m}(\mathbf{x})$ involving spatial fluctuations. However, before doing so, it is first necessary to acquire some familiarity with the method of Gaussian functional integration, the basic machinery of statistical (and quantum) field theory.

2.3 Gaussian and Functional Integration

▷ INFO: Before defining the Gaussian functional integral, it is useful to recall some results involving integration over discrete variables. We begin with the Gaussian integral involving a single (real) variable ϕ,

$$\mathcal{Z}_1 = \int_{-\infty}^{\infty} d\phi \ \exp\left[-\frac{\phi^2}{2G} + h\phi\right] = \sqrt{2\pi G} \ \exp\left[\frac{Gh^2}{2}\right].$$

Now derivatives of $\mathcal{Z}_1$ on h generate Gaussian integrals involving powers of ϕ. Thus, if the integrand represents the probability distribution of a random variable ϕ, logarithmic derivatives can be used to generate moments ϕ. In particular,

$$\langle\phi\rangle \equiv \frac{\partial \ln \mathcal{Z}_1}{\partial h} = hG.$$

Subjecting $\ln \mathcal{Z}_1$ to a second derivative obtains (exercise)

$$\frac{\partial^2 \ln \mathcal{Z}_1}{\partial h^2} = \langle\phi^2\rangle - \langle\phi\rangle^2 = G.$$

Note that, in general, the second derivative does not simply yield the second moment. In fact it obtains an object known as the ‘second cumulant’, the physical significance of which will become clear later. However, in the present case, it is simple to deduce from the expansion, $\langle\phi\rangle = hG$, and $\langle\phi^2\rangle = h^2G^2 + G$.

Higher moments are more conveniently expressed by the **cumulant expansion**[2]

$$\boxed{\langle\phi^r\rangle_c = \frac{\partial^r}{\partial k^r}\Big|_{k=0} \ln\left\langle e^{k\phi}\right\rangle}$$

Applied to the first two cumulants, one obtains $\langle\phi\rangle_c = \langle\phi\rangle = hG$, and $\langle\phi^2\rangle_c = \langle\phi^2\rangle - \langle\phi\rangle^2 = G$ (as above), while $\langle\phi^r\rangle_c = 0$ for $r > 2$. The average $\langle e^{k\phi}\rangle$ is known as the **moment generating function**.

Gaussian integrals involving N (real) variables

$$\mathcal{Z}_N = \int_{-\infty}^{\infty} \prod_{i=1}^{N} d\phi_i \exp\left[-\frac{1}{2}\phi^T \mathbf{G}^{-1}\phi + \mathbf{h}\cdot\phi\right], \tag{2.3}$$

can be reduced to a product of N one-dimensional integrals by diagonalising the (real symmetric) matrix $\mathbf{G}^{-1}$. (Convergence of the Gaussian integration is assured only when the eigenvalues are positive definite.) Denoting the unitary matrices that diagonalise $\mathbf{G}$ by $\mathbf{U}$, the matrix

[2] The moments are related to the cumulants by the identity

$$\langle\phi^n\rangle = \sum_P \prod_\alpha \langle\phi^{n_\alpha}\rangle_c,$$

where $\sum_P$ represents the sum over all partitions of the product ϕ^n into subsets ϕ^{n_α} labelled by α.

$\widetilde{\mathbf{G}}^{-1} = \mathbf{U}\mathbf{G}^{-1}\mathbf{U}^{-1}$ represents the diagonal matrix of eigenvalues. Making use of the identity (i.e. completing the square)

$$\frac{1}{2}\phi^T\mathbf{G}^{-1}\phi - \mathbf{h}\cdot\phi = \frac{1}{2}\chi^T\widetilde{\mathbf{G}}^{-1}\chi - \frac{1}{2}\mathbf{h}^T\mathbf{U}^{-1}\widetilde{\mathbf{G}}\mathbf{U}\mathbf{h},$$

where $\chi = \mathbf{U}\phi - \widetilde{\mathbf{G}}\mathbf{U}\mathbf{h}$, and changing integration variables (since the transformation is unitary, the corresponding Jacobian is unity) we obtain

$$\begin{aligned}\mathcal{Z}_N &= \int_{-\infty}^{\infty}\prod_{i=1}^{N} d\chi_i \exp\left[-\frac{1}{2}\chi^T\widetilde{\mathbf{G}}^{-1}\chi + \frac{1}{2}\mathbf{h}^T\mathbf{U}^{-1}\widetilde{\mathbf{G}}\mathbf{U}\mathbf{h}\right],\\ &= \det(2\pi\mathbf{G})^{1/2}\exp\left[\frac{1}{2}\mathbf{h}^T\mathbf{G}\mathbf{h}\right].\end{aligned} \tag{2.4}$$

Regarding $\mathcal{Z}_N$ as the partition function of a set of N Gaussian distributed random variables, $\{\phi_i\}$, the corresponding cumulant expansion is generated by

$$\boxed{\langle\phi_i\cdots\phi_j\rangle_c = \frac{\partial}{\partial k_i}\cdots\frac{\partial}{\partial k_j}\bigg|_{\mathbf{k}=0}\ln\left\langle e^{\mathbf{k}\cdot\phi}\right\rangle,}$$

where the moment generatingfunction is equal to

$$\boxed{\left\langle e^{\mathbf{k}\cdot\phi}\right\rangle = \exp\left[\mathbf{h}^T\mathbf{G}\mathbf{k} + \frac{1}{2}\mathbf{k}^T\mathbf{G}\mathbf{k}\right].} \tag{2.5}$$

Applying this result we find that the first two cumulants are given by

$$\langle\phi_i\rangle_c = \sum_j G_{ij}h_j, \qquad \langle\phi_i\phi_j\rangle_c = G_{ij}, \tag{2.6}$$

while, as for the case $N = 1$, cumulants higher than the second vanish. The latter is a unique property of Gaussian distributions. Applying Eq. (2.5), we can further deduce the important result that for any linear combination of Gaussian distributed variables $A = \mathbf{a}\cdot\phi$,

$$\boxed{\langle e^A\rangle = e^{\langle A\rangle_c + \langle A^2\rangle_c/2}.}$$

Now Gaussian **functional integrals** are a limiting case of the above. Consider the points i as the sites of a d-dimensional lattice and let the spacing go to zero. In the continuum limit, the set $\{\phi_i\}$ translates to a function $\phi(\mathbf{x})$, and the matrix G_{ij}^{-1} is replaced by an **operator** kernel or **propagator** $G^{-1}(\mathbf{x},\mathbf{x}')$. The natural generalisation of Eq. (2.4) is

$$\begin{aligned}&\int D\phi(\mathbf{x})\exp\left[-\frac{1}{2}\int d\mathbf{x}\int d\mathbf{x}'\ \phi(\mathbf{x})\ G^{-1}(\mathbf{x},\mathbf{x}')\ \phi(\mathbf{x}') + \int d\mathbf{x}\ h(\mathbf{x})\phi(\mathbf{x})\right]\\ &\qquad\qquad \propto (\det\hat{\mathbf{G}})^{1/2}\exp\left[\frac{1}{2}\int d\mathbf{x}\int d\mathbf{x}'\ h(\mathbf{x})\ G(\mathbf{x},\mathbf{x}')\ h(\mathbf{x}')\right],\end{aligned}$$

where the inverse kernel $G(\mathbf{x},\mathbf{x}')$ satisfies the equation

$$\boxed{\int d\mathbf{x}'\ G^{-1}(\mathbf{x},\mathbf{x}')\ G(\mathbf{x}',\mathbf{x}'') = \delta^d(\mathbf{x}-\mathbf{x}'').} \tag{2.7}$$

The notation $D\phi(\mathbf{x})$ is used to denote the measure of the functional integral. Although the constant of proportionality $(2\pi)^N$ left out is formally divergent in the thermodynamic limit, it does not affect averages that are obtained from derivatives of such integrals. For Gaussian distributed functions, Eq. (2.6) then generalises to

$$\boxed{\langle\phi(\mathbf{x})\rangle_c = \int d\mathbf{x}\; G(\mathbf{x},\mathbf{x}')\; h(\mathbf{x}'), \qquad \langle\phi(\mathbf{x})\phi(\mathbf{x}')\rangle_c = G(\mathbf{x},\mathbf{x}').}$$

Later, in dealing with small fluctuations in the Ginzburg-Landau Hamiltonian, we will frequently encounter the quadratic form,

$$\boxed{\beta H[\phi] = \frac{1}{2}\int d\mathbf{x}\left[(\nabla\phi)^2 + \xi^{-2}\phi^2\right] \equiv \frac{1}{2}\int d\mathbf{x}\int d\mathbf{x}'\; \phi(\mathbf{x}')\delta^d(\mathbf{x}-\mathbf{x}')(-\nabla^2+\xi^{-2})\;\phi(\mathbf{x}),} \quad (2.8)$$

which (integrating by parts) implies an operator kernel

$$\boxed{G^{-1}(\mathbf{x},\mathbf{x}') = K\delta^d(\mathbf{x}-\mathbf{x}')(-\nabla^2+\xi^{-2}).}$$

Substituting into Eq. (2.7) and integrating we obtain $K(-\nabla^2+\xi^{-2})G(\mathbf{x}) = \delta^d(\mathbf{x})$. The propagator can thus be identified as nothing but the **Green's function**.

In the present case, translational invariance of the propagator suggests the utility of the Fourier representation[3]

$$\boxed{\phi(\mathbf{x}) = \sum_{\mathbf{q}}\phi_{\mathbf{q}}\; e^{i\mathbf{q}\cdot\mathbf{x}}, \qquad \phi_{\mathbf{q}} = \frac{1}{L^d}\int_0^L d\mathbf{x}\;\phi(\mathbf{x})\; e^{-i\mathbf{q}\cdot\mathbf{x}},}$$

where $\mathbf{q} = (q_1,\cdots q_d)$, with the Fourier elements taking values $q_i = 2\pi m/L$, m integer. In this representation, making use of the identity $\int_0^L d\mathbf{x}\; e^{-i(\mathbf{q}+\mathbf{q}')\cdot\mathbf{x}} = L^d\delta_{\mathbf{q},-\mathbf{q}'}$, the quadratic form above becomes diagonal in $\mathbf{q}$[4]

$$\beta H[\phi] = \frac{1}{2}\sum_{\mathbf{q}}(\mathbf{q}^2+\xi^{-2})|\phi_{\mathbf{q}}|^2,$$

[3] Here the system is supposed to be confined to a square box of dimension d and volume L^d. In the thermodynamic limit $L\to\infty$, the Fourier series becomes the transform

$$\boxed{\phi(\mathbf{x}) = \int_{-\infty}^{\infty}\frac{d\mathbf{q}}{(2\pi)^d}\;\phi(\mathbf{q})\; e^{i\mathbf{q}\cdot\mathbf{x}}, \qquad \phi(\mathbf{q}) = \int_{-\infty}^{\infty} d\mathbf{x}\;\phi(\mathbf{x})\; e^{-i\mathbf{q}\cdot\mathbf{x}}.}$$

Similarly,

$$\boxed{\int_{-\infty}^{\infty} d\mathbf{x}\; e^{i(\mathbf{q}+\mathbf{q}')\cdot\mathbf{x}} = (2\pi)^d\delta^d(\mathbf{q}+\mathbf{q}'), \qquad \int_{-\infty}^{\infty}\frac{d\mathbf{q}}{(2\pi)^d}\; e^{-i\mathbf{q}\cdot(\mathbf{x}+\mathbf{x}')} = \delta^d(\mathbf{x}+\mathbf{x}').}$$

In the formulae above, the arrangements of $(2\pi)^d$ is not occasional. In defining the Fourier transform, it is wise to declare a convention and stick to it. The convention chosen here is one in which factors of $(2\pi)^d$ are attached to the $\mathbf{q}$ integration, and to the δ-function in $\mathbf{q}$.

[4] Similarly, in the thermodynamic limit, the Hamiltonian takes the form

$$\beta H[\phi] = \int_{-\infty}^{\infty}\frac{d\mathbf{q}}{(2\pi)^d}\frac{1}{2}(\mathbf{q}^2+\xi^{-2})|\phi(\mathbf{q})|^2.$$

where, since $\phi(\mathbf{x})$ is real, $\phi_{-\mathbf{q}} = \phi^*_{\mathbf{q}}$. The corresponding propagator is given by $G(\mathbf{q}) = (\mathbf{q}^2 + \xi^{-2})^{-1}$. Thus in real space, the correlation function is given by

$$G(\mathbf{x}, \mathbf{x}') \equiv \langle \phi(\mathbf{x})\phi(\mathbf{x}')\rangle_c = \sum_{\mathbf{q}} e^{i\mathbf{q}\cdot(\mathbf{x}-\mathbf{x}')} G(\mathbf{q}).$$

Here we have kept L finite and the modes discrete to emphasize the connection between the discrete Gaussian integrations $\mathcal{Z}_N$ and the functional integral. Hereafter, we will focus on the thermodynamic limit $L \to \infty$.

2.4 Derivation of GL Hamiltonian for the Ising model

We now illustrate how a coarse-grained GL Hamiltonian can arise from a microscopic model with a first principles derivation. We will use the Ising model as a convenient example. The partition function of the Ising model takes the following form

$$\mathcal{Z} = \sum_{\{\sigma_i = \pm 1\}} e^{K \sum_{\langle ij \rangle} \sigma_i \sigma_j + h \sum_i \sigma_i}. \tag{2.9}$$

Step 1 — Introducing the order parameter via Hubbard-Stratonovich decoupling

$$\mathcal{Z} = \det \left[2\pi G_{ij}^{-1}\right]^{-\frac{1}{2}} \sum_{\{\sigma_i = \pm 1\}} \int \left(\prod_i d\Psi_i\right) \, e^{-\frac{1}{2}\sum_{ij} G_{ij}^{-1} \Psi_i \Psi_j} \, e^{\sum_i (\Psi_i + h)\sigma_i}, \tag{2.10}$$

where $G_{ij} = K$ for nearest neighbours ij and vanishes otherwise.

Step 2 — Integrating out the original microscopic variables

The partition function factorises, allowing us to carry out the sum over σ_i

$$\begin{aligned} \mathcal{Z} &\propto \sum_{\{\sigma_i = \pm 1\}} \int \left(\prod_i d\Psi_i\right) \, e^{-\frac{1}{2}\sum_{ij} G_{ij}^{-1} \Psi_i \Psi_j} \, \left(\prod_i e^{\sigma_i(\Psi_i + h)}\right) \\ &= \int \left(\prod_i d\Psi_i\right) \, e^{-\frac{1}{2}\sum_{ij} G_{ij}^{-1} \Psi_i \Psi_j} \left(\prod_i 2\cosh\left(\Psi_i + h\right)\right). \end{aligned} \tag{2.11}$$

Step 3 — Re-expontiating to obtain the GL Hamiltonian

$$\mathcal{Z} \propto \int \left(\prod_i d\Psi_i\right) \, e^{-\frac{1}{2}\sum_{ij} G_{ij}^{-1} \Psi_i \Psi_j} \, e^{\sum_i \ln\cosh(\Psi_i + h)}. \tag{2.12}$$

Step 4 — Expanding in the order parameter and its gradients close to the critical point

$$\mathcal{Z} = \int \left(\prod_i d\Psi_i \right) \, e^{-\frac{1}{2}\sum_{ij} G^{-1}_{ij} \Psi_i \Psi_j} \, e^{\sum_i \left(\frac{1}{2}\Psi_i^2 - \frac{1}{12}\Psi_i^4 + h\Psi_i \right)}, \tag{2.13}$$

where we have kept terms up to fourth order in Ψ_i (and up to linear order in h). It is convenient to work in Fourier space and to find the Fourier transform of G_{ij} before inverting it; this can be done either directly or by computing

$$\sum_{ij} G_{ij} \phi_i \phi_j = \sum_{\mathbf{q}\in \mathrm{BZ},\alpha} 2K \cos(q_\alpha a) \phi_{\mathbf{q}} \phi_{-\mathbf{q}}, \tag{2.14}$$

where $\phi_i = \frac{1}{\sqrt{N}} \sum_{\mathbf{q}\in\mathrm{BZ}} e^{i\mathbf{q}\cdot\mathbf{r}} \phi_{\mathbf{q}}$ is a generic (vector) variable and q_α is one of the d Cartesian components of $\mathbf{q}$. Sufficiently close to the critical point, the relevant modes will be long-wavelength $|\mathbf{q}|a \ll 1$ modes

$$\sum_{ij} G_{ij} \phi_i \phi_j = \sum_{\mathbf{q}\in\mathrm{BZ}} 2Kd \left(1 - \frac{|\mathbf{q}|^2 a^2}{2d} \right) \Psi_{\mathbf{q}} \Psi_{-\mathbf{q}} + \mathcal{O}(|\mathbf{q}|^4 a^4) \, . \tag{2.15}$$

We can now easily invert the matrix in Fourier space

$$\begin{aligned} G_{\mathbf{q},\mathbf{q}'} &= \delta_{\mathbf{q}+\mathbf{q}'} 2Kd \left(1 - \frac{|\mathbf{q}|^2 a^2}{2d} \right), \\ G^{-1}_{\mathbf{q},\mathbf{q}'} &= \delta_{\mathbf{q}+\mathbf{q}'} \frac{1}{2Kd} \left(1 + \frac{|\mathbf{q}|^2 a^2}{2d} \right), \\ \frac{1}{2} \sum_{ij} G^{-1}_{ij} \Psi_i \Psi_j &= \frac{1}{4Kd} \sum_{\mathbf{q}\in\mathrm{BZ}} \left(1 + \frac{|\mathbf{q}|^2 a^2}{2d} \right) |\Psi_{\mathbf{q}}|^2. \end{aligned} \tag{2.16}$$

Returning to real space and replacing sums with integrals $\sum_i \to \int \frac{d^d\mathbf{r}}{a^d}$, $\sum_{\mathbf{q}\in\mathrm{BZ}} \to \int_{\mathrm{BZ}} \frac{N a^d d^d\mathbf{q}}{(2\pi)^d}$, $\Psi_{\mathbf{q}} \to \frac{\Psi(\mathbf{q})}{\sqrt{N}\, a^d}$, and $\Psi(\mathbf{q}) = \int d^d\mathbf{r} \, \Psi(\mathbf{r}) e^{-i\mathbf{q}\cdot\mathbf{r}}$, which is valid for long-wavelength fluctuations, we obtain

$$\mathcal{Z} \propto \int \mathcal{D}\Psi(\mathbf{r}) \, e^{-\beta H[\Psi(\mathbf{r})]}, \tag{2.17}$$

where $\beta H[\Psi(\mathbf{r})]$ is the Ising model Ginzburg-Landau Hamiltonian

$$\beta H[\Psi(\mathbf{r})] = \int \frac{d^d\mathbf{r}}{a^d} \left[\frac{t}{2} \Psi^2(\mathbf{r}) + \frac{a^2}{8Kd^2} \left(\nabla\Psi(\mathbf{r}) \right)^2 + \frac{1}{12} \Psi^4(\mathbf{r}) - h\Psi(\mathbf{r}) \right] .$$

The reduced temperature $t = \frac{1}{2Kd} - 1$ identifies $1/K_C = 2d$ as the critical temperature in the mean-field approximation.

2.5 Symmetry Breaking: Goldstone Modes

With these important mathematical preliminaries, we return to the consideration of the influence of spatial fluctuations on the stability of the mean-field analysis. Even for $h = 0$, when βH has full rotational symmetry, the ground state of the Ginzburg-Landau Hamiltonian is ordered along some given direction for $T < T_c$ — a direction of 'magnetisation' is specified. One can say that the onset of **long-range order** is accompanied by the **spontaneous breaking** of the rotational symmetry. The presence of a degenerate manifold of ground states obtained by a *global* rotation of the order parameter implies the existence of low energy excitations corresponding to slowly varying rotations in the spin space. Such excitations are characteristic of systems with a broken *continuous* symmetry and are known as **Goldstone modes**. In magnetic systems the Goldstone modes are known as **spin-waves**, while in solids, they are the vibrational or *phonon* modes.

The influence of Goldstone modes can be explored by treating fluctuations within the framework of the Ginzburg-Landau theory. For a fixed magnitude of the n-component order parameter or, in the spin model, the magnetic moment $\mathbf{m} = \bar{m}\hat{\mathbf{e}}_h$, the transverse fluctuations can be parametrized in terms of a set of $n-1$ angles. One-component, or **Ising** spins have only a discrete symmetry and possess no low energy excitations. Two-component, or XY-spins, where the moment lies in a plane, are defined by a single angle θ, $\mathbf{m} = \bar{m}(\cos\theta, \sin\theta)$ (cf. the complex phase of a 'superfluid' order parameter). In this case the Ginzburg-Landau free energy functional takes the form

$$\boxed{\beta H[\theta(\mathbf{x})] = \beta H_0 + \tfrac{\bar{K}}{2}\int d\mathbf{x}\ (\nabla\theta)^2,} \tag{2.18}$$

where $\bar{K} = K\bar{m}^2/2$.

Although superficially quadratic, the multi-valued nature of the transverse field $\theta(\mathbf{x})$ makes the evaluation of the partition function problematic. However, at low temperatures, taking the fluctuations of the fields to be small $\theta(\mathbf{x}) \ll 2\pi$, the functional integral can be taken as Gaussian. Following on from our discussion of the Gaussian functional integral, the operator kernel or propagator can be identified simply as the Laplacian operator. The latter is diagonalised in Fourier space, and the corresponding degrees of freedom are associated with spin-wave modes.

Then, employing the results of the previous section, we immediately find the average phase vanishes $\langle\theta(\mathbf{x})\rangle = 0$, and the correlation function takes the form

$$G(\mathbf{x}, \mathbf{x}') \equiv \langle\theta(\mathbf{x})\theta(\mathbf{x}')\rangle = -\frac{C_d(\mathbf{x}-\mathbf{x}')}{\bar{K}}, \qquad \nabla^2 C_d(\mathbf{x}) = \delta^d(\mathbf{x})$$

where C_d denotes the Coulomb potential for a δ-function charge distribution. Exploiting the symmetry of the field, and employing Gauss' law, $\int_V d\mathbf{x}\ \nabla^2 C_d(\mathbf{x}) = \oint dS \cdot \nabla C_d$, we find that C_d depends only on the radial coordinate x, and

$$\frac{dC_d}{dx} = \frac{1}{x^{d-1}S_d}, \qquad C_d(x) = \frac{x^{2-d}}{(2-d)S_d} + \text{const.}, \tag{2.19}$$

where $S_d = 2\pi^{d/2}/\Gamma(d/2)$ denotes the surface area of a unit d-dimensional ball.[5] Hence

$$\left\langle [\theta(\mathbf{x}) - \theta(0)]^2 \right\rangle = 2\left[\langle \theta(0)^2\rangle - \langle \theta(\mathbf{x})\theta(0)\rangle\right] \stackrel{|\mathbf{x}|>a}{=} \frac{2(|\mathbf{x}|^{2-d} - a^{2-d})}{\bar{K}(2-d)S_d},$$

where the cut-off, a, is of the order of the lattice spacing. Note that, in the case where $d = 2$, the combination $|\mathbf{x}|^{2-d}/(2-d)$ must be interpreted as $\ln|\mathbf{x}|$.

The long distance behaviour changes dramatically at $d = 2$. For $d > 2$, the phase fluctuations approach some finite constant as $|\mathbf{x}| \to \infty$, while they become asymptotically large for $d \leq 2$. Since the phase is bounded by 2π, it implies that long-range order (predicted by the mean-field theory) is destroyed. This result becomes more apparent by examining the effect of phase fluctuations on the two-point correlation function,

$$\langle \mathbf{m}(\mathbf{x}) \cdot \mathbf{m}(0)\rangle = \bar{m}^2 \mathrm{Re}\ \left\langle e^{i[\theta(\mathbf{x})-\theta(0)]}\right\rangle.$$

(Since amplitude fluctuations are neglected, we are in fact looking at the **transverse correlation function**.) For Gaussian distributed variables (with zero mean) we have already seen that $\langle \exp[\alpha\theta]\rangle = \exp[\alpha^2\langle\theta^2\rangle/2]$. We thus obtain

$$\langle \mathbf{m}(\mathbf{x}) \cdot \mathbf{m}(0)\rangle = \bar{m}^2 \exp\left[-\frac{1}{2}\langle[\theta(\mathbf{x}) - \theta(0)]^2\rangle\right] = \bar{m}^2 \exp\left[-\frac{(x^{2-d} - a^{2-d})}{\bar{K}(2-d)S_d}\right],$$

implying a power-law decay of correlations in $d = 2$, and an exponential decay in $d < 2$,

$$\boxed{\lim_{|\mathbf{x}|\to\infty} \langle \mathbf{m}(\mathbf{x}) \cdot \mathbf{m}(0)\rangle = \begin{cases} \bar{m}'^2 & d > 2, \\ 0 & d \leq 2. \end{cases}}$$

The saddle-point approximation to the order parameter, $\bar{m}$ was obtained by neglecting fluctuations. The result above demonstrates that the inclusion of phase fluctuations leads to a reduction in the degree of order in $d = 2$, and to its complete destruction in $d < 2$. This result typifies a more general result known as the **Mermin-Wagner Theorem** (N. D. Mermin and H. Wagner, Phys. Rev. Lett. **17**, 1133 (1967)). The theorem states that there is no spontaneous breaking of a continuous symmetry in systems with short-range interactions in dimensions $d \leq 2$. Corollaries to the theorem include:

[5] An important consequence of Eq. (2.19) is the existence of an unphysical **ultraviolet divergence** of the theory (i.e. $x \to 0 \longleftrightarrow q \to \infty$) in dimensions $d \geq 2$. In the present case, this divergence can be traced to the limited form of the effective free energy which accommodates short-range fluctuations of arbitrary magnitude. In principle one can account for the divergence by introducing additional terms in the free energy which control the short-range behaviour more precisely. Alternatively, and in keeping with the philosophy that lies behind the Ginzburg-Landau theory, we can introduce a short-length scale cut-off into the theory, a natural candidate being the "lattice spacing" a of the coarse-grained free energy. Note, however, that were the free energy a microscopic one — i.e. a free field theory — we would be forced to make sense of the ultraviolet divergence. Indeed finding a renormalisation scheme to control ultraviolet aspects of the theory is the subject of high energy quantum field theory. In condensed matter physics our concern is more naturally with the **infrared**, long-wavelength divergence of the theory which, in the present case (2.19), appears in dimensions $d \leq 2$.

- The borderline dimensionality of two, known as the **lower critical dimension** d_l has to be treated carefully. As we shall show in Chapter 5, there is in fact a phase transition for the two-dimensional XY-model (or superfluid), although there is no true long-range order.

- There are no Goldstone modes when the broken symmetry is discrete (e.g. for $n = 1$). In such cases long-range order is possible down to the lower critical dimension of $d_l = 1$.

2.6 Fluctuations, Correlations & Susceptibilities

Our study of Landau mean-field theory showed that the most probable configuration was spatially uniform with $\mathbf{m}(\mathbf{x}) = \bar{m}\hat{\mathbf{e}}_1$, where $\hat{\mathbf{e}}_1$ is a unit vector ($\bar{m}$ is zero for $t > 0$, and equal to $\sqrt{-t/4u}$ for $t < 0$). The role of small fluctuations around such a configuration can be examined by setting

$$\boxed{\mathbf{m}(\mathbf{x}) = [\bar{m} + \phi_l(\mathbf{x})]\,\hat{\mathbf{e}}_1 + \sum_{\alpha=2}^{n} \phi_{t,\alpha}(\mathbf{x})\hat{\mathbf{e}}_\alpha,}$$

where ϕ_l and ϕ_t refer respectively to fluctuations **longitudinal** and **transverse** to the axis of order $\hat{\mathbf{e}}_1$. The transverse fluctuations can take place along any of the $n-1$ directions perpendicular to $\hat{\mathbf{e}}_1$.

After substitution into the Ginzburg-Landau Hamiltonian, a quadratic expansion of the free energy functional with

$$\begin{aligned}
(\nabla\mathbf{m})^2 &= (\nabla\phi_l)^2 + (\nabla\phi_t)^2,\\
\mathbf{m}^2 &= \bar{m}^2 + 2\bar{m}\phi_l + \phi_l^2 + \phi_t^2,\\
\mathbf{m}^4 &= \bar{m}^4 + 4\bar{m}^3\phi_l + 6\bar{m}^2\phi_l^2 + 2\bar{m}^2\phi_t^2 + O(\phi_l^3, \phi_l\phi_t^2),
\end{aligned}$$

generates the perturbative expansion of the Hamiltonian

$$\begin{aligned}
\beta H = V\left(\tfrac{t}{2}\bar{m}^2 + u\bar{m}^4\right) &+ \int d\mathbf{x}\,\left[\tfrac{K}{2}(\nabla\phi_l)^2 + \tfrac{t+12u\bar{m}^2}{2}\phi_l^2\right]\\
&+ \int d\mathbf{x}\,\left[\tfrac{K}{2}(\nabla\phi_t)^2 + \tfrac{t+4u\bar{m}^2}{2}\phi_t^2\right] + O(\phi_l^3, \phi_l\phi_t^2).
\end{aligned} \tag{2.20}$$

For spatially uniform fluctuations, one can interpret the prefactors of the quadratic terms in ϕ as "masses" or "restoring forces" (cf. the action of a harmonic oscillator). These effective masses for the fluctuations can be associated with a length scale defined by

$$\begin{aligned}
\frac{K}{\xi_l^2} &\equiv t + 12u\bar{m}^2 = \begin{cases} t & t > 0,\\ -2t & t < 0,\end{cases}\\
\frac{K}{\xi_t^2} &\equiv t + 4u\bar{m}^2 = \begin{cases} t & t > 0,\\ 0 & t < 0.\end{cases}
\end{aligned} \tag{2.21}$$

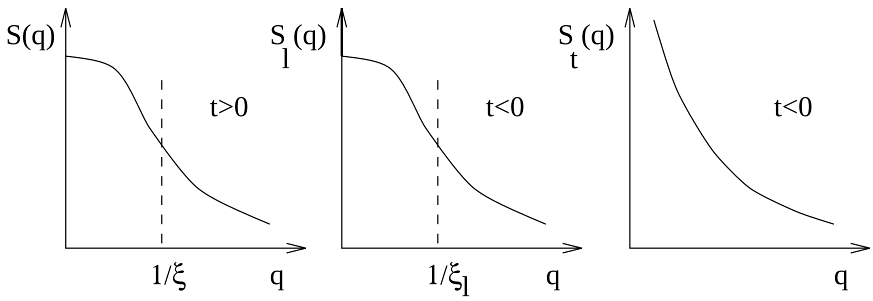


Figure 2.2: Typical neutron scattering amplitude for $t > 0$ and $t < 0$.

(The physical significance of the length scales ξ_l and ξ_t will soon become apparent.) Note that there is no distinction between longitudinal and transverse components in the paramagnetic phase ($t > 0$), while below the transition ($t < 0$), there is no restoring force for the transverse fluctuations (a consequence of the massless Goldstone degrees of freedom discussed previously).

To explore spatial fluctuations and correlation functions, it is convenient to switch to the Fourier representation, wherein the Hamiltonian becomes diagonal (cf. discussion of Gaussian functional integration). After the change of variables

$$\phi(\mathbf{x}) = \int_{-\infty}^{\infty} \frac{d\mathbf{q}}{(2\pi)^d}\, e^{i\mathbf{q}\cdot\mathbf{x}}\, \phi(\mathbf{q}),$$

the quadratic Hamiltonian becomes separable into longitudinal and transverse modes,

$$\beta H[\phi_l, \phi_t] = \int \frac{d\mathbf{q}}{(2\pi)^d} \frac{K}{2} \left[\left(\mathbf{q}^2 + \xi_l^{-2}\right) |\phi_l(\mathbf{q})|^2 + \left(\mathbf{q}^2 + \xi_t^{-2}\right) |\phi_t(\mathbf{q})|^2 \right].$$

Thus, each mode behaves as a Gaussian distributed random variable with zero mean, while the two-point correlation function assumes the form of a **Lorentzian**,

$$\boxed{\langle \phi_\alpha(\mathbf{q})\phi_\beta(\mathbf{q}')\rangle = \delta_{\alpha\beta}\ (2\pi)^d\ \delta^d(\mathbf{q}+\mathbf{q}')\ G_\alpha(\mathbf{q}), \qquad G_\alpha^{-1}(\mathbf{q}) = K(\mathbf{q}^2 + \xi_\alpha^{-2})} \tag{2.22}$$

where the indices α, β denote longitudinal and transverse components. In fact, this equation describing correlations of an order parameter in the vicinity of a critical point was first proposed by **Ornstein and Zernike** as a means to explain the phenomenon of critical opalescence in the light scattering from a fluid in the vicinity of a liquid-gas transition. To understand the mechanism by which ξ sets the characteristic length scale of fluctuations let us consider the scattering amplitude.

In the case of the ferromagnetic model, the two-point correlation function of magnetisation can be observed directly using spin-polarised scattering experiments. The scattering amplitude is related to the Fourier density of scatterers $S(\mathbf{q}) \propto \langle |\mathbf{m}(\mathbf{q})|^2\rangle$ (see Fig. 2.2). The Lorentzian form predicted above usually provides an excellent fit to scattering line shapes away from the critical point. Eq. (2.21) indicates that in the ordered

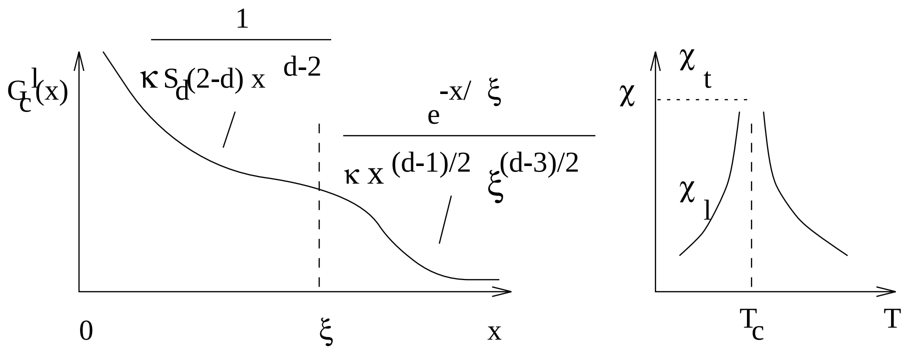


Figure 2.3: Decay of the two-point correlation of magnetisation, and the divergence of the longitudinal and transverse susceptibility in the vicinity of T_c.

phase longitudinal scattering still gives a Lorentzian form (on top of a δ-function at $\mathbf{q} = 0$ due to the spontaneous magnetisation), while transverse scattering always grows as $1/\mathbf{q}^2$. The same power law decay is also predicted to hold at the critical point, $t = 0$. In fact, actual experimental fits yield a power law of the form

$$\boxed{S(\mathbf{q}, T = T_c) \propto \frac{1}{|\mathbf{q}|^{2-\eta}},}$$

with a small positive value of the universal exponent η.

Turning to real space, we find that the average magnetisation is left unaffected by fluctuations, $\langle \phi_\alpha(\mathbf{x}) \rangle \equiv \langle m_\alpha(\mathbf{x}) - \bar{m}_\alpha \rangle = 0$, while the connected part of the two-point correlation function takes the form $G^c_{\alpha\beta}(\mathbf{x}, \mathbf{x}') \equiv \langle (m_\alpha(\mathbf{x}) - \bar{m}_\alpha)(m_\beta(\mathbf{x}') - \bar{m}_\beta) \rangle = \langle \phi_\alpha(\mathbf{x}) \phi_\beta(\mathbf{x}') \rangle$ where

$$\langle \phi_\alpha(\mathbf{x}) \phi_\beta(\mathbf{x}') \rangle = -\frac{\delta_{\alpha\beta}}{K} I_d(\mathbf{x} - \mathbf{x}', \xi_\alpha), \qquad I_d(\mathbf{x}, \xi) = -\int \frac{d\mathbf{q}}{(2\pi)^d} \frac{e^{i\mathbf{q}\cdot\mathbf{x}}}{\mathbf{q}^2 + \xi^{-2}}. \tag{2.23}$$

The detailed profile of this equation[6] is left as an exercise, but leads to the asymptotics

[6] This Fourier transform is discussed in Chaikin and Lubensky p 156. However, some clue to understanding the form of the transform can be found from the following: Expressed in terms of the modulus q and $d - 1$ angles θ_d, the d-dimensional integration measure takes the form

$$d\mathbf{q} = q^{d-1} dq \ \sin^{d-2}\theta_{d-1} \ d\theta_{d-1} \ \sin^{d-3}\theta_{d-2} \ d\theta_{d-2} \cdots d\theta_1,$$

where $0 < \theta_k < \pi$ for $k > 1$, and $0 < \theta_1 < 2\pi$. Thus, by showing that

$$I_d(\mathbf{x}, \xi) = -\frac{1}{(2\pi)^{d/2} |\mathbf{x}|^{d/2-1}} \int_0^{1/a} \frac{q^{d/2} dq}{q^2 + \xi^{-2}} J_{d/2-1}(q|\mathbf{x}|),$$

one can obtain Eq. (2.24) by asymptotic expansion. A second approach is to present the correlator as

$$I_d(\mathbf{x}, \xi) = -\int_0^\infty dt \int \frac{d\mathbf{q}}{(2\pi)^d} e^{i\mathbf{q}\cdot\mathbf{x} - t(\mathbf{q}^2 + \xi^{-2})},$$

integrate over $\mathbf{q}$, and employ a saddle-point approximation.

(see Fig. 2.6)

$$\boxed{I_d(\mathbf{x},\xi) \simeq \begin{cases} C_d(\mathbf{x}) = \frac{|\mathbf{x}|^{2-d}}{(2-d)S_d} & |\mathbf{x}| \ll \xi, \\ \frac{\xi^{2-d}}{(2-d)S_d}\,\frac{\exp[-|\mathbf{x}|/\xi]}{|\mathbf{x}/\xi|^{(d-1)/2}} & |\mathbf{x}| \gg \xi. \end{cases}} \qquad (2.24)$$

From the form of this equation we can interpret the length scale ξ as the **correlation length**.

Using Eq. (2.21) we see that close to the critical point the longitudinal correlation length behaves as

$$\boxed{\xi_l = \begin{cases} (K/t)^{1/2} & t > 0, \\ (-K/2t)^{1/2} & t < 0. \end{cases}}$$

The singularities can be described by $\xi_\pm \simeq \xi_0 B_\pm |t|^{-\nu_\pm}$, where $\nu_\pm = 1/2$ and the ratio $B_+/B_- = \sqrt{2}$ are universal, while $\xi_0 \propto \sqrt{K}$ is not. The transverse correlation length is equivalent to ξ_l for $t > 0$, while it is infinite for all $t < 0$. Eq. (2.24) implies that precisely at T_c, the correlations decay as $1/|\mathbf{x}|^{d-2}$. Again, the experimental decay exponent is usually given by $1/|\mathbf{x}|^{d-2-\eta}$.

These results imply a longitudinal susceptibility of the form (see Fig. 2.6)

$$\boxed{\chi_l \propto \int d\mathbf{x}\ \overbrace{\langle \phi_l(\mathbf{x})\phi_l(0)\rangle}^{G_l^c(\mathbf{x})} \propto \int_0^{\xi_l} \frac{d\mathbf{x}}{|\mathbf{x}|^{d-2}} \propto \xi_l^2 \simeq A_\pm t^{-1}}$$

The universal exponents and amplitude ratios are again recovered from this equation. For $T < T_c$ there is no upper cut-off length for transverse fluctuations, and the divergence of the transverse susceptibility can be related to the system size L, as

$$\boxed{\chi_t \propto \int d\mathbf{x}\ \overbrace{\langle \phi_l(\mathbf{x})\phi_l(0)\rangle}^{G_t^c(\mathbf{x})} \propto \int_0^{L} \frac{d\mathbf{x}}{|\mathbf{x}|^{d-2}} \propto L^2} \qquad (2.25)$$

2.7 Comparison of Theory and Experiment

The validity of the mean-field approximation is assessed in the table below by comparing the results with (approximate) exponents for $d = 3$ from experiment.

Transition type	Material	α	β	γ	ν
		$C \sim \|t\|^{-\alpha}$	$\langle m\rangle \sim \|t\|^{\beta}$	$\chi \sim \|t\|^{-\gamma}$	$\xi \sim \|t\|^{-\nu}$
Ferromag. ($n = 3$)	Fe, Ni	-0.1	0.34	1.4	0.7
Superfluid ($n = 2$)	He^4	0	0.3	1.3	0.7
Liquid-gas ($n = 1$)	CO_2, Xe	0.11	0.32	1.24	0.63
Superconductors		0	1/2	1	1/2
Mean-field		0	1/2	1	1/2

The discrepancy between the mean-field results and experiment signal the failure of the saddle-point approximation. Indeed, the results suggest a dependence of the critical exponents on n (and d). Later we will try to explore ways of going beyond the mean-field approximation. However, before doing so, the experimental results above leave a dilemma. Why do the critical exponents obtained from measurements of the superconducting transition agree so well with mean field theory? Indeed, why do they differ from other transitions which apparently belong to the same universality class? To understand the answer to these questions, it is necessary to examine more carefully the role of fluctuations on the saddle-point.

2.8 Fluctuation Corrections to the Saddle-Point

We are now in a position to determine the corrections to the saddle-point from fluctuations at quadratic order. To do so, it is necessary to determine the fluctuation contribution to the free energy. Applying the matrix (or functional) identity $\ln\det\mathbf{G}^{-1} = -\mathrm{tr}\ln\mathbf{G}$ to Eq. (2.20) we obtain the following estimate for the free energy density

$$f = -\frac{\ln\mathcal{Z}}{V} = \frac{t}{2}\bar{m}^2 + u\bar{m}^4 + \frac{1}{2}\int\frac{d\mathbf{q}}{(2\pi)^d}\,\ln[K(\mathbf{q}^2+\xi_l^{-2})] + \frac{n-1}{2}\int\frac{d\mathbf{q}}{(2\pi)^d}\,\ln[K(\mathbf{q}^2+\xi_t^{-2})].$$

Inserting the dependence of the correlation lengths on reduced temperature, the singular component of the heat capacity is given by

$$C_{\text{sing.}} \propto -\frac{\partial^2 f}{\partial t^2} = \begin{cases} 0 + \frac{n}{2}\int\frac{d\mathbf{q}}{(2\pi)^d}\,\frac{1}{(Kq^2+t)^2} & t>0, \\ \frac{1}{8u} + 2\int\frac{d\mathbf{q}}{(2\pi)^d}\,\frac{1}{(Kq^2-2t)^2} & t<0. \end{cases} \tag{2.26}$$

The behaviour of the integral correction changes dramatically at $d = 4$. For $d > 4$ the integral diverges at large $\mathbf{q}$ and is dominated by the upper cut-off $\Lambda \approx 1/a$, while for $d < 4$, the integral is convergent in both limits. It can be made dimensionless by rescaling $\mathbf{q}$ by ξ^{-1}, and is hence proportional to ξ^{4-d}. Therefore

$$\boxed{\delta C \simeq \frac{1}{K^2}\begin{cases} a^{4-d} & d>4, \\ \xi^{4-d} & d<4. \end{cases}} \tag{2.27}$$

In dimensions $d > 4$ fluctuation corrections to the heat capacity add a constant term to the background on each side of the transition. However, the primary form of the discontinuity in $C_{\text{sing.}}$ is unchanged. For $d < 4$, the divergence of $\xi \propto t^{-1/2}$ at the transition leads to a correction term that dominates the original discontinuity. Indeed, the correction term suggests an exponent $\alpha = (4-d)/2$. But even this is not reliable — a treatment of higher order corrections will lead to yet more severe divergences. In fact the divergence of δC implies that the conclusions drawn from the saddle-point approximation

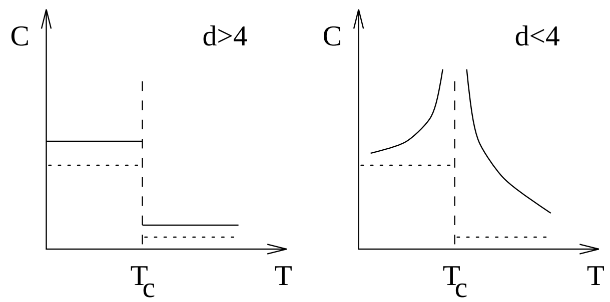


Figure 2.4: Sketch of the heat capacity in the vicinity of the critical point.

are simply no longer reliable in dimensions $d < 4$. One says that Ginzburg-Landau models which belong to this universality class exhibit an **upper critical dimension** d_u of four. Although we reached this conclusion by examining the heat capacity the same conclusion would have been reached for any physical quantity such as magnetisation, or susceptibility.

2.9 Ginzburg Criterion

We have thus established the importance of fluctuations as the probable reason for the failure of the saddle-point approximation to correctly describe the observed exponents. How, therefore, it is possible to account for materials such as superconductors in which the exponents agree well with mean-field theory?

Eq. (2.27) suggests that fluctuations become important when the correlation length begins to diverge. Within the saddle-point approximation, the correlation length diverges as $\xi \simeq \xi_0 |t|^{-1/2}$, where $\xi_0 \approx \sqrt{K}$ represents the microscopic length scale. The importance of fluctuations can be assessed by comparing the two terms in Eq. (2.26), the saddle-point discontinuity $\Delta C_{\rm sp} \propto 1/u$, and the correction, δC. Since $K \propto \xi_0^2$, and $\delta C \propto \xi_0^{-d}|t|^{-(4-d)/2}$, fluctuations become important when

$$\boxed{\left(\frac{\xi_0}{a}\right)^{-d} t^{(d-4)/2} \gg \left(\frac{\Delta C_{\rm sp}}{k_B}\right) \Longrightarrow |t| \ll t_G \approx \frac{1}{[(\xi_0/a)^d(\Delta C_{\rm sp}/k_B)]^{2/(4-d)}}.}$$

This inequality is known as the **Ginzburg Criterion**. Naturally, in $d < 4$ it is satisfied sufficiently close to the critical point. However, the resolution of the experiment may not be good enough to get closer than the Ginzburg reduced temperature t_G. If so, the apparent singularities at reduced temperatures $t > t_G$ may show saddle-point behaviour.

In principle, ξ_0 can be deduced experimentally from scattering line shapes. It has to approximately equal the size of the units that undergo ordering at the phase transition. For the liquid-gas transition, ξ_0 can be estimated by $v_c^{1/3}$, where v_c is the critical atomic volume. In superfluids, ξ_0 is approximately equal to the thermal wavelength $\lambda(T)$. Taking $\Delta C_{\rm sp}/k_B \sim 1$ per particle, and $\lambda \sim 2-3$Å we obtain $t_G \sim 10^{-1}-10^{-2}$, a value accessible in

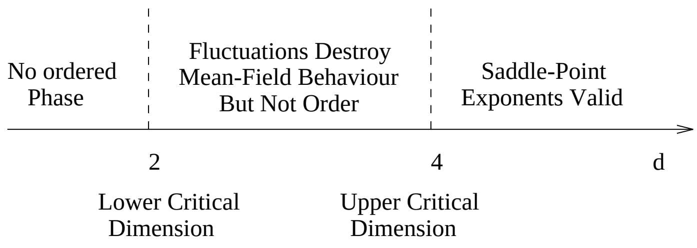


Figure 2.5: Summary of results for the Ginzburg-Landau theory based on mean-field and Gaussian fluctuations.

experiment. However, for a superconductor, the underlying length scale is the separation of Cooper pairs which, as a result of Coulomb repulsion, typically gives $\xi_0 \approx 10^3$Å. This implies $t_G \sim 10^{-16}$, a degree of resolution inaccessible by experiment.

The Ginzburg criterion allows us to restore some credibility to the mean-field theory. As we will shortly see, a theoretical estimate of the critical exponents below the upper critical dimension is typically a challenging endeavour. Yet, for many purposes, a good qualitative understanding of the thermodynamic properties of the experimentally relevant regions of the phase diagram can be understood from the mean-field theory alone.

Self-consistent mean-field: More generally, mean-field theories can be checked for self-consistency as follows. We begin by writing a general Hamiltonian

$$\beta H = \int d\mathbf{x} \int d\mathbf{x}' J(\mathbf{x}-\mathbf{x}') m(\mathbf{x}) m(\mathbf{x}').$$

We can then decompose the field into its mean-field part and the fluctuation part

$$m(\mathbf{x}) = \bar{m} + \phi(\mathbf{x}).$$

In the mean-field approximation second-order fluctuation terms are neglected. This is self-consistent provided

$$\int d\mathbf{x} \int d\mathbf{x}' J(\mathbf{x}-\mathbf{x}') \langle \phi(\mathbf{x})\phi(\mathbf{x}')\rangle_{\rm MF} \ll V J \bar{m}^2,$$

where $\int d\mathbf{x} J(\mathbf{x}) = J$.

Because, in the vicinity of the critical point the potential $J(\mathbf{x}-\mathbf{x}')$ is much more short-ranged than the correlation function, we can approximate the left-hand-side by

$$\int d\mathbf{x} \int d\mathbf{x}' J(\mathbf{x}-\mathbf{x}') \langle \phi(\mathbf{x})\phi(\mathbf{x}')\rangle_{\rm MF} \approx JV \langle \phi^2(\mathbf{0})\rangle_{\rm MF} \propto JV \int \frac{d^d\mathbf{q}}{K\left(\mathbf{q}^2+\xi^{-2}\right)}.$$

The integral can be split up as follows into a constant and temperature-dependent part

$$\begin{aligned}\frac{JV}{K}\int \frac{d^d\mathbf{q}}{\mathbf{q}^2+\xi^{-2}} &= \frac{JV}{K}\int \frac{d^d\mathbf{q}}{\mathbf{q}^2} - \frac{JV\xi^{-2}}{K}\int \frac{d^d\mathbf{q}}{\mathbf{q}^2(\mathbf{q}^2+\xi^{-2})} \\ &= \text{const.} + \frac{JV}{K}\xi^{2-d}.\end{aligned}$$

Since $\bar{m}^2 \propto t \propto K\xi^{-2}$, we conclude that the mean-field approximation is valid when

$$\begin{aligned}\frac{JV}{K}\xi^{2-d} &\ll JVK\xi^{-2}\\ \xi^{4-d} &\ll \xi_0^4,\end{aligned}$$

where $K = \xi_0^2$. For $d < 4$ mean-field theory breaks down when $\xi \sim \xi_0^{\frac{4}{4-d}}$, which for systems with large interaction range ξ_0, such as superconductors, takes place very close to the critical point. Note that the temperature-independent term that we have neglected, although non-singular, might still be large and result in a shift in the critical temperature away from its mean-field value, even when $d > 4$.

2.10 Summary

A summary of our findings for the Ginzburg-Landau Hamiltonian based on mean-field theory and Gaussian fluctuations is shown in Fig. 2.5.

Chapter 3

The Scaling Hypothesis

*Previously, we found that singular behaviour in the vicinity of a second order critical point was characterised by a set of critical exponents $\{\alpha, \beta, \gamma, \delta, \cdots\}$. These power law dependencies of thermodynamic quantities are a symptom of **scaling behaviour**. Mean-field estimates of the critical exponents were found to be unreliable due to fluctuations. However, since the various thermodynamic quantities are related, these exponents can not be completely independent of each other. The aim of this chapter is to employ scaling ideas to uncover relationships between them.*

3.1 Homogeneity

The non-analytic structure of the Ginzburg-Landau model was found to be a coexistence line for $t < 0$ and $h = 0$ that terminates at the critical point $h = t = 0$. Thermodynamic quantities $Q(t, h)$ in the vicinity of the critical point are characterised by various exponents. In particular, within the saddle-point approximation we found that the free energy density was given by

$$f \equiv \frac{\beta F}{V} = \min_{\mathbf{m}} \left[\tfrac{t}{2}\mathbf{m}^2 + u\mathbf{m}^4 - \mathbf{h}\cdot\mathbf{m}\right] \sim \begin{cases} -t^2/u, & h = 0,\ t < 0, \\ -h^{4/3}/u^{1/2} & h \neq 0,\ t = 0. \end{cases} \tag{3.1}$$

In fact, the free energy can be described by a single **homogeneous** function[1] in t and h

$$f(t, h) = t^2 g_f(h/t^{\Delta}), \tag{3.2}$$

where Δ is known as the "Gap exponent". Comparison with Eq. (3.1) shows that, if we set $\Delta = 3/2$, the correct asymptotic behaviour of f is obtained,

$$\begin{aligned} \lim_{x\to 0} g_f(x) &\sim -\frac{1}{u}, & f(t, h = 0) &\sim -\frac{t^2}{u}, \\ \lim_{x\to\infty} g_f(x) &\sim \frac{x^{4/3}}{u^{1/3}}, & f(t = 0, h) &\sim t^2\left(\frac{h}{t^{\Delta}}\right)^{4/3} \sim h^{4/3}. \end{aligned}$$

[1] A function $f(x)$ is said to be homogeneous of degree k if it satisfies the relation $f(bx) = b^k f(x)$.

The assumption of homogeneity is that, on going beyond the saddle-point approximation, the singular form of the free energy (and of any other thermodynamic quantity) retains a homogeneous form

$$\boxed{f_{\text{sing.}}(t,h) = t^{2-\alpha} g_f\left(\frac{h}{t^{\Delta}}\right),} \tag{3.3}$$

where the actual exponents α and Δ depend on the critical point being considered.

Heat Capacity: For example, the dependence on t is chosen to reproduce the heat capacity singularity at $h=0$. The singular part of the energy is obtained from

$$E_{\text{sing.}} \sim \frac{\partial f}{\partial t} \sim (2-\alpha)t^{1-\alpha} g_f(h/t^{\Delta}) - \Delta h t^{1-\alpha-\Delta} g_f'(h/t^{\Delta}) \equiv t^{1-\alpha} g_E(h/t^{\Delta}),$$

where the prime denotes the derivative of the function with respect to the argument. Thus, the derivative of one homogeneous function is another. Similarly, the second derivative takes the form

$$C_{\text{sing.}} \sim -\frac{\partial^2 f}{\partial t^2} \sim t^{-\alpha} g_C(h/t^{\Delta}),$$

reproducing the scaling $C_{\text{sing.}} \sim t^{-\alpha}$ as $h \to 0$.[2]

Magnetisation: Similarly the magnetisation is obtained from Eq. (3.3) using the expression

$$m(t,h) \sim \frac{\partial f}{\partial h} \sim t^{2-\alpha-\Delta} g_m(h/t^{\Delta}).$$

In the limit $x \to 0$, $g_m(x)$ is a constant, and $m(t,h=0) \sim t^{2-\alpha-\Delta}$ (i.e. $\beta = 2-\alpha-\Delta$). On the other hand, if $x \to \infty$, $g_m(x) \sim x^p$, and $m(t=0,h) \sim t^{2-\alpha-\Delta}(h/t^{\Delta})^p$. Since this limit is independent of t, we must have $p\Delta = 2-\alpha-\Delta$. Hence $m(t=0,h) \sim h^{(2-\alpha-\Delta)/\Delta}$ (i.e. $\delta = \Delta/(2-\alpha-\Delta) = \Delta/\beta$).

Susceptibility: Finally, calculating the susceptibility we obtain

$$\chi(t,h) \sim \frac{\partial m}{\partial h} \sim t^{2-\alpha-2\Delta} g_\chi(h/t^{\Delta}) \Rightarrow \chi(t,h=0) \sim t^{2-\alpha-2\Delta} \Rightarrow \gamma = 2\Delta - 2 + \alpha.$$

Thus the consequences of homogeneity are:

- The singular parts of all critical quantities, $Q(t,h)$ are homogeneous, with the same exponents above and below the transition.
- Because of the interconnections via thermodynamic derivatives, the same gap exponent, Δ occurs for all such quantities.
- All critical exponents can be obtained from only *two* independent ones, e.g. α, Δ.

[2]It may appear that we have the freedom to postulate a more general form, $C_\pm = t^{-\alpha_\pm} g_\pm(h/t_\pm^{\Delta})$ with different functions for $t>0$ and $t<0$ that match at $t=0$. However, this can be ruled out by the condition that the free energy is analytic everywhere except on the coexistence line $h=0$ and $t<0$.

- As a result of above, one obtains a number of *exponent identities*:

$$\boxed{\alpha + 2\beta + \gamma = 2.} \qquad \text{(Rushbrooke's Identity)}$$

$$\boxed{\delta - 1 = \gamma/\beta.} \qquad \text{(Widom's Identity)}$$

These identities can be checked against the following table of critical exponents. The first three rows are based on a number of theoretical estimates in $d = 3$; the last row comes from an exact solution in $d = 2$. The exponent identities are approximately consistent with these values, as well as with all reliable experimental data.

			α	β	γ	δ	ν	η
$d = 3$	$n = 1$	Ising	0.12	0.31	1.25	5	0.64	0.05
	$n = 2$	XY-spin	0.00	0.33	1.33	5	0.66	0.00
	$n = 3$	Heisenberg	-0.14	0.35	1.4	5	0.7	0.04
$d = 2$	$n = 1$	Ising	0	1/8	7/4	15	1	1/4

3.2 Hyperscaling and the Correlation Length

The homogeneity assumption relates to the free energy and quantities derived from it. It says nothing about correlation functions. An important property of a critical point is the divergence of the correlation length, which is responsible for (and can be deduced from) the divergence of response functions. In order to obtain an identity involving the exponent ν describing the divergence of the correlation length, we replace the homogeneity assumption for the free energy with the following *two* conditions:

1. The correlation length has a homogeneous form,

$$\boxed{\xi(t, h) \sim t^{-\nu} g_\xi \left(\frac{h}{t^\Delta} \right).}$$

   For $t = 0$, ξ diverges as $h^{-\nu_h}$ with $\nu_h = \nu/\Delta$.

2. Close to criticality, the correlation length ξ is the most important length scale, and is *solely* responsible for singular contributions to thermodynamic quantities.

The second condition determines the singular part of the free energy. Since $\ln \mathcal{Z}(t, h)$ is *dimensionless* and *extensive* (i.e. scales in proportion with the volume L^d), it must take the form

$$\ln \mathcal{Z} = \left(\frac{L}{\xi} \right)^d \times g_s + \left(\frac{L}{a} \right)^d \times g_a,$$

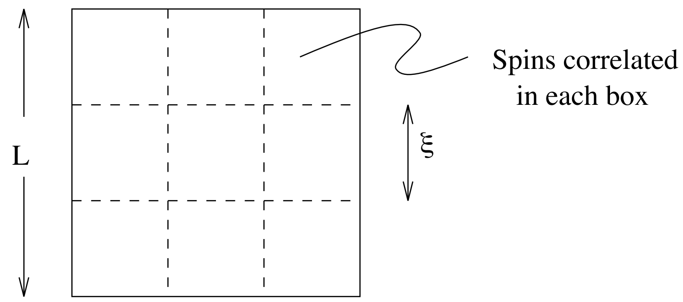


Figure 3.1: Within each cell of size ξ spins are correlated.

where g_s and g_a are non-singular functions of dimensionless parameters (a is an appropriate microscopic length). The singular part of the free energy comes from the first term and behaves as

$$f_{\text{sing.}}(t,h) \sim \frac{\ln \mathcal{Z}}{L^d} \sim \xi^{-d} \sim t^{d\nu} g_f(t/h^{\Delta}). \tag{3.4}$$

A simple interpretation of this result is obtained by dividing the system into units of the size of the correlation length (Fig. 3.2). Each unit is then regarded as an independent random variable, contributing a constant factor to the critical free energy. The number of units grows as $(L/\xi)^d$.

The consequences of Eq. (3.4) are:

- Homogeneity of $f_{\text{sing.}}$ emerges naturally.
- We obtain the additional exponent relation

$$\boxed{2-\alpha = d\nu.} \qquad \text{(Josephson's Idenitity)}$$

Identities obtained from the generalised homogeneity assumption involve the space dimension d, and are known as **hyperscaling relations**. The relation between α and ν is consistent with the exponents in the table above. However, it does not agree with the mean-field values, $\alpha = 0$ and $\nu = 1/2$, which are valid for $d > 4$. Any theory of critical behaviour must therefore account for the validity of this relation in low dimensions, and its breakdown in $d > 4$.

3.3 Correlation Functions and Self-Similarity

So far we have not accounted for the exponent η which describes the decay of correlation functions at criticality. Exactly at the critical point the correlation length is infinite, and there is no other length scale to cut-off the decay of correlation functions. Thus all correlations decay as a power of the separation. As discussed in the previous chapter, the magnetisation falls off as

$$\boxed{G_c(\mathbf{x}) \equiv \langle \mathbf{m}(\mathbf{x}) \cdot \mathbf{m}(0) \rangle - \langle \mathbf{m}^2 \rangle \sim \frac{1}{|\mathbf{x}|^{d-2+\eta}},}$$

where η was deduced from the form factor.

Away from criticality, the power laws are cut-off for distances $|\mathbf{x}| \gg \xi$. As the response functions can be obtained from integrating the connected correlation functions, there are additional exponent identities such as Fisher's identity

$$\chi \sim \int d^d\mathbf{x}\ G_c(\mathbf{x}) \sim \int^{\xi} \frac{d^d\mathbf{x}}{|\mathbf{x}|^{d-2+\eta}} \sim \xi^{2-\eta} \sim t^{-\nu(2-\eta)} \Longrightarrow \boxed{\gamma = (2-\eta)\nu.}$$

Therefore, two *independent* exponents are sufficient to describe all singular critical behaviour.

An important consequence of these scaling ideas is that the critical system has an additional **dilation symmetry**. Under a change of scale, the critical correlation functions behave as

$$\boxed{G_{\text{critical}}(\lambda\mathbf{x}) = \lambda^p G_{\text{critical}}(\mathbf{x}).}$$

This implies a **scale invariance** or **self-similarity**: If a snapshot of the critical system is enlarged by a factor of λ, apart from a change of contrast (λ^p), the resulting snapshot is statistically similar to the original. Such statistical self-similarity is the hallmark of **fractal** geometry. The Ginzburg-Landau functional was constructed on the basis of **local** symmetries such as rotational invariance. If we could add to the list of constraints the requirement of dilation symmetry, the resulting probability would indeed describe the critical point. Unfortunately, it is not in general possible to see directly how such a requirement constrains the effective Hamiltonian.[3] We shall instead prescribe a less direct route by following the effects of the dilation operation on the effective energy; a procedure known as the **renormalisation group**.

[3]One notable exception is in $d = 2$, where dilation symmetry implies conformal symmetry.

Chapter 4

Renormalisation Group

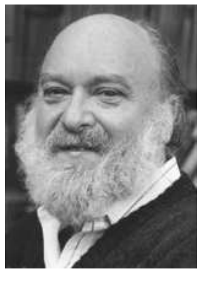
Previously, our analysis of the Ginzburg-Landau Hamiltonian revealed a formal breakdown of mean-field theory in dimensions below some upper critical dimension. Although the integrity of mean-field theory is sometimes extended by resolution limitations in experiment, the breakdown of mean-field theory is often associated with the appearance of qualitatively new critical behaviour. In the previous section, we saw that a simple scaling hypothesis can lead to useful insight into critical behaviour below the upper critical dimension. However, to complement the ideas of scaling, a formal theoretical approach to the analysis of the Ginzburg-Landau Hamiltonian is required. In this section we will introduce a general scheme which allows one to explore beyond the realms of mean-field theory. Yet the method, known as the Renormalisation Group, is not exact nor completely controlled. Instead, it should be regarded as largely conceptual — i.e. its application, which relies fundamentally only on scaling, can be tailored to the particular application at hand.

4.1 Conceptual Approach

The success of the scaling theory in correctly predicting various exponent identities strongly supports the contention that close to the critical point the correlation length ξ is the only important length scale, and that the microscopic lengths are irrelevant. The critical behaviour is governed by fluctuations that are statistically self-similar up to the scale ξ. Can this self-similarity be used to develop a theory of critical phenomena below the upper critical dimension? Kadanoff[1] suggested taking advantage of the self-similarity to gradually eliminate the correlated degrees of freedom at length scales $x \ll \xi$, until one

[1]

Leo Kadanoff: recipient of the 1999 National Medal of Science and the 1998 Lars Onsager Prize "for his numerous and profound contributions to statistical physics, including the introduction of the concepts of universality and block spin scaling that are central to the modern understanding of the critical phenomena".



is left with the relatively simple uncorrelated degrees of freedom at length scale ξ. This is achieved through a procedure known as the **Renormalisation Group** (RG), whose conceptual foundation is outlined below:

1. **Coarse-Grain**: The first step of the RG is to decrease the resolution by changing the minimum length scale from the microscopic scale a to ba where $b > 1$. This is achieved by integrating out fluctuations of the fields $\mathbf{m}$ which occur on length scales finer than ba. The result is a renormalisation of the Hamiltonian βH which leads to an effective Hamiltonian expressed in terms of a 'coarse-grained' magnetisation field
$$\bar{\mathbf{m}}(\mathbf{x}) = \frac{1}{(ba)^d} \int_{\text{Cell}} d\mathbf{y}\ \mathbf{m}(\mathbf{y}),$$
where the integral runs over a cell of size $(ba)^d$ centred on $\mathbf{x}$.

2. **Rescale**: Due to the change in resolution, the coarse-grained "picture" is grainier than the original. The original resolution a can be restored by decreasing all length scales by a factor b, i.e. defining
$$\mathbf{x}' = \frac{\mathbf{x}}{b}.$$
Thus, at each position $\mathbf{x}'$ we have defined an average moment $\bar{\mathbf{m}}(\mathbf{x}')$.

3. **Renormalise**: The relative size of the fluctuations of the rescaled magnetisation profile is in general different from the original, i.e. there is a change in contrast between the pictures. This can be remedied by introducing a factor ζ, and defining a renormalised magnetisation
$$\mathbf{m}'(\mathbf{x}') = \frac{1}{\zeta}\bar{\mathbf{m}}(\mathbf{x}').$$
The choice of ζ will be discussed later.

By following these steps, for each configuration $\mathbf{m}(\mathbf{x})$ one generates a renormalised configuration $\mathbf{m}'(\mathbf{x}')$. It can be regarded as a mapping of one set of random variables to another, and can be used to construct the probability distribution. Kadanoff's insight was to realise that since, on length scales less than ξ, the renormalised configurations are statistically similar to the original ones, they must be distributed by a Hamiltonian that is also close to the original. In particular, if the original Hamiltonian βH is at a critical point, $t = h = 0$, the new $\beta H'$ is also at criticality since no new length scale is generated in the renormalisation procedure, i.e. $t' = h' = 0$.

However, if the Hamiltonian is originally off criticality, then the renormalisation takes us further away from criticality because $\xi' = \xi/b$ is smaller. The next assumption is that since any transformation only involves changes at the shortest length scales it can not produce singularities. The renormalised parameters must be *analytic* functions, and hence expandable as

$$\begin{cases} t(b;t,h) = A(b)t + B(b)h + O(t^2, h^2, th), \\ h(b;t,h) = C(b)t + D(b)h + O(t^2, h^2, th). \end{cases}$$

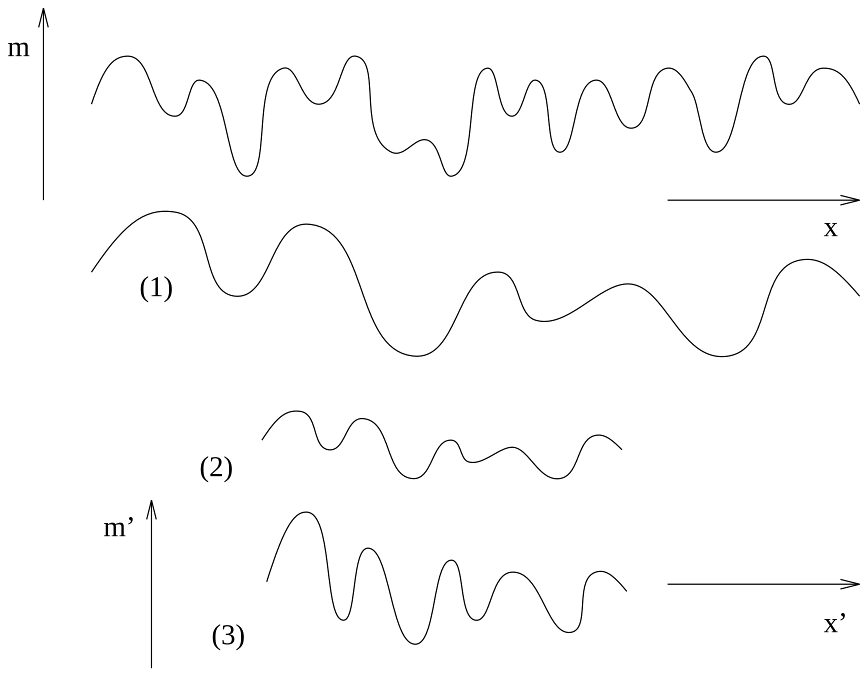


Figure 4.1: Schematic diagram showing the three steps of Kadanoff's renormalisation procedure.

However, the known behaviour at $t = h = 0$ rules out a constant term in the expansion, and to prevent a spontaneously broken symmetry we further require $C(b) = B(b) = 0$. Finally, rescaling by b_1 and then by b_2 ought to give the same result as rescaling by $b = b_1 b_2$; therefore $A(b_1 b_2) = A(b_1)A(b_2)$, and similarly for the other parameters, which implies $A(b) = b^{y_t}$ and $D(b) = b^{y_h}$, for some exponents y_t, y_h. So, to lowest order

$$\begin{cases} t(b) = b^{y_t} t, \\ h(b) = b^{y_h} h, \end{cases} \tag{4.1}$$

where $y_t, y_h > 0$ (to ensure that ξ diminishes under the RG procedure). As a consequence:

1. **The free energy**: Since the statistical Boltzmann weight of the new configuration, $\exp[\beta H'[\mathbf{m}']]$ is obtained by summing the weights $\exp[\beta H[\mathbf{m}]]$ of old ones, the partition function is preserved

$$\mathcal{Z} = \int D\mathbf{m}\; e^{-\beta H[\mathbf{m}]} = \int D\mathbf{m}'\; e^{-\beta H'[\mathbf{m}']} = \mathcal{Z}'.$$

From this it follows that the free energies density takes the form

$$f(t,h) = -\frac{\ln \mathcal{Z}}{V} = -\frac{\ln \mathcal{Z}'}{V' b^d} = b^{-d} f(t(b), h(b)) = b^{-d} f(b^{y_t} t, b^{y_h} h), \tag{4.2}$$

where we have assumed that the two free energies are obtained from the *same Hamiltonian* in which only the parameters t and h have changed according to Eq. (4.1). Eq. (4.2) describes a *homogeneous* function of t and h. This is made apparent by choosing a rescaling factor b such that $b^{y_t}t$ is a constant, say unity, i.e. $b = t^{-1/y_t}$, and

$$\boxed{f(t,h) = t^{d/y_t} f(1, h/t^{y_h/y_t}) \equiv t^{d/y_t} g_f(h/t^{y_h/y_t}).}$$

We have thus recovered the scaling form of Eq. (3.2) and can identify the exponents

$$\boxed{2-\alpha = d/y_t, \qquad \Delta = y_h/y_t} \tag{4.3}$$

So if y_t and y_h are known we can generate all critical exponents.

2. **Correlation Length**: All length scales are reduced by a factor of b during the RG transformation. This is also true of the correlation length $\xi' = \xi/b$ implying

$$\boxed{\xi(t,h) = b\,\xi(b^{y_t}t, b^{y_h}h) = t^{-1/y_t}\xi(1, h/t^{y_h/y_t}) = t^{-1/y_t} g_\xi(h/t^{y_t/y_h}).}$$

This identifies $\nu = 1/y_t$ and using Eq. (4.3), the hyperscaling identity $2-\alpha = d\nu$ is recovered.

3. **Magnetisation**: From the homogeneous form of the free energy we can obtain other bulk quantities such as magnetisation. Alternatively, from the RG results for $\mathcal{Z}$, V, and h we conclude

$$\boxed{m(t,h) = \frac{1}{V}\frac{\partial \ln \mathcal{Z}(t,h)}{\partial h} = \frac{1}{b^d V'}\frac{1}{b^{-y_h}}\frac{\partial \ln Z'(t',h')}{\partial h'} = b^{y_h-d} m(b^{y_t}t, b^{y_h}h)}$$

Choosing $b = t^{-1/y_t}$, we find $m(t,h) = t^{-(y_h-d)/y_t} g_m(h/t^{y_h/y_t})$ which implies that $\beta = (y_h - d)/y_t$ and $\Delta = y_h/y_t$ as before.

4. **Heat Capacity**: The singular part of the heat capacity can be obtained by differentiating Eq. (1)

$$C_{\text{sing.}} \sim -\frac{\partial^2 f}{\partial t^2} \sim t^{\frac{d}{y_t}-2} g_C(h/t^{\frac{y_h}{y_t}}),$$

reproducing the scaling $C_{\text{sing.}} \sim t^{-\alpha}$ as $h \to 0$ with $\alpha = 2 - \frac{d}{y_t}$.

5. **Susceptibility**: Finally, calculating the susceptibility we obtain

$$\chi(t,h) \sim \frac{\partial m}{\partial h} \sim t^{\frac{d-2y_h}{y_t}} g_\chi(h/t^{\frac{y_h}{y_t}}) \Rightarrow \chi(t, h=0) \sim t^{\frac{d-2y_h}{y_t}} \Rightarrow \gamma = -\frac{d-2y_h}{y_t}.$$

It is therefore apparent that quite generally, a quantity X will have a homogeneous form

$$X(t,h) = b^{y_X} X(b^{y_t}t, b^{y_h}h) = t^{-y_X/y_t} g_X(h/t^{y_h/y_t}). \tag{4.4}$$

In general, for any conjugate pair of variables contributing a term $\int d\mathbf{x}\ \mathbf{F}\cdot\mathbf{X}$ to the Hamiltonian (e.g. $\mathbf{m}\cdot\mathbf{h}$), the **scaling dimensions** are related by $y_X + y_F = d$.

4.2 Formal Approach

In the previous section we found that all critical properties can be abstracted from a scaling relation. Though conceptually appealing, it is not yet clear how such a procedure can be formally implemented. In particular, why should the form of the two Hamiltonians be identical, and why are the two parameters t and h sufficient to describe the transition? In this section we outline a more formal procedure for identifying the effects of the dilation operation on the Hamiltonian. The various steps of the program are as follows:

1. Start with the most general Hamiltonian allowed by symmetry. For example, in the presence of rotational symmetry,

$$\beta H[\mathbf{m}] = \int d\mathbf{x}\left[\frac{t}{2}\mathbf{m}^2 + u\mathbf{m}^4 + v\mathbf{m}^6 + \cdots + \frac{K}{2}(\nabla\mathbf{m})^2 + \frac{L}{2}(\nabla^2\mathbf{m})^2 + \cdots\right]. \quad (4.5)$$

2. Apply the three steps of the renormalisation in configuration space: (i) Coarse grain by b; (ii) rescale, $\mathbf{x}' = \mathbf{x}/b$; and (iii) renormalise, $\mathbf{m}' = \mathbf{m}/\zeta$. This defines a change of variables

$$\mathbf{m}'(\mathbf{x}') = \frac{1}{\zeta b^d}\int_{\substack{\text{Cell centred}\\ \text{at } b\mathbf{x}'}} d\mathbf{x}\ \mathbf{m}(\mathbf{x}).$$

Given the Boltzmann weight $\exp[-\beta H[\mathbf{m}(\mathbf{x})]]$ of the original configurations, we can use the change of variables above to construct the corresponding weight $\exp[-\beta H'[\mathbf{m}'(\mathbf{x}')]]$ of the new configurations. Naturally this is the most difficult step in the program.

3. Since rotational symmetry is preserved by the RG procedure, the rescaled Hamiltonian must also be described by a point in parameter space,

$$\beta H'[\mathbf{m}'] = \int d\mathbf{x}'\left[\frac{t'}{2}\mathbf{m}'^2 + u'\mathbf{m}'^4 + v'\mathbf{m}'^6 + \cdots + \frac{K'}{2}(\nabla\mathbf{m}')^2 + \frac{L'}{2}(\nabla^2\mathbf{m}')^2 + \cdots\right].$$

The renormalised coefficients are functions of the original ones, i.e. $t' = t(b; t, u, \cdots)$; $u' = u(b; t, u, \cdots)$, etc., defining a mapping $\mathbf{S}' \mapsto \mathbf{R}_b\mathbf{S}$ in parameter space (where $\mathbf{S}$ and $\mathbf{S}'$ are the full sets of parameters that the Hamiltonians H and H' depend on). In general such a mapping is non-linear.

4. The operation $\mathbf{R}_b$ describes the effects of dilation on the Hamiltonian of the system. Hamiltonians that describe statistically self-similar configurations must thus correspond to **fixed points** $\mathbf{S}^*$ such that $\mathbf{R}_b\mathbf{S}^* = \mathbf{S}^*$. Since the correlation length, a function of Hamiltonian parameters, is reduced by b under the RG operation (i.e. $\xi(\mathbf{S}) = b\ \xi(\mathbf{R}_b\mathbf{S})$), the correlation length at a fixed point must be zero or infinity. Fixed points with $\xi^* = 0$ describe independent fluctuations at each point and correspond to complete disorder (infinite temperature), or complete order (zero temperature). Fixed points with $\xi^* = \infty$ describe critical points ($T = T_c$).

5. Eq. (4.1) represents a simplified case in which the parameter space is two-dimensional. The point $t = h = 0$ is a fixed point, and the lowest order terms in these equations describe the behaviour in the neighbourhood of the fixed point. In general, we can study the stability of a fixed point by *linearising* the **recursion relations** in its vicinity: under RG, a point $\mathbf{S}^* + \delta\mathbf{S}$ is transformed to

$$S_i^* + \delta S_i' = S_i^* + \sum_j [\mathbf{R}_b]_{ij}\, \delta S_j + \cdots, \qquad (\mathbf{R}_b)_{ij} \equiv \frac{\partial S_i'}{\partial S_j}\Big|_{\mathbf{S}^*}.$$

Because of the semi (i.e. irreversible)-group property we have

$$\mathbf{R}_b \mathbf{R}_{b'} \mathbf{O}_i = \lambda_i(b)\lambda_i(b')\mathbf{O}_i = \mathbf{R}_{bb'}\mathbf{O}_i = \lambda_i(bb')\mathbf{O}_i,$$

where $\mathbf{O}_i$ denote the eigenvectors of $[\mathbf{R}_b]_{ij}$ with the eigenvalues $\lambda_i(b)$. Together with the condition $\lambda_i(b = 1) = 1$, the equation above implies $\lambda_i(b) = b^{y_i}$.

The vectors $\mathbf{O}_i$ are called **scaling directions** associated with the fixed point S^*, and y_i are the corresponding **anomalous dimensions**. Any Hamiltonian in the vicinity of the fixed point can be described by a set of parameters $\mathbf{S} = \mathbf{S}^* + \sum_i g_i \mathbf{O}_i$. The renormalised Hamiltonian has the interaction parameters $\mathbf{S}' = \mathbf{S}^* + \sum_i g_i b^{y_i} \mathbf{O}_i$.

If $y_i > 0$, g_i *increases* under scaling, and O_i is a **relevant operator**.

If $y_i < 0$, g_i *decreases* under scaling, and O_i is a **irrelevant operator**.

If $y_i = 0$, O_i is a **marginal operator**, and higher order terms are necessary to track the behaviour.

The subspace spanned by the irrelevant directions is called the **basin of attraction** of the fixed point $\mathbf{S}^*$. Since ξ always decreases under RG ($\xi' = \xi/b$), and $\xi(\mathbf{S}^*) = \infty$, ξ is also infinite for any point on the basin of attraction of a critical fixed point $\mathbf{S}^*$. The surface defines the phase transition — it is equivalent to varying β (i.e. the temperature) at different values of the parameters and eventually meeting the surface.

In fact, for a general point in the vicinity of S^*, the correlation length satisfies the relation

$$\xi(g_1, g_2, \cdots) = b\xi(b^{y_1} g_1, b^{y_2} g_2, \cdots). \tag{4.6}$$

For sufficiently large b all the irrelevant operators scale to zero. The leading singularities of ξ are then determined by the remaining set of *relevant* operators. In particular, if the operators are indexed in order of decreasing dimensions, we can choose b such that $b^{y_1} g_1 = 1$. In this case Eq. (4.6) implies

$$\xi(g_1, g_2, \cdots) = g_1^{-1/y_1} f(g_2/g_1^{y_2/y_1}, \cdots).$$

We have thus obtained an exponent $\nu_1 = 1/y_1$ for the divergence of ξ, and a generalised set of gap exponents $\Delta_\alpha = y_\alpha/y_1$ associated with g_α.

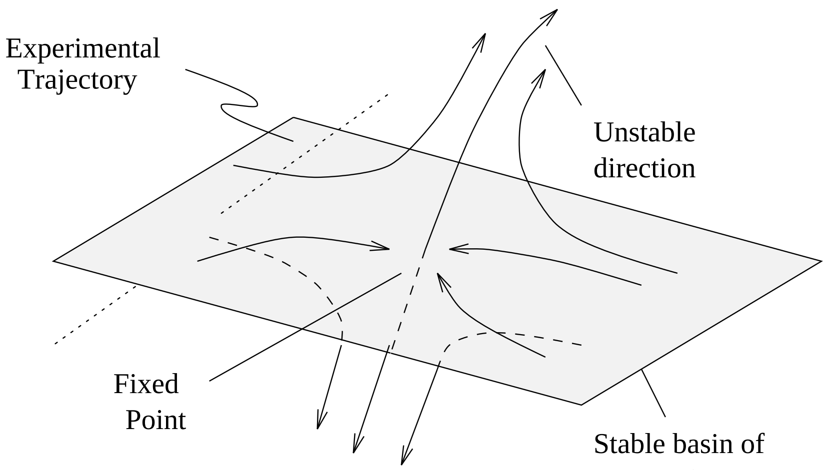


Figure 4.2: Schematic representation of RG flows in a high-dimensional space. Fixed-points describing ordered or disordered phases generally have basins of attraction with dimensions equal to that of the space of potentials. Fixed points describing critical points have a basin of attraction of lower dimensionality.

Let us imagine that the fixed point $\mathbf{S}^*$ describes the critical point of the magnet in Eq. (4.5) at zero magnetic field. As the temperature, or some other control parameter, is changed, the coefficients of the Hamiltonian are altered, and the point S follows a different trajectory in parameter space under renormalisation (see Fig. 4.2). Except for a single point (at the critical temperature) the magnet has a finite correlation length. This can be achieved if the experimental trajectory of the unrenormalised parameters $\mathbf{S}$ intersects the basin of attraction of $\mathbf{S}^*$ only at one point. To achieve this the basin must have co-dimension one, i.e. the fixed point S^* must have one and only one relevant operator.

This provides an explanation of **universality** in that the very many microscopic details of the system make up a huge space of irrelevant operators comprising the basin of attraction. In the presence of a magnetic field, two system parameters must be adjusted to reach the critical point, ($T = T_c$ and $h = 0$). Thus the magnetic field corresponds to an additional relevant operator of $\mathbf{S}^*$. *In general, for fixed points describing second-order critical points, there are two relevant parameters: the temperature and the field conjugate to the order parameter* (for the magnet it is the magnetic field).

Although the formal procedure outlined in this section is quite rigorous, it suffers from some quite obvious shortcomings: how do we actually implement the RG transformations analytically? There are an infinite number of interactions allowed by symmetry, and hence the space of parameters of $\mathbf{S}$ is inconveniently large. How do we know *a priori* that there are fixed points for the RG transformation; that $\mathbf{R}_b$ can be linearised; that relevant operators are few; etc? The way forward was presented by Wilson[2] who showed

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how these steps can be implemented (at least perturbatively) in the Ginzburg-Landau model.

4.3 The Gaussian Model

In this section we will apply the RG approach to study the **Gaussian theory** obtained by retaining only the terms to quadratic order in the Ginzburg-Landau Hamiltonian,

$$\mathcal{Z} = \int D\mathbf{m}(\mathbf{x}) \exp\left\{-\int d^d\mathbf{x}\left[\frac{t}{2}\mathbf{m}^2 + \frac{K}{2}(\nabla\mathbf{m})^2 - \mathbf{h}\cdot\mathbf{m}\right]\right\}, \tag{4.7}$$

where, as usual, $\mathbf{m}$ represents an n-component vector field. The absence of a term at order m^4 makes the Hamiltonian meaningful only for $t \geq 0$. The singularity at $t = 0$ can be considered as representing the ordered side of the phase transition.

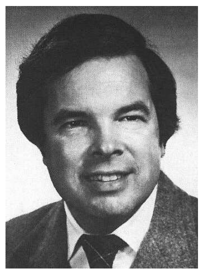
4.3.1 Exact Solution

Before turning to the RG analysis, let us first obtain the exact homogeneous form for the free energy density. Being of quadratic form, the Hamiltonian is diagonalised in Fourier space and generates the partition function[3]

$$\mathcal{Z} = \int D\mathbf{m}(\mathbf{q}) e^{-\beta H[\mathbf{m}]}, \qquad \beta H[\mathbf{m}] = \int \frac{d\mathbf{q}}{(2\pi)^d}\frac{1}{2}\left(t + K\mathbf{q}^2\right)|\mathbf{m}(\mathbf{q})|^2 - \mathbf{h}\cdot\mathbf{m}(\mathbf{q}=0).$$

Performing the Gaussian integral, and neglecting the constant factor $(2\pi)^{nN/2}$ arising from the Gaussian functional integral, we obtain the free energy density,

$$f(t,h) = -\frac{\ln\mathcal{Z}}{V} = \frac{n}{2}\int\frac{d\mathbf{q}}{(2\pi)^d}\ln(t + K\mathbf{q}^2) - \frac{h^2}{2t}.$$



Kenneth G. Wilson, 1936-: Recipient of the 1982 Nobel Prize in Physics, awarded for "discoveries he made in understanding how bulk matter undergoes phase transition, i.e., sudden and profound structural changes resulting from variations in environmental conditions". Wilson's background ranges from elementary particle theory and condensed matter physics (critical phenomena and the Kondo problem) to quantum chemistry and computer science.

[3]Setting $\mathbf{m}(\mathbf{x}) = \int (d\mathbf{q}/(2\pi)^d)\,\mathbf{m}(\mathbf{q})\,e^{i\mathbf{q}\cdot\mathbf{x}}$, $\mathbf{m}(\mathbf{q}) = \int d\mathbf{x}\,\mathbf{m}(\mathbf{x})\,e^{-i\mathbf{q}\cdot\mathbf{x}}$,

$$\begin{aligned}\int d\mathbf{x}\;\mathbf{m}(\mathbf{x})\cdot\mathbf{m}(\mathbf{x}) &= \int\frac{d\mathbf{q}}{(2\pi)^d)}\int\frac{d\mathbf{q}'}{(2\pi)^d}\mathbf{m}(\mathbf{q})\cdot\mathbf{m}(\mathbf{q}')\overbrace{\int\frac{d\mathbf{x}}{L^d}e^{i(\mathbf{q}+\mathbf{q}')\cdot\mathbf{x}}}^{(2\pi)^d\delta(\mathbf{q}+\mathbf{q}')}\\ &= \int\frac{d\mathbf{q}}{(2\pi)^d}\,\mathbf{m}(\mathbf{q})\cdot\mathbf{m}(-\mathbf{q}) = \int\frac{d\mathbf{q}}{(2\pi)^d}\,|\mathbf{m}(\mathbf{q})|^2,\end{aligned}$$

where we have used in the identity $\mathbf{m}^*(\mathbf{q}) = \mathbf{m}(-\mathbf{q})$.

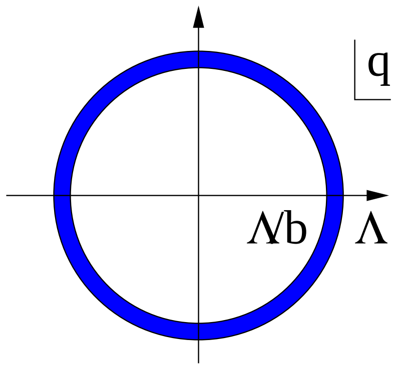


Figure 4.3: Diagram showing the shell in Fourier space that is integrated out in the renormalisation procedure.

Although the integral runs over the whole Fourier space $\mathbf{q}$, the important singular contributions originate from long wavelength modes (i.e. those around $\mathbf{q} = 0$). To study the non-analytic contributions to f, it is convenient to approximate the domain of integration by a "hypersphere" of radius $\Lambda \approx \pi/a$ where a denotes the short-length scale cut-off. The functional form of the integral can be obtained on dimensional grounds by rescaling $\mathbf{q}$ by a factor $\sqrt{t/K}$. Neglecting the upper limit to the integral, and logarithmic factors, the free energy takes the scaling form

$$f_{\text{sing.}}(t,h) = t^{d/2}\left[A + B\frac{h^2}{t^{1+d/2}}\right] \equiv t^{2-\alpha} g_f(h/t^{\Delta}),$$

where A and B represent dimensionless constants.

Thus, matching the points ($h = 0$, $t = 0^+$) and ($h \to 0$), the singular part of the free energy is described by the exponents

$$\boxed{\alpha_+ = 2 - d/2, \qquad \Delta = (2+d)/4.}$$

Since the ordered phase for $t < 0$ is not stable, the exponent β is undefined. The susceptibility, $\chi \propto \partial^2 f/\partial h^2 \propto 1/t$, diverges with an exponent $\gamma_+ = 1$.

4.3.2 The Gaussian Model via RG

The RG of the Gaussian model is most conveniently performed in terms of the Fourier modes. The goal is to evaluate the partition function (4.7) indirectly via the three steps of the RG:

1. **Coarse-Grain:** The first step involves the elimination of fluctuations at scales $a < |\mathbf{x}| < ba$. In spirit, it is similar to removing Fourier modes with wavenumbers

$\Lambda/b < |\mathbf{q}| < \Lambda$ (see Fig. 4.3.2). We thus separate the fields into slowly and rapidly varying functions, $\mathbf{m}(\mathbf{q}) = \mathbf{m}_>(\mathbf{q}) + \mathbf{m}_<(\mathbf{q})$, with

$$\mathbf{m}(\mathbf{q}) = \begin{cases} \mathbf{m}_<(\mathbf{q}) & 0 < |\mathbf{q}| < \Lambda/b, \\ \mathbf{m}_>(\mathbf{q}) & \Lambda/b < |\mathbf{q}| < \Lambda. \end{cases}$$

The partition function can be re-expressed in the form

$$\mathcal{Z} = \int D\mathbf{m}_<(\mathbf{q}) \int D\mathbf{m}_>(\mathbf{q}) e^{-\beta H[\mathbf{m}_<, \mathbf{m}_>]}.$$

Since the two sets of modes are decoupled in the Gaussian model, the integration is straightforward, and gives

$$\mathcal{Z} = \mathcal{Z}_> \int D\mathbf{m}_<(\mathbf{q}) \exp\left[-\int_0^{\Lambda/b} \frac{d\mathbf{q}}{(2\pi)^d} \left(\frac{t + K\mathbf{q}^2}{2} \right) |\mathbf{m}_<(\mathbf{q})|^2 + \mathbf{h} \cdot \mathbf{m}_<(0) \right],$$

where $\mathcal{Z}_> = \exp[-(nV/2) \int_{\Lambda/b}^{\Lambda} (d\mathbf{q}/(2\pi)^d) \ln(t + k\mathbf{q}^2)]$.

2. **Rescale:** The partition function for the modes $\mathbf{m}_<(\mathbf{q})$ is similar to the original, except that the upper cut-off has decreased to Λ/b, reflecting the coarse-graining in resolution. The rescaling, $\mathbf{x}' = \mathbf{x}/b$ in real space, is equivalent to $\mathbf{q}' = b\mathbf{q}$ in momentum space, and restores the cut-off to the original value.

3. **Renormalise:** The final step of the RG involves the renormalisation of magnetisation field, $\mathbf{m}'(\mathbf{x}') = \mathbf{m}_<(\mathbf{x}')/\zeta$. Alternatively, we can renormalise the Fourier modes according to $\mathbf{m}'(\mathbf{q}') = \mathbf{m}_<(\mathbf{q}')/z$, resulting in

$$\mathcal{Z} = \mathcal{Z}_> \int D\mathbf{m}'(\mathbf{q}') e^{-\beta H'[\mathbf{m}'(\mathbf{q}')]},$$
$$\beta H' = \int_0^{\Lambda} \frac{d\mathbf{q}'}{(2\pi)^d} b^{-d} z^2 \left(\frac{t + Kb^{-2}\mathbf{q}'^2}{2} \right) |\mathbf{m}'(\mathbf{q}')|^2 - z\mathbf{h} \cdot \mathbf{m}'(0).$$

The constant factor change from the Jacobian, as well as $\mathcal{Z}_>$, can be neglected in favour of the singular contribution from the exponent.

This procedure has transformed from a set of parameters $\mathbf{S} = \{K, t, h\}$ to a new set

$$\mathbf{S}' = \begin{cases} K' = Kb^{-d-2} z^2, \\ t' = tb^{-d} z^2, \\ h' = hz. \end{cases}$$

(Note that in general, such transformations can and often will lead to the appearance of new terms absent in the original Hamiltonian.) The singular point $t = h = 0$ is mapped onto itself as expected. To make the fluctuations scale invariant at this point, we must ensure that the remaining parameter in the Hamiltonian, K, stays fixed. This is achieved by the choice $z = b^{1+d/2}$ which implies that

$$\begin{cases} t' = b^2 t & y_t = 2, \\ h' = b^{1+d/2} h & y_h = 1 + d/2. \end{cases}$$

For the fixed point $t = t' = \infty$, K becomes weaker and the spins become uncorrelated — the high temperature phase.

From these equations, we can predict the scaling of the Free energy

$$\begin{aligned} f_{\text{sing.}}(t, h) &= b^{-d} f_{\text{sing.}}(b^2 t, b^{1+d/2} h) \qquad (b^2 t = 1) \\ &= t^{d/2} g_f(h/t^{1/2+d/4}). \end{aligned}$$

This implies the exponents: $2 - \alpha = d/2$, $\Delta = y_h/y_t = 1/2 + d/4$, $\nu = 1/y_t = 1/2$, $\gamma = 1$ and $\delta = \frac{d+2}{d-2}$. Comparing with the results from the exact solution we can confirm the validity of the RG. Further, a naive application of RG scaling gives $\beta = (d-2)/4$, even though the magnetisation is unbounded for $t < 0$ as the Gaussian theory is unstable. As expected, all of the exponents are fixed by two anomalous dimensions y_t, y_h, and therefore, the critical exponent identities apply.

At the fixed point ($t = h = 0$) the Hamiltonian must be scale invariant. This allows us to find the scaling of the renormalisation parameter ζ. By dimensional analysis $\mathbf{x} = b\mathbf{x}'$, $\mathbf{m}(\mathbf{x}) = \zeta \mathbf{m}'(\mathbf{x}')$ and

$$\beta H^* = \frac{K}{2} b^{d-2} \zeta^2 \int d\mathbf{x}' \, (\nabla \mathbf{m}')^2, \qquad \zeta = b^{1-d/2}.$$

Therefore, for small perturbations

$$\beta H^* + u_p \int d\mathbf{x} \, |\mathbf{m}(\mathbf{x})|^p \to \beta H^* + u_p b^d \zeta^p \int d\mathbf{x}' \, |\mathbf{m}'(\mathbf{x}')|^p.$$

Thus, in general $u_p \mapsto u_p' = b^d b^{p-pd/2} u_p = b^{y_p} u_p$, where $y_p = p - d(p/2 - 1)$, in agreement with our earlier findings that $y_1 \equiv y_h = 1 + d/2$ and $y_2 \equiv y_t = 2$. For the Ginzburg-Landau Hamiltonian, the quartic term scales with an exponent $y_4 = 4 - d$ and is therefore relevant for $d < 4$ and irrelevant for $d > 4$. Sixth order perturbations scale with an exponent $y_6 = 6 - 2d$ and is therefore irrelevant for $d > 3$.

Dangerous Irrelevant Couplings: Note that not all of the Gaussian fixed point exponents are consistent with mean-field exponents for $d > 4$. There is only perfect agreement at the upper critical dimension $d = 4$. Even though formally u is an irrelevant variable above $d = 4$, it must be included in the RG treatment to obtain correct critical exponents. Such a variable is known as a *dangerous irrelevant coupling*. Close to a general fixed point $t = h = 0, u = u^*$, the free energy scales as follows

$$\begin{aligned} f(t,h,u) &= b^{-d} f\left(b^{y_t} t, b^{y_h} h, u^* + b^{y_u}(u-u^*)\right) \\ &= b^{-d} f(b^{y_t} t, b^{y_h} h, u^*) + b^{y_u}(u-u^*) \left(\frac{\partial f}{\partial u}\right)_{u=u^*} \\ &\overset{b^{y_t} t = 1}{=} t^{d/y_t} g_f(h/t^{y_h/y_t}) + t^{-y_u/y_t}(u-u^*)\left(\frac{\partial f}{\partial u}\right)_{u=u^*} \end{aligned} \tag{4.8}$$

and so the irrelevant ($y_u < 0$) variable u can be neglected close to the fixed point $t = h = 0, u = u^*$, provided the free energy is *analytic* in u around that fixed point. As we will see, this is indeed the case at the Wilson-Fisher fixed point which develops in dimensions $d < 4$. In that case, the singular parts of the thermodynamic variables only depend on two exponents y_t, y_h and all the exponent identities derived previously hold. In dimensions $d > 4$, on the other hand, where mean-field behaviour takes hold, the free energy is *singular* in u at the Gaussian fixed point $t = h = u = 0$ and the critical exponents depend on all three anomalous dimensions y_t, y_h, y_u. Josephson's identity does not apply in this case. We demonstrate this for the heat capacity, although a similar derivation can be easily performed for the other thermodynamic variables

$$\begin{aligned} C = \left.\frac{\partial^2 f}{\partial t^2}\right|_{h=0} &= t^{d/y_t - 2} g_C(u/t^{y_u/y_t}) \\ &\overset{t\to 0}{=} t^{d/y_t - 2 - y_u/y_t}/u \\ &\overset{1/y_t = \nu}{=} t^{d\nu - 2 + \nu y_u}/u \end{aligned} \tag{4.9}$$

where, from mean-field theory, $g_C(u) \propto \frac{1}{u}$ for small u. Substituting in $y_u = 4 - d$, we find $\alpha = 4\nu - 2$ (cf. Josephson's identity) above the upper critical dimension. Further, substituting in the mean-field $\nu = \frac{1}{2}$, we find the mean-field heat capacity exponent $\alpha = 0$. [Note that both the mean-field correlation length and the susceptibility are independent of u. Hence, Gaussian exponents and mean-field exponents coincide in the case of γ and ν and by extension η.]

4.4 Wilson's Perturbative Renormalisation Group

In this section we will assess the extent to which the higher order terms in the Ginzburg-Landau expansion can be treated as a perturbation of the Gaussian model. Our method will be to combine the momentum space RG with a perturbative treatment of the Hamiltonian.

Since the unperturbed part of the Hamiltonian is diagonal in Fourier space, it is convenient to switch to that representation and re-express

$$\beta H[\mathbf{m}] = \overbrace{\int d\mathbf{x} \left[\frac{t}{2}\mathbf{m}^2 + \frac{K}{2}(\nabla \mathbf{m})^2\right]}^{\beta H_0} + \overbrace{u \int d\mathbf{x}\ \mathbf{m}^4}^{U},$$

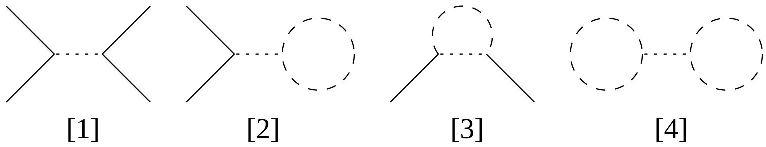


Figure 4.4: Diagrammatic representation of the correlators appearing in the text.

as

$$\beta H_0 = \int \frac{d\mathbf{q}}{(2\pi)^d}\frac{1}{2}\left(t + K\mathbf{q}^2\right)|\mathbf{m}(\mathbf{q})|^2,$$
$$U = u\int \frac{d\mathbf{q}_1}{(2\pi)^d}\int \frac{d\mathbf{q}_2}{(2\pi)^d}\int \frac{d\mathbf{q}_3}{(2\pi)^d}\ \mathbf{m}(\mathbf{q}_1)\cdot\mathbf{m}(\mathbf{q}_2)\ \mathbf{m}(\mathbf{q}_3)\cdot\mathbf{m}(-\mathbf{q}_1-\mathbf{q}_2-\mathbf{q}_3).$$

To implement the perturbative RG we proceed, as before, in three steps

1. **Coarse-Grain**: Subdividing the fluctuations into two components $\mathbf{m}(\mathbf{q}) = \mathbf{m}_<(\mathbf{q}) + \mathbf{m}_>(\mathbf{q})$, the contribution to the unperturbed (Gaussian) part of the Hamiltonian is separable while the perturbation mixes the terms. Integrating, we obtain

$$\begin{aligned}\mathcal{Z} &= \mathcal{Z}_0^> \int D\mathbf{m}_< e^{-\beta H_0[\mathbf{m}_<]}\overbrace{\frac{1}{\mathcal{Z}_0^>}\int D\mathbf{m}_> e^{-\beta H_0[\mathbf{m}_>]-U[\mathbf{m}_<,\mathbf{m}_>]}}^{\left\langle e^{-U[\mathbf{m}_<,\mathbf{m}_>]}\right\rangle_{\mathbf{m}_>}}\\ &= \mathcal{Z}_0^> \int D\mathbf{m}_< e^{-\beta H_0[\mathbf{m}_<]+\ln\left\langle e^{-U[\mathbf{m}_<,\mathbf{m}_>]}\right\rangle_{\mathbf{m}_>}},\end{aligned}$$

where $\mathcal{Z}_0^>$ denotes the contribution to the Gaussian (unperturbed) partition function arising from $\mathbf{m}_>$.

In general, the renormalisation of the Hamiltonian would call for the expansion

$$\ln\left\langle e^{-U}\right\rangle = -\langle U\rangle + \frac{1}{2}\left(\langle U^2\rangle - \langle U\rangle^2\right) + \cdots + \frac{(-1)^\ell}{\ell!}\left\langle U^\ell\right\rangle_c + \cdots,$$

where $\langle U^\ell\rangle_c$ denotes the ℓth cummulant. However, for simplicity, we will stop here at leading order in the perturbation from which we obtain

$$\beta H[\mathbf{m}_<] = \beta H_0[\mathbf{m}_<] - \ln[\mathcal{Z}_0^>] + \langle U\rangle_{\mathbf{m}_>} + O(u^2).$$

Only terms which are of an even order in $\mathbf{m}_>$ contribute to the average $\langle U\rangle_{\mathbf{m}_>}$. In particular, we will require averages of the form

$$\begin{aligned}C_1(\{\mathbf{q}_i\}) &= \langle \mathbf{m}_<(\mathbf{q}_1)\cdot\mathbf{m}_<(\mathbf{q}_2)\ \mathbf{m}_<(\mathbf{q}_3)\cdot\mathbf{m}_<(\mathbf{q}_4)\rangle_{\mathbf{m}_>},\\ C_2(\{\mathbf{q}_i\}) &= \langle \mathbf{m}_>(\mathbf{q}_1)\cdot\mathbf{m}_>(\mathbf{q}_2)\ \mathbf{m}_<(\mathbf{q}_3)\cdot\mathbf{m}_<(\mathbf{q}_4)\rangle_{\mathbf{m}_>},\\ C_3(\{\mathbf{q}_i\}) &= \langle \mathbf{m}_>(\mathbf{q}_1)\cdot\mathbf{m}_<(\mathbf{q}_2)\ \mathbf{m}_>(\mathbf{q}_3)\cdot\mathbf{m}_<(\mathbf{q}_4)\rangle_{\mathbf{m}_>},\\ C_4(\{\mathbf{q}_i\}) &= \langle \mathbf{m}_>(\mathbf{q}_1)\cdot\mathbf{m}_>(\mathbf{q}_2)\ \mathbf{m}_>(\mathbf{q}_3)\cdot\mathbf{m}_>(\mathbf{q}_4)\rangle_{\mathbf{m}_>}.\end{aligned}$$

C_1 simply generates $U[\mathbf{m}_<]$ while C_4 gives some constant independent of $\mathbf{m}_<$. The important contributions arise from C_2 and C_3 which can be represented diagrammatically as in Fig. 4.4.

For the unperturbed Hamiltonian the two-point expectation value is equal to

$$\langle m_\alpha(\mathbf{q}) m_\beta(\mathbf{q}')\rangle_0 = \delta_{\alpha\beta}\ (2\pi)^d \delta^d(\mathbf{q}+\mathbf{q}')\ G_0(\mathbf{q}), \qquad G_0(\mathbf{q}) = \frac{1}{t+K\mathbf{q}^2},$$

where the subscript zero indicates that the average is with respect to the unperturbed (Gaussian) Hamiltonian.[4] Using the results above we find

$$\begin{aligned} C_2(\{\mathbf{q}_i\}) &= nG_0(\mathbf{q}_1)\ (2\pi)^d\delta^d(\mathbf{q}_1+\mathbf{q}_2)\ \mathbf{m}_<(\mathbf{q}_3)\cdot\mathbf{m}_<(\mathbf{q}_4),\\ C_3(\{\mathbf{q}_i\}) &= G_0(\mathbf{q}_1)\ (2\pi)^d\delta^d(\mathbf{q}_1+\mathbf{q}_3)\ \mathbf{m}_<(\mathbf{q}_2)\cdot\mathbf{m}_<(\mathbf{q}_4). \end{aligned}$$

Dropping the irrelevant constant terms, C_4 and $\ln \mathcal{Z}_0^>$ we find that no new relevant terms appear in the coarse-grained Hamiltonian $\beta H[\mathbf{m}_<]$, and the coefficients K and u are unrenormalised, while

$$t \mapsto \widetilde{t} = t + 4u(n+2)\int_{\Lambda/b}^{\Lambda} \frac{d\mathbf{q}}{(2\pi)^d} G_0(\mathbf{q}),$$

the factor of $4(n+2)$ arising from enumerating all permutations.

[4]In general, the expectation value involving any product of $\vec{m}$'s can be obtained from the identity for Gaussian distributed random variables with zero mean

$$\boxed{\left\langle \exp\left[\int d\mathbf{x}\ \mathbf{a}(\mathbf{x})\cdot\mathbf{m}(\mathbf{x})\right]\right\rangle_0 = \exp\left[\int d\mathbf{x}\int d\mathbf{x}'\frac{1}{2}\ a_\alpha(\mathbf{x})\ \langle m_\alpha(\mathbf{x}) m_\beta(\mathbf{x}')\rangle_0\ a_\beta(\mathbf{x}')\right]}$$

Expanding both sides in powers of $\{\mathbf{a}(\mathbf{x})\}$ we obtain **Wick's theorem**

$$\left\langle \prod_{i=1}^{\ell} m_{\alpha_i}(x_i)\right\rangle_0 = \begin{cases} 0 & \ell \text{ odd},\\ \text{sum over all pairwide contractions} & \ell \text{ even}.\end{cases}$$

For example

$$\begin{aligned} \left\langle m_{\alpha_i}(x_i)m_{\alpha_j}(x_j)m_{\alpha_k}(x_k)m_{\alpha_l}(x_l)\right\rangle_0 &= \left\langle m_{\alpha_i}(x_i)m_{\alpha_j}(x_j)\right\rangle_0 \langle m_{\alpha_k}(x_k)m_{\alpha_l}(x_l)\rangle_0\\ &+ \left\langle m_{\alpha_i}(x_i)m_{\alpha_j}(x_k)\right\rangle_0 \langle m_{\alpha_k}(x_j)m_{\alpha_l}(x_l)\rangle_0 + \langle m_{\alpha_i}(x_k)m_{\alpha_l}(x_l)\rangle_0 \langle m_{\alpha_k}(x_k)m_{\alpha_l}(x_j)\rangle_0 . \end{aligned}$$

Moreover, in the presence of a perturbation U, the expectation value of any operator O can be expressed using the identity

$$\begin{aligned} \langle O\rangle &= \frac{\int Dm\ O\ e^{-\beta H}}{\int Dm\ e^{-\beta H}} = \frac{\int Dm\ O\ [1-U+U^2/2-\cdots]e^{-\beta H_0}}{\int Dm\ [1-U+U^2/2-\cdots]e^{-\beta H_0}}\\ &= \frac{\mathcal{Z}_0[\langle O\rangle_0 - \langle OU\rangle_0 + \langle OU^2/2\rangle_0 - \cdots]}{\mathcal{Z}_0[1-\langle U\rangle_0 + \langle U^2/2\rangle_0 - \cdots]} \equiv \sum_n \frac{(-1)^n}{n!}\langle OU^n\rangle_0^c = \left\langle Oe^{-U}\right\rangle_0^c, \end{aligned}$$

where the different orders in the expansion define the *connected average* denoted by the superscript c.

2. **Rescale**: As usual we set $\mathbf{q}' = b\mathbf{q}$.

3. **Renormalise**: Finally we set $\mathbf{m}' = \mathbf{m}_<(\mathbf{q}')/z$ and obtain

$$\beta H'[\mathbf{m}'] = \int_0^\Lambda \frac{d\mathbf{q}'}{(2\pi)^d} b^{-d} z^2 \left(\frac{\widetilde{t} + Kb^{-2}\mathbf{q}'^2}{2} \right) |\mathbf{m}'(\mathbf{q}')|^2$$
$$+ uz^4 b^{-3d} \int_0^\Lambda \frac{d\mathbf{q}_1'}{(2\pi)^d} \int_0^\Lambda \frac{d\mathbf{q}_2'}{(2\pi)^d} \int_0^\Lambda \frac{d\mathbf{q}_3'}{(2\pi)^d} \, \mathbf{m}'(\mathbf{q}_1') \cdot \mathbf{m}'(\mathbf{q}_2') \, \mathbf{m}'(\mathbf{q}_3') \cdot \mathbf{m}'(-\mathbf{q}_1' - \mathbf{q}_2' - \mathbf{q}_3').$$

The renormalised Hamiltonian is defined by

$$t' = b^{-d} z^2 \widetilde{t}, \qquad K' = b^{-d-2} z^2 K, \qquad u' = b^{-3d} z^4 u.$$

As in the Gaussian model, if we set $z = b^{1+d/2}$ such that $K' = K$, there is a fixed point at $t^* = u^* = 0$. The recursion relations for t and u in the vicinity of this point are given by

$$t' \equiv t(b) = b^2 \left[t + 4u(n+2) \int_{\Lambda/b}^\Lambda \frac{d^d\mathbf{q}}{(2\pi)^d} G_0(\mathbf{q}) \right],$$
$$u' \equiv u(b) = b^{4-d} u.$$

The recursion relation for u at this order is identical to that obtained by dimensional analysis; but that of t is modified. It is conventional to convert the above discrete recursion relations to continuous differential equations by setting $b = e^\ell$. For an infinitesimal $\delta\ell$,

$$t(b) \equiv t(1 + \delta\ell + \cdots) = t + \delta\ell \frac{dt}{d\ell} + O(\delta\ell^2),$$
$$u(b) = u + \delta\ell \frac{du}{d\ell} + O(\delta\ell^2).$$

Expanding the recursion relations, we obtain[5]

$$\frac{dt}{d\ell} = 2t + \frac{4u(n+2)K_d\Lambda^d}{t + K\Lambda^2},$$
$$\frac{du}{d\ell} = (4-d)u,$$

where $K_d \equiv S_d/(2\pi)^d$. Integrated, the second equation gives $u(\ell) = u_0 e^{(4-d)\ell} = u_0 b^{4-d}$.

[5]Here we have made use of the approximation

$$\int_{\Lambda/b}^\Lambda \frac{d\mathbf{q}}{(2\pi)^d} G_0(\mathbf{q}) \simeq \left(\Lambda - \frac{\Lambda}{b}\right) \Lambda^{d-1} \frac{S_d}{(2\pi)^d} \frac{1}{K\Lambda^2 + t}$$

and set $\Lambda(1 - e^{-\delta\ell}) \simeq \Lambda \, \delta\ell + \cdots$.

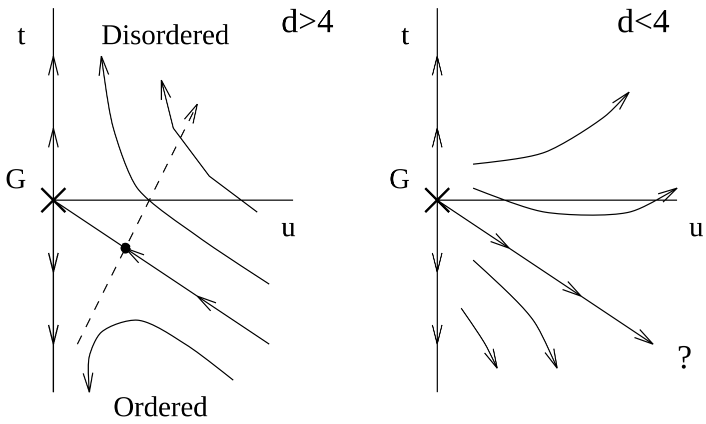


Figure 4.5: Perturbative RG flow of the Ginzburg-Landau model treated within the "one-loop" approximation.

The recursion relations can be linearised in the vicinity of the fixed point $t^* = u^* = 0$ by setting $t = t^* + \delta t$ and $u = u^* + \delta u$, as

$$\frac{d}{d\ell}\begin{pmatrix}\delta t\\ \delta u\end{pmatrix} = \begin{pmatrix}2 & 4(n+2)K_d\Lambda^{d-2}/K\\ 0 & 4-d\end{pmatrix}\begin{pmatrix}\delta t\\ \delta u\end{pmatrix}.$$

In the differential form, the eigenvalues of the matrix that enter the recursion relations determine the relevance of the operators. Since the matrix above has zero elements on one side, its eigenvalues are the diagonal elements and, as in the Gaussian model, we can identify $y_t = 2$, and $y_u = 4 - d$. The results at this order are identical to those obtained from dimensional analysis of the Gaussian model. The only difference is in the eigen-directions. The exponent $y_t = 2$ is still associated with $u = 0$, while $y_u = 4 - d$ is actually associated with the direction $t = 4u(n+2)K_d\Lambda^{d-2}/(2-d)K$.

For $d > 4$ the Gaussian fixed point has only one unstable direction associated with y_t. It thus correctly describes the phase transition. For $d < 4$ it has two relevant directions and is unstable. Unfortunately, the recursion relations have no other fixed point at this order and it appears that we have learned little from the perturbative RG. However, since we are dealing with a perturbative series alternating in sign, we can anticipate that the recursion relations at the next order are modified according to

$$\begin{aligned}\frac{dt}{d\ell} &= 2t + \frac{4u(n+2)K_d\Lambda^d}{t + K\Lambda^2} - Au^2,\\ \frac{du}{d\ell} &= (4-d)u - Bu^2,\end{aligned}$$

with A and B both positive. There is now an additional fixed point at $u^* = (4-d)/B$ for $d < 4$. For a systematic perturbation theory we need to keep the parameter u small. Thus the new fixed point can be explored systematically only for $\epsilon = 4 - d$; we are led to consider an expansion in the dimension of space in the vicinity of $d = 4$! For a calculation valid at $O(\epsilon)$ we have to keep track of terms of second order in the recursion relation for u, but only first order in t. It would thus be unnecessary to calculate the term A in the expression above.

4.5 †The ϵ-Expansion

▷ INFO: It is left as an exercise (see problem set II) to show that the expansion to second order ("two-loop") in u leads to the identity

$$B = -\frac{4(n+8)K_d\Lambda^d}{(t+K\Lambda^2)^2}.$$

Thus, in addition to the Gaussian fixed point at $u^* = t^* = 0$, there is now a non-trivial fixed point ($dt/d\ell = du/d\ell = 0$) at

$$\begin{cases} u^* = \frac{(t^*+K\Lambda^2)^2}{4(n+8)K_d\Lambda^d}\epsilon = \frac{K^2}{4(n+8)K_4}\epsilon + O(\epsilon^2), \\ t^* = -\frac{2u^*(n+2)K_d\Lambda^d}{t^*+K\Lambda^2} = -\frac{(n+2)}{2(n+8)}K\Lambda^2\epsilon + O(\epsilon^2), \end{cases}$$

where only those terms at leading order in $\epsilon = 4-d$ have been retained.

Linearising the recursion relations in the vicinity of the new fixed point we obtain

$$\frac{d}{d\ell}\begin{pmatrix}\delta t\\ \delta u\end{pmatrix} = \begin{pmatrix} 2-\frac{n+2}{n+8}\epsilon & \cdots \\ 0 & -\epsilon\end{pmatrix}\begin{pmatrix}\delta t\\ \delta u\end{pmatrix}.$$

The first eigenvalue is positive controlling the instability of the fixed point

$$\boxed{y_t = 2 - \frac{n+2}{n+8}\epsilon + O(\epsilon^2)}$$

while the second eigenvalue

$$\boxed{y_u = -\epsilon + O(\epsilon^2)}$$

is negative for $d<4$. The new fixed point thus has co-dimension one and can describe the phase transition in these dimensions. Although the position of the fixed point depends on microscopic parameters such as K and Λ, the final eigenvalues are pure numbers that depend only on n and $d = 4-\epsilon$. These eigenvalues characterise the **universality classes** of rotational symmetry breaking in $d<4$.

Continuing it is possible to obtain better estimates for critical exponents. However, even at second order, the ϵ-expansion does not make numerically accurate predictions in physical dimensions. Why then should one bother with such calculations? Their great virtue is that they provide a relatively straightforward way of determining what types of universality classes exist. Although the numerical values of the critical exponents change considerably as one moves away from the upper critical dimension, the topology of the flow diagrams does not. Thus one can investigate which interactions will lead to new universality classes and which will not. It is in this sense that the ϵ-expansion is largely responsible for our rather detailed understanding of critical phenomena.

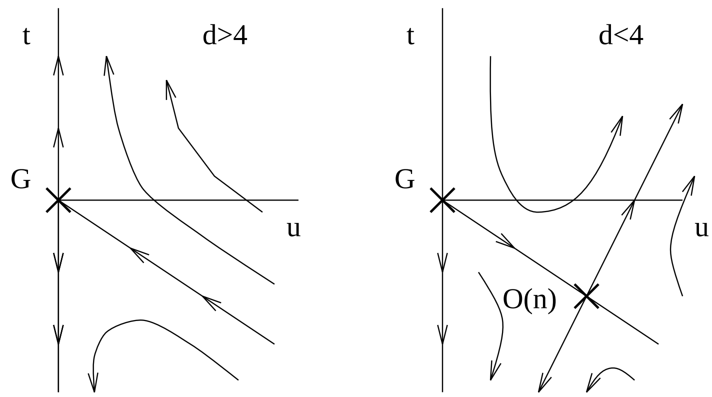


Figure 4.6: Perturbative RG flow of the Ginzburg-Landau model treated within the two-loop approximation.

The perturbative implementation of the RG procedure for the Ginzburg-Landau Hamiltonian was first performed by K. G. Wilson in the early 1970's, while the ϵ-expansion was developed jointly with M. E. Fisher.[6]

Wilson was awarded the Nobel prize in 1982. Historical details can be found in his Nobel lecture reprinted in Rev. Mod. Phys. **55**, 583 (1983). This concludes our investigation of the scaling theory and renormalisation group.

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[6] Michael E. Fisher: recipient of the 1995 Lars Onsager Prize "for his numerous and seminal contributions to statistical mechanics, including but not restricted to the theory of phase transitions and critical phenomena, scaling laws, critical exponents, finite size effects, and the application of the renormalisation group to many of the above problems".

Chapter 5

Topological Phase Transitions

Previously, we have seen that the breaking of a continuous symmetry is accompanied by the appearance of massless Goldstone modes. Fluctuations of the latter lead to the destruction of long-range order at any finite temperature in dimensions $d \leq 2$ — the Mermin-Wagner theorem. However, our perturbative analysis revealed only a power-law decay of spatial correlations in precisely two-dimensions — "quasi long-range order". Such cases admit the existence of a new type of continuous phase transition driven by the proliferation of topological defects. The aim of this section is to discuss the phenomenology of this type of transition which lies outside the usual classification scheme.

In classifying states of condensed matter, we usually consider two extremes: on the one hand there are crystalline solids in which atoms form a perfectly periodic array that extends to infinity in all directions. Such phases are said to possess **long-range order** (LRO). On the other hand there are fluids or glasses, in which the atoms are completely disordered and the system is both orientationally and positionally isotropic — that is the materials look the same when viewed from any direction. However, an intermediate state of matter is possible. In such a state the atoms are distributed at random, as in a fluid or glass, but the system is orientationally anisotropic on a macroscopic scale, as in a crystalline solid. This means that some properties of the fluid are different in different directions. Order of this sort is known as **bond-orientational order**.

This type of **quasi long-range order** is manifest in properties of superfluid and superconducting films (i.e. two-dimensions) and in the crystallisation properties of fluid membranes. As we have seen, according to the Mermin-Wagner theorem, fluctuations of a two-component or complex order parameter destroy LRO at all finite temperatures. However, at temperatures below T_c, quasi-LRO is maintained. The nature of this **topological phase transition** was first resolved by Berezinskii (Sov. Phys. JETP **32**, 493, (1971)) and later generalised to encompass a whole class of systems by Kosterlitz and Thouless[1] (J. Phys. C **5**, L124 (1972); **6**, 1181 (1973)). These include the melting of a two-dimensional crystal, with dislocations taking the place of vortices (Halperin and Nelson, Phys. Rev. Lett. **41**, 121 (1978)).

---

[1]

In this chapter, we will exploit a magnetic analogy to explore this unconventional type of phase transition which is driven by the condensation of **topological defects** known as vortices. Note that this type of phase transition is qualitatively quite different from those we have met previously.

5.1 Continuous Spins Near Two-Dimensions

Suppose unit n-component spins $\mathbf{S}_i = (s_{i1}, s_{i2}, \cdots s_{in})$ ($\mathbf{S}_i^2 = 1$) which occupy the sites i of a lattice and interact ferromagnetically with their neighbours.

$$-\beta H = K \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j = -\frac{K}{2} \sum_{\langle ij \rangle} \left[(\mathbf{S}_i - \mathbf{S}_j)^2 - 2 \right].$$

5.1.1 High Temperature Series

As usual we can try to confirm the existence of two separate phases, at high and low temperatures, by respectively treating β as a small or large parameter in the partition function. In the former case, we can expand the exponential in the partition function as follows

$$\mathcal{Z} = \int D\mathbf{S}_i \; \delta(\mathbf{S}^2 - 1) \; e^{-\beta H} = \int D\mathbf{S}_i \; \delta(\mathbf{S}^2 - 1) \left[1 + K \sum_{<ij>} S_i^\mu S_j^\mu + O(K^2) \right],$$

where we have used the notation $\delta(\mathbf{S}^2 - 1)$ to represent a "functional δ-function" — i.e., at all spatial coordinates, $\mathbf{S}(\mathbf{x})^2 = 1$. Summation over repeated Cartesian components μ is implied.

The high temperature expansion can be used to estimate the spin-spin correlation function $\langle \mathbf{S}_0 \cdot \mathbf{S}_\mathbf{x} \rangle$. The terms in the high temperature series are products of factors. Each factor in a given product corresponds to a lattice bond $\langle ij \rangle$. To leading order, only those products with factors which join sites 0 and $\mathbf{r}$ will survive and give a contribution. This is because once the integral over $\mathbf{S}_i$ is taken we have $\langle S_i^\mu S_j^\nu \rangle = \frac{1}{n} \delta_{\mu\nu} \delta_{ij}$, where the average is taken with respect to all possible configurations of $\mathbf{S}_i$.

$$\boxed{\langle \mathbf{S}_0 \cdot \mathbf{S}_\mathbf{x} \rangle \sim \left(\frac{K}{n} \right)^{|\mathbf{x}|} \sim \exp\left[-|\mathbf{x}|/\xi \right]}$$


John Michael Kosterlitz and David James Thouless: together with Duncan Haldane co-recipients of the 2016 Nobel Prize in Physics "for theoretical discoveries of topological phase transitions and topological phases of matter".

where $\xi^{-1} = \ln(n/K)$. This result implies an *exponential decay* of the spin-spin correlation function in the *disordered phase*. Note that that the number of possible lattice paths that connect two points can scale with at most $d^{|\mathbf{x}|}$ — we have neglected these non-universal lattice effects.

5.1.2 Low Temperature Series

At zero temperature the presumption is that the ground state configuration is ferromagnetic with all spins aligned along some direction (say $\mathbf{S}_i = \hat{\mathbf{e}}_n \equiv (0, 0, \cdots, 1)$). At low temperatures statistical fluctuations involve only low energy long wavelength modes which can be treated within a continuum approximation. Accordingly the Hamiltonian can be replaced by

$$\boxed{-\beta H[\mathbf{S}] = -\beta E_0 - \frac{K}{2}\int d\mathbf{x}\ (\nabla \mathbf{S})^2,}$$

where the discrete lattice index i has been replaced by a continuous vector $\mathbf{x} \in R^d$. The corresponding partition function is given by the so-called **non-linear σ-model**,

$$\boxed{\mathcal{Z} = \int D\mathbf{S}(\mathbf{x})\ \delta(\mathbf{S}^2 - 1)\ e^{-\beta H[\mathbf{S}]}.}$$

Here we have used the notation $\delta(\mathbf{S}^2 - 1)$ to represent a "functional δ-function" — i.e. at all spatial coordinates, $\mathbf{S}(\mathbf{x})^2 = 1$.

Fluctuations transverse to the ground state spin orientation $\hat{\mathbf{e}}_n$ are described by $n-1$ **Goldstone modes**. Adopting the parameterisation $\mathbf{S}(\mathbf{x}) = (\pi_1(\mathbf{x}), \cdots \pi_{n-1}(\mathbf{x}), (1 - \pi^2)^{1/2}) \equiv (\pi, (1-\pi^2)^{1/2})$, and expanding to quadratic order in π we obtain the following expression for the average transverse fluctuation (cf. section 2.5)

$$\begin{aligned}
\langle|\pi(\mathbf{x})|^2\rangle &= \int \frac{d^d\mathbf{q}}{(2\pi)^d}\langle|\pi(\mathbf{q})|^2\rangle = \int \frac{d^d\mathbf{q}}{(2\pi)^d}\frac{n-1}{K\mathbf{q}^2} \\
&= \frac{n-1}{K}\frac{S_d}{(2\pi)^d}\frac{a^{2-d} - L^{2-d}}{d-2} \xrightarrow{L\to\infty} \frac{(n-1)K_d}{K}\begin{cases} a^{2-d} \propto T & d > 2, \\ L^{2-d} \to \infty & d \le 2. \end{cases}
\end{aligned}$$

This result suggests that in more than two dimensions we can always find a temperature where the magnitude of the fluctuations is small while in dimensions of two or less fluctuations always destroy long-range order. This is in accord with the Mermin-Wagner theorem discussed in section 2.5 which predicted the absence of long-range order in $d \le 2$. Even so, for $d = 2$ the low temperature analysis still indicates the presence of a low-temperature phase which is distinct from the high-temperature phase with a finite correlation length. This phase, rather than exhibiting true long-range order has **quasi long-range order** (power-law order)

$$\langle \mathbf{S}(\mathbf{0}) \cdot \mathbf{S}(\mathbf{x})\rangle \approx e^{-\frac{n-1}{2\pi K}\ln\left(\frac{\mathbf{x}}{a}\right)} = \left(\frac{a}{|\mathbf{x}|}\right)^{\frac{n-1}{2\pi K}} \tag{5.1}$$

This analysis is in fact incorrect for $n > 2$ as higher order interaction terms between the $n-1$ Goldstone mode branches are relevant. For $n = 2$ there is only one Goldstone mode branch and the low temperature expansion is stable – the power-law phase extends to finite temperatures. The mechanism behind the phase transition responsible for loss of power-law order at high temperatures will be the subject of the next section. We now demonstrate in the case of $n = 3$ that interactions between two different Goldstone mode branches are relevant. (This argument carries through to $n > 3$).

$$
\begin{aligned}
\beta H[\mathbf{S}(\mathbf{x})] &= \frac{K}{2}\int d^d\mathbf{x}\,(\mathbf{e}_\theta\partial_\mu\theta + \mathbf{e}_\phi\sin\theta\partial_\mu\phi)\cdot(\mathbf{e}_\theta\partial_\mu\theta + \mathbf{e}_\phi\sin\theta\partial_\mu\phi) \\
&\overset{\substack{\theta\to\frac{\pi}{2}+\theta \\ K=T^{-1}}}{=} \frac{1}{2T}\int d^d\mathbf{x}\left[\partial_\mu\theta\partial^\mu\theta + \partial_\mu\phi\partial^\mu\phi - \frac{1}{2}\theta^2\partial_\mu\phi\partial^\mu\phi + \mathcal{O}(\theta^4\phi^2)\right] \\
&\overset{\substack{\theta\to\sqrt{T}\theta \\ \phi\to\sqrt{T}\phi}}{=} \int d^d\mathbf{x}\left[\partial_\mu\theta\partial^\mu\theta + \partial_\mu\phi\partial^\mu\phi - \frac{T}{2}\theta^2\partial_\mu\phi\partial^\mu\phi + \mathcal{O}(\theta^4\phi^2)\right]
\end{aligned}
\tag{5.2}
$$

where $\theta(\mathbf{r})$ and $\phi(\mathbf{r})$ are the spherical polar angles of the spin vector $\mathbf{S}(\mathbf{r})$, $\mathbf{e}_\theta$, $\mathbf{e}_\phi$ the corresponding unit direction vectors, and $(\theta = \pi/2, \phi = 0)$ is the globally uniform configuration around which we are expanding. We have also explicitly shown that the quartic interaction term is small in T. This is why T is referred to as the **coupling** as it is a measure of the interaction strength between the Goldstone modes. Under naive RG scaling of $(\theta,\phi) \to b^{\frac{2-d}{2}}(\theta,\phi)$ and $\mathbf{x} \to b\mathbf{x}$, it is clear that this term is relevant in $d \leq 2$. In fact, Polyakov [Phys. Lett. **59**B, 79 (1975)] developed a perturbative RG expansion close to two-dimensions that shows that the interactions between these Goldstone modes lead to the instability of the low-temperature fixed point for $d \leq 2$, i.e., the system flows towards the high-temperature $K = 0$ fixed point as soon as K becomes finite.[2]

The excitation of Goldstone modes therefore rules out spontaneous order in two-dimensional models with a continuous symmetry. An RG analysis of the non-linear σ-model indeed confirms that the transition temperature of n-component spins vanishes as $T^* = 2\pi\epsilon/(n-2)$ for $\epsilon = (d-2) \to 0$ (see problem set 2). This unstable fixed point that separates the low and high temperature phases moves to a finite temperature as d is increased above 2. The RG also indicates that the behaviour for $n = 2$ is in some sense marginal.

RG flow for $n = 3$ and $d = 2$: We now analyse the RG flow equation, derived by Polyakov, in more detail in the case of $n = 3$ and $d = 2$ (see problem set 2)

$$\boxed{\frac{dT}{dl} = \frac{T^2}{2\pi},} \tag{5.3}$$

[2]Polyakov's work provided one of the milestones in the study of critical phenomena. The $\epsilon = d-2$ expansion employed in the perturbative RG approach set the framework for numerous subsequent investigations. A description of the RG calculation can be found in Chaikin and Lubensky and is assigned as a question in the problem set 2.

where $T = K^{-1}$. Integrating the above equation we obtain

$$\frac{1}{T} - \frac{1}{T'} = \frac{l}{2\pi}, \tag{5.4}$$

where $T' = T$ at $l = 0$. We can also write down separate flow equations for the correlation length ξ and the momentum p

$$\begin{aligned} \xi' &= \xi e^{-l}, \\ p' &= p e^{l}. \end{aligned} \tag{5.5}$$

If we choose $T \sim \mathcal{O}(1)$, then $\xi \sim a$. We thus obtain

$$\boxed{\xi' \sim a e^{\frac{2\pi}{T'}},} \tag{5.6}$$

for the divergence of the correlation length as $T' \to 0$. This divergence is non-perturbative, i.e., it could not have been obtained from any finite order of perturbation theory.

Running coupling: In general, we can map correlation functions at momentum p and coupling T to ones at momentum p' and coupling T'. The change of correlators with l can be obtained from the RG flow equations and is described by the Callan-Symanzik equation. We will demonstrate this idea by considering the flow of the following non-linear σ model correlator for the case $n = 3$, $d = 2$

$$G(x,T) = \langle \mathbf{S}(\mathbf{x}) \cdot \mathbf{S}(0) \rangle_T \approx \langle 1 + 2\phi(\mathbf{x})\phi(0) - 2\phi^2(0) \rangle_T, \tag{5.7}$$

where $\phi(\mathbf{x})$ is the azimuthal angle of the three-component spin and to leading order its renormalisation factor $\zeta = 1$ (see problem set 3). Note that, to leading order, the fast and slow parts of $\phi(\mathbf{x})$ separate. Neglecting the quartic terms, we can write down

$$\langle 1 + 2\phi(\mathbf{x})\phi(0) - 2\phi^2(0) \rangle_T \approx \langle 1 + 2\phi_<(\mathbf{x})\phi_<(0) - 2\phi_<^2(0) \rangle \langle 1 + 2\phi_>(\mathbf{x})\phi_>(0) - 2\phi_>^2(0) \rangle\,. \tag{5.8}$$

Considering the flow of the correlator from $l = 0$ to δl, we obtain for $\delta l \ll 1$

$$\begin{aligned} G(x,T) &= G\left(xe^{-\delta l}, T'(\delta l)\right)\left(1 - 2\langle \phi^2(0) - \phi(\mathbf{x})\phi(0) \rangle_>\right) \\ &= G\left(xe^{-\delta l}, T'(\delta l)\right)\left(1 - 2\int_{\Lambda e^{-\delta l}}^{\Lambda} \frac{d^2\mathbf{q}}{(2\pi)^2}\frac{T}{\mathbf{q}^2}\left(1 - e^{i\mathbf{q}\cdot\mathbf{x}}\right)\right) \\ &\overset{\Lambda|\mathbf{x}|\gg 1}{=} G\left(xe^{-\delta l}, T'(\delta l)\right)\left(1 - 2\int_{\Lambda e^{-\delta l}}^{\Lambda} \frac{d^2\mathbf{q}}{(2\pi)^2}\frac{T}{\mathbf{q}^2}\right) \\ &= G\left(xe^{-\delta l}, T'(\delta l)\right) e^{-\frac{T}{\pi}\delta l}, \end{aligned} \tag{5.9}$$

where the factor is the result of integrating out fluctuations $\Lambda e^{-l} \leq |\mathbf{q}| \leq \Lambda$, which are not present in the correlator that is evaluated with the renormalised parameters. Taking the Fourier transform of both sides of the equation, we obtain

$$G(p,T) = e^{-\frac{T}{\pi}\delta l + 2\delta l} G(pe^{\delta l}, T'(\delta l))\,. \tag{5.10}$$

Considering a succession of RG transformations we thus obtain

$$G(p,T) = e^{2l}\Gamma(l)G(pe^l, T'(l)), \tag{5.11}$$

where Γ is the amplitude factor accumulated through a series of integrations over the short-distance fluctuations

$$\Gamma(l) = \exp\left[-\int_0^l \frac{T'(l)}{\pi} dl\right], \tag{5.12}$$

and the integrand in the exponential $\gamma(T) = -\frac{T}{\pi}$ is known as the **gamma function**.

Choosing an l such that $pe^l = p'$, we obtain

$$G(p,T) = \Gamma\left(\ln\frac{p'}{p}\right)\left(\frac{p'}{p}\right)^2 G\left(p', T'\left(\ln\frac{p'}{p}\right)\right), \tag{5.13}$$

where

$$\boxed{T'\left(\ln\frac{p'}{p}\right) = \frac{1}{\frac{1}{T}+\frac{1}{2\pi}\ln\frac{p}{p'}} \to \frac{2\pi}{\ln\frac{p}{p'}} \quad \text{as} \quad \frac{p}{p'} \to \infty} \tag{5.14}$$

is known as the running (or effective) coupling constant at momentum p and its derivative $\frac{dT'}{d\ln\frac{p}{p'}} = \beta(T')$ is known as the **beta function**. Hence, in the limit $p/p' \to \infty$ ($p' \sim \mathcal{O}(1)$ is kept fixed and the lattice cutoff $1/a$ has been taken to infinity), we can expand $G\left(p', T'\left(\ln\frac{p'}{p}\right)\right)$ in small T'. In the limit $T \to 0$ the correlation length ξ diverges and the correlator $G(x, T\to 0) \to \frac{1}{x^{T/\pi}}$ at a fixed lengthscale $x \ll \xi$, and its Fourier transform is therefore $G(p,T) \to 1/p^{2-T/\pi}$

$$G\left(p', T'\left(\ln\frac{p'}{p}\right)\right) = \frac{1}{p'^2} + \mathcal{O}\left(\frac{1}{\ln p/p'}\right), \tag{5.15}$$

$$G(p,T) = \Gamma\left(\ln\frac{p'}{p}\right)\left[\frac{1}{p^2} + \mathcal{O}\left(\frac{1}{\ln p/p'}\right)\right]. \tag{5.16}$$

The correlators tend to those of a purely quadratic theory in the large momentum limit with logarithmically small corrections. In other words, the effective (or **running**) coupling becomes logarithmically small at large momenta.

Exercise for the Reader:
Show that the gamma function gives rise to logarithmic corrections $\Gamma\left(\ln\frac{p'}{p}\right) \propto \ln^2\frac{p'}{p}$ as $\frac{p'}{p} \to \infty$.

5.2 Topological Defects in the XY-Model

The first indication of unusual behaviour in the two-dimensional XY-model ($n = 2$) appeared in an analysis of the high temperature series expansion by Stanley and Kaplan (1971). The series appeared to indicate a divergence of susceptibility at a finite temperature, seemingly in contradiction with the absence of symmetry breaking. It was this contradiction that led Wigner to explore the possibility of a *phase transition without symmetry breaking*. It is the study of this novel and important type of phase transition to which we now turn. We begin our analysis with a study of the asymptotic behaviour of the partition function at high and low temperatures using a series expansion.

5.2.1 High Temperature Series

In two-dimensions it is convenient to parameterise the spins by their angle with respect to the direction of one of the ground state configurations $\mathbf{S} = (\cos\theta, \sin\theta)$. The spin Hamiltonian can then be presented in the form

$$\boxed{-\beta H = K \sum_{\langle ij \rangle} \cos(\theta_i - \theta_j).}$$

At high temperatures the partition function can be expanded in powers of K

$$\mathcal{Z} = \int_0^{2\pi} \prod_i \frac{d\theta_i}{2\pi} e^{-\beta H} = \int_0^{2\pi} \prod_i \frac{d\theta_i}{2\pi} \prod_{\langle ij \rangle} \left[1 + K\cos(\theta_i - \theta_j) + O(K^2)\right].$$

Each term in the product can be represented by a "bond" that connects neighbouring sites i and j. To the lowest order in K, each bond on the lattice contributes either a factor of one, or $K\cos(\theta_i - \theta_j)$. But, since $\int_0^{2\pi}(d\theta_1/2\pi)\cos(\theta_1 - \theta_2) = 0$ any graph with a single bond emanating from a site vanishes. On the other hand, a site at which two-bonds meet yields a factor $\int_0^{2\pi}(d\theta_2/2\pi)\cos(\theta_1 - \theta_2)\cos(\theta_2 - \theta_3) = \cos(\theta_1 - \theta_3)/2$. The first non-vanishing contributions to the partition function arise from closed loop configurations that encircle one plaquette.

The high temperature expansion can be used to estimate the spin-spin correlation function $\langle \mathbf{S}_0 \cdot \mathbf{S}_\mathbf{x} \rangle = \langle \cos(\theta_\mathbf{x} - \theta_0) \rangle$. To leading order, only those graphs which join sites 0 and $\mathbf{r}$ will survive and give a contribution

$$\boxed{\langle \mathbf{S}_0 \cdot \mathbf{S}_\mathbf{x} \rangle \sim \left(\frac{K}{2}\right)^{|\mathbf{x}|} \sim \exp\left[-|\mathbf{x}|/\xi\right],}$$

where $\xi^{-1} = \ln(2/K)$. This result implies an *exponential decay* of the spin-spin correlation function in the *disordered phase*.

5.2.2 Low Temperature Series

At low temperature the cost of small fluctuations around the ground state is obtained within a quadratic expansion which yields the Hamiltonian corresponding to Eq. (2.18)

$$-\beta H = \frac{K}{2}\int d\mathbf{x}(\nabla\theta)^2,$$

in the continuum limit. Note that the integration measure $d^2\mathbf{x}$ is in units of a. According to the standard rules of Gaussian integration

$$\langle \mathbf{S}(0)\cdot\mathbf{S}(\mathbf{x})\rangle = \mathrm{Re}\left\langle e^{i(\theta(0)-\theta(\mathbf{x}))}\right\rangle = \mathrm{Re}\left[e^{-\langle(\theta(0)-\theta(\mathbf{x}))^2\rangle/2}\right].$$

In section 2.5 we saw that in two-dimensions Gaussian fluctuations grow logarithmically $\langle(\theta(0)-\theta(\mathbf{x}))^2\rangle/2 = \ln(|\mathbf{x}|/a)/2\pi K$, where a denotes a short distance cut-off (i.e. lattice spacing). Therefore, at low temperatures the spin-spin correlation function decays *algebraically* as opposed to exponential.

$$\boxed{\langle \mathbf{S}(0)\cdot\mathbf{S}(\mathbf{x})\rangle \simeq \left(\frac{a}{|\mathbf{x}|}\right)^{1/2\pi K}.}$$

A power law decay of correlations implies self-similarity (i.e. no correlation length), as is usually associated with a critical point. Here it arises from the logarithmic growth of angular fluctuations, which is specific to two-dimensions.

The distinction between the nature of the asymptotic decays allows for the possibility of a finite temperature phase transition. However, the arguments so far put forward are not specific to the XY-model. Any continuous spin model in $d = 2$ will exhibit exponential decay of correlations at high temperature, and a power law decay in a low temperature Gaussian approximation. Strictly speaking, to show that Gaussian behaviour persists to low temperatures we must prove that it is not modified by the additional terms in the gradient expansion. Quartic terms, such as $\int d^d\mathbf{x}(\nabla\theta)^4$, generate interactions between Goldstone modes belonging to the same branch and naive RG scaling suggests they are irrelevant in $d = 2$. This can be confirmed using perturbative RG (see problem set 2).

Exercise for the Reader:
Show that naive RG scaling suggests that terms $\int d^d\mathbf{x}(\nabla\theta)^4$ are irrelevant.

We have already seen that the zero temperature fixed point in $d = 2$ is unstable for all $n > 2$ but apparently stable for $n = 2$. (There is only one branch of Goldstone modes for $n = 2$. It is the interactions between different branches of these modes for $n > 2$ that are relevant and lead to instability towards high temperature behaviour.) The low temperature phase of the XY-model is said to possess **quasi-long range order**, as opposed to **true long range order** that accompanies finite magnetisation.

What is the mechanism for the disordering of the quasi-long range ordered phase? Since the RG suggests that higher order terms in the gradient expansion are not relevant it is necessary to search for other relevant operators.

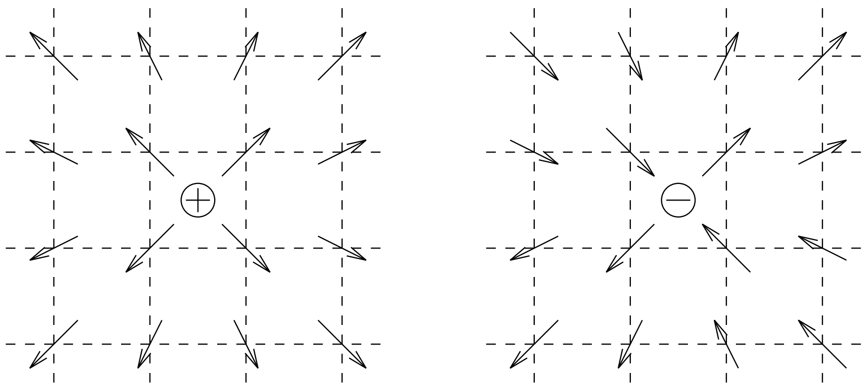

Figure 5.1: Spin configurations of the two-dimensional XY-model showing vortices of charge ±1.

5.3 Vortices

The gradient expansion describes the energy cost of *small* deformations around the ground state and applies to configurations that can be continuously deformed to the uniformly ordered state. Berezinskii, and later Kosterlitz and Thouless, suggested that the disordering is caused by **topological defects** that can not be obtained from such deformations.

Since the angle describing the orientation of a spin is defined up to an integer multiple of 2π, it is possible to construct spin configurations in which the traversal of a closed path will see the angle rotate by $2\pi n$. The integer n is the **topological charge** enclosed by the path. The discrete nature of the charge makes it impossible to find a continuous deformation which returns the state to the uniformly ordered configuration in which the charge is zero. (More generally, topological defects arise in any model with a compact group describing the order parameter — e.g. a 'skyrmion in an $O(3)$' or three-component spin Heisenberg Ferromagnet, or a dislocation in a crystal.)

The elementary defect, or **vortex**, has a unit charge. In completing a circle centred on the defect the orientation of the spin changes by $\pm 2\pi$ (see Fig. 5.1). If the radius r of the circle is sufficiently large, the variations in angle will be small and the lattice structure can be ignored. By symmetry $\nabla\theta$ has uniform magnitude and points along the azimuthal direction. The magnitude of the distortion is obtained by integrating around a path that encloses the defect,

$$\boxed{\oint \nabla\theta \cdot d\ell = 2\pi n \quad \Longrightarrow \quad \nabla\theta = \frac{n}{r}\hat{\mathbf{e}}_r \times \hat{\mathbf{e}}_z,}$$

where $\hat{\mathbf{e}}_r$ and $\hat{\mathbf{e}}_z$ are unit vectors respectively in the plane and perpendicular to it. This (continuum) approximation fails close to the centre (core) of the vortex, where the lattice structure is important.

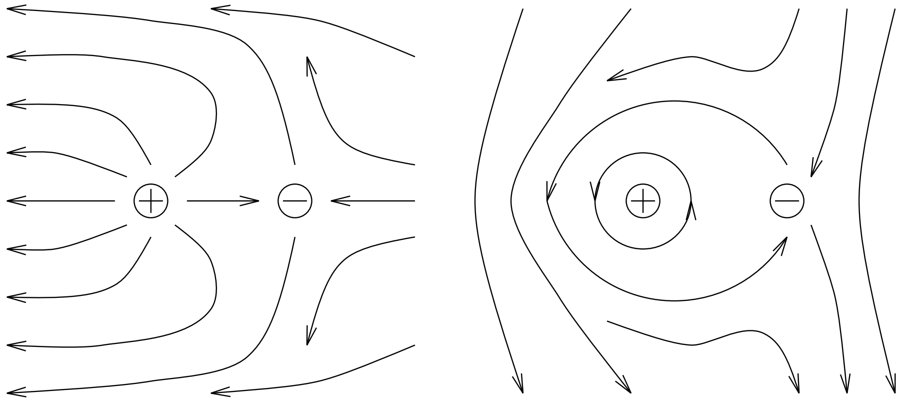

Figure 5.2: Spin configurations of vortex/antivortex pairs.

The energy cost from a single vortex of charge n has contributions from the core region, as well as from the relatively uniform distortions away from the centre. The distinction between regions inside and outside the core is arbitrary, and for simplicity, we shall use a circle of radius a to distinguish the two, i.e.

$$\boxed{\beta E_n = \beta E_n^0(a) + \frac{K}{2}\int_a d\mathbf{x}(\nabla\theta)^2 = \beta E_n^0(a) + \pi K n^2 \ln\left(\frac{L}{a}\right).}$$

The dominant part of the energy comes from the region outside the core and diverges logarithmically with the system size L.[3] The large energy cost associated with the defects prevents their spontaneous formation close to zero temperature. The partition function for a configuration with a single vortex of charge n is

$$\mathcal{Z}_1(n) \approx \left(\frac{L}{a}\right)^2 \exp\left[-\beta E_n^0(a) - \pi K n^2 \ln\left(\frac{L}{a}\right)\right], \tag{5.17}$$

where the factor of $(L/a)^2$ results from the *configurational entropy* of possible vortex locations in an area of size L^2. The entropy and energy of a vortex both grow as $\ln L$, and the free energy is dominated by one or the other. At low temperatures, large K, energy dominates and $\mathcal{Z}_1$, a measure of the weight of configurations with a single vortex, vanishes. At high enough temperatures, $K < K_n = 2/(\pi n^2)$, the entropy contribution is large enough to favour spontaneous formation of vortices. On increasing temperature, the first vortices that appear correspond to $n = \pm 1$ at $K_c = 2/\pi$. Beyond this point many vortices appear and Eq. (5.17) is no longer applicable.

In fact this estimate of K_c represents only a *lower bound* for the stability of the system towards the condensation of topological defects. This is because pairs (dipoles) of defects may appear at larger couplings. Consider a pair of charges ± 1 separated by a distance

[3]Notice that if the spin degrees of freedom have three components or more, the energy cost of a defect is finite.

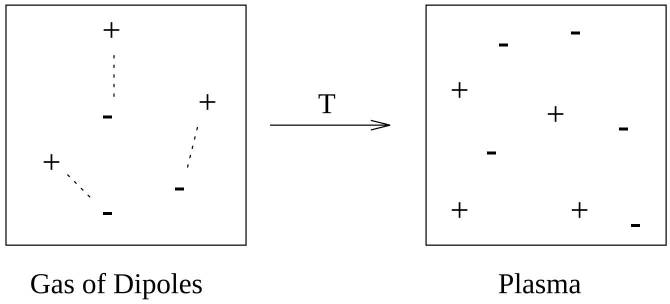

Figure 5.3: Schematic diagram showing the deconfinement of vortex pairs.

d. Distortions far from the core $|\mathbf{r}| \gg d$ can be obtained by superposing those of the individual vortices (see fig. 5.2)

$$\nabla\theta = \nabla\theta_+ + \nabla\theta_- \approx 2\mathbf{d}\cdot\nabla\left(\frac{\hat{\mathbf{e}}_r \times \hat{\mathbf{e}}_z}{|\mathbf{r}|}\right),$$

which decays as $d/|\mathbf{r}|^2$. Integrating this distortion leads to a *finite* energy, and hence dipoles appear with the appropriate Boltzmann weight at any temperature. The low temperature phase should therefore be visualised as a gas of tightly bound dipoles (see fig. 5.3), their density and size increasing with temperature. The high temperature phase constitutes a plasma of unbound vortices. A theory of the Berezinskii-Kosterlitz-Thouless transition based on an RG description can be found in Chaikin and Lubensky.

5.3.1 Coulomb Gas Description of the XY Model

Vortex Interactions: In deriving long-distance vortex-vortex interactions, we can take the continuum $a \to 0$ and thermodynamic $L \to \infty$ limits. The flow field $\mathbf{v}$ of a single vortex with integer charge q at $\mathbf{r} = \mathbf{0}$ satisfies the following equation

$$\mathbf{v} = \nabla\theta = \frac{q}{r}\mathbf{e}_\phi, \tag{5.18}$$

with

$$\nabla\times\mathbf{v} = 2\pi q\delta(\mathbf{r})\mathbf{e}_z. \tag{5.19}$$

For multiple vortices with charges q_i at locations $\mathbf{r}_i$, we therefore have

$$\boxed{\nabla\times\mathbf{v} = 2\pi\sum_i q_i\delta(\mathbf{r}-\mathbf{r}_i)\mathbf{e}_z.} \tag{5.20}$$

We now introduce a scalar potential $\Psi(\mathbf{r})$ to parametrise the flow field $\mathbf{v}$

$$\mathbf{v} = \nabla\times\Psi\mathbf{e}_z. \tag{5.21}$$

Eq. (5.20) thus leads to Laplace's equation for $\Psi(\mathbf{r})$ with the following unique solution

$$\boxed{\begin{aligned} &\nabla^2\Psi = -2\pi \sum_i q_i \delta(\mathbf{r}-\mathbf{r}_i), \\ &\Psi = -\sum_i q_i \ln|\mathbf{r}-\mathbf{r}_i|. \end{aligned}} \tag{5.22}$$

The energy of this multiple vortex configuration is given by

$$\begin{aligned} \beta H &= \frac{K}{2}\int d^2\mathbf{r}\, \mathbf{v}^2 = \frac{K}{2}\int d^2\mathbf{r}\, \left[(\partial_x\Psi)^2 + (\partial_y\Psi)^2\right] \\ &= -\frac{K}{2}\int d^2\mathbf{r}\, \Psi\left(\partial_x^2+\partial_y^2\right)\Psi + \frac{K}{2}\int_S (\Psi\nabla\Psi)\cdot d\mathbf{S} \\ &= -\pi K\sum_{i,j} q_i q_j \ln|\mathbf{r}_i - \mathbf{r}_j|, \end{aligned} \tag{5.23}$$

where the surface integral vanishes for configurations that are overall charge neutral $\sum_i q_i = 0$ (we have imposed periodic boundary conditions). As expected, the above formula gives us a divergent result for $\mathbf{r}_i = \mathbf{r}_j$ (because $L/a \to \infty$ in the continuum picture), but gives the correct asymptotic limit ($|\mathbf{r}_i - \mathbf{r}_j|/a \gg 1$) of the vortex-vortex interaction.

In the large K limit vortices will come in tightly bound vortex-antivortex pairs. We can regularise the above expression by considering the energy of a single vortex-antivortex pair

$$\beta H_{\text{pair}} = 2Eq^2 - 4\pi^2 q^2 K C(\mathbf{x}), \tag{5.24}$$

where q, $-q$ are the charges of the vortex and the anitvortex respectively, and $2E$ is the self-energy of a dipole of size a. The function $C(\mathbf{x}) = 0$ for $|\mathbf{x}| \le a$ and $C(\mathbf{x}) = \frac{1}{2\pi}\ln(|\mathbf{x}|/a)$ for $|\mathbf{x}| \ge a$. Note that we also need to enforce that the vortex separation is $|\mathbf{x}| \ge a$, because otherwise the vortices could annihilate and the above Hamiltonian would no longer give the correct energy.

In a system with multiple vortex-antivortex pairs we then have

$$\beta H = E\sum_i q_i^2 - 2\pi^2 K \sum_{i\neq j} q_i q_j C(\mathbf{x}_i - \mathbf{x}_j), \tag{5.25}$$

where E can now be interpreted as the core vortex self-energy. As the vortex-antivortex separation is increased the energy increases logarithmically indicating that there are 2D Coulomb forces between the vortices which are inversely proportional to their separation. It is important to note that the parameter K that determines the long-distance vortex interactions is the same parameter that enters the long-wavelength Gaussian limit of the original XY model, whereas the parameter E that determines the vortex core energy is directly related to the nearest-neighbour microscopic interactions of the original XY model (a cosine potential).

Dilute 2D Coulomb Gas: In the large K limit, vortices are dilute and come in tightly bound vortex-antivortex pairs. In this limit, we can write down the following partition function as a good approximation of the XY model

$$\boxed{\mathcal{Z} = \sum_{N=0}^{\infty} \frac{y^N}{((N/2)!)^2} \int \prod_{i=1}^{N} d^2\mathbf{x}_i \, e^{2\pi^2 K \sum_{i\neq j} q_i q_j C(\mathbf{x}_i - \mathbf{x}_j)},} \tag{5.26}$$

where $y = e^{-E}$ is the vortex *fugacity* and $\mathcal{Z}$ is the partition function of the dilute 2D Coulomb gas. In the limit of $y \ll 1$ configurations with $q_i = \pm 1$ dominate and only such configurations are included in the partition function. Furthermore, as explained above, we enforce charge neutrality $\sum_i q_i = 0$.

We want to explore the instability of the XY model around the fixed point $y = 0$, $K = 2/\pi$ caused by unbinding of vortex-antivortex pairs. The singular properties associated with this point are therefore captured by the above partition function, valid in the limit $y \ll 1$. Thus, the critical properties of the XY model are those of the dilute 2D Coulomb gas. We now explore this critical behaviour by following an RG scheme, originally due to Kosterlitz.

5.3.2 Perturbative RG for the Dilute Coulomb Gas

The RG scheme can be summarised as follows. We first integrate out vortex-antivortex pairs whose size ranges from a to ba and look at the renormalisation of K that results. We then rescale $\mathbf{x} = b\mathbf{x}'$ to restore the original cut-off a, which leads to the renormalisation of fugacity y.

Renormalisation of K: We will follow a slightly indirect approach here. We will introduce two external unit charges to the Coulomb gas at positions $\mathbf{x}$ and $\mathbf{x}'$ and compute their potential energy $V(\mathbf{x}, \mathbf{x}')$. This is a *physically* measurable quantity and must be constant under renormalisation. By looking at how screening from vortex-antivortex pairs contributes to this potential energy, we can *deduce* the RG transformation for K. Perturbatively in the fugacity y we only need to include corrections from a single vortex-antivortex pair

$$\begin{aligned} e^{-\beta V(\mathbf{x}-\mathbf{x}')} &= e^{-4\pi^2 K C(\mathbf{x}-\mathbf{x}')} \times \\ &\frac{\left[1 + y^2 \int d^2\mathbf{y} d^2\mathbf{y}' e^{-4\pi^2 K C(\mathbf{y}-\mathbf{y}') + 4\pi^2 K [C(\mathbf{x}-\mathbf{y}) - C(\mathbf{x}-\mathbf{y}') - C(\mathbf{x}'-\mathbf{y}) + C(\mathbf{x}'-\mathbf{y}')]} + \mathcal{O}(y^4)\right]}{\left[1 + y^2 \int d^2\mathbf{y} d^2\mathbf{y}' e^{-4\pi^2 K C(\mathbf{y}-\mathbf{y}')} + \mathcal{O}(y^4)\right]} \\ &= e^{-4\pi^2 K C(\mathbf{x}-\mathbf{x}')} \left[1 + y^2 \int d^2\mathbf{y} d^2\mathbf{y}' e^{-4\pi^2 K C(\mathbf{y}-\mathbf{y}')} \left(e^{4\pi^2 K D(\mathbf{x},\mathbf{x}';\mathbf{y},\mathbf{y}')} - 1\right) + \mathcal{O}(y^4)\right]. \end{aligned} \tag{5.27}$$

In the small fugacity limit, the size of the *internal* vortex-antivortex dipoles $\mathbf{r} = \mathbf{y}' - \mathbf{y}$ is small. We can thus approximate

$$D(\mathbf{x}, \mathbf{x}'; \mathbf{y}, \mathbf{y}') = C(\mathbf{x} - \mathbf{R} + \frac{\mathbf{r}}{2}) - C(\mathbf{x} - \mathbf{R} - \frac{\mathbf{r}}{2}) - C(\mathbf{x}' - \mathbf{R} + \frac{\mathbf{r}}{2}) + C(\mathbf{x}' - \mathbf{R} - \frac{\mathbf{r}}{2})$$

as:

$$-\mathbf{r}\cdot\nabla_{\mathbf{R}}C(\mathbf{x}-\mathbf{R})+\mathbf{r}\cdot\nabla_{\mathbf{R}}C(\mathbf{x}'-\mathbf{R})+\mathcal{O}(r^3) \tag{5.28}$$

where $\mathbf{R}=(\mathbf{y}+\mathbf{y}')/2$ is the dipole centre of mass. Substituting the dipole approximation for $D(\mathbf{x},\mathbf{x}';\mathbf{y},\mathbf{y}')$ into Eq. (5.27), we obtain

$$\begin{aligned} e^{-\beta V(\mathbf{x}-\mathbf{x}')} &= e^{-4\pi^2 KC(r)}\Big(1+8\pi^4K^2y^2\int d^2\mathbf{r}\,d^2\mathbf{R}\,e^{-4\pi^2KC(r)} \\ &\quad\times\left[\mathbf{r}\cdot\nabla_{\mathbf{R}}C(\mathbf{x}-\mathbf{R})-\mathbf{r}\cdot\nabla_{\mathbf{R}}C(\mathbf{x}'-\mathbf{R})\right]^2\Big), \end{aligned} \tag{5.29}$$

where the integral over the linear term in $\mathbf{r}$ vanishes. Carrying out the angular part of the $\mathbf{r}$ integration, we obtain

$$\begin{aligned} e^{-\beta V(\mathbf{x}-\mathbf{x}')} &= e^{-4\pi^2 KC(r)}\Big(1+8\pi^5K^2y^2\int r^3e^{-4\pi^2KC(r)}dr \\ &\quad\times\int d^2\mathbf{R}\,\left[\nabla_{\mathbf{R}}C(\mathbf{x}-\mathbf{R})-\nabla_{\mathbf{R}}C(\mathbf{x}'-\mathbf{R})\right]^2. \end{aligned} \tag{5.30}$$

The second integral is proportional to the energy of a vortex and anti-vortex at locations $\mathbf{x}$ and $\mathbf{x}'$ (see Eq. (5.23)), and is equal to $2C(\mathbf{x}-\mathbf{x}')$ in the long distance limit. Note that $C(\mathbf{0})=0$.

We thus obtain the following correction to the potential $V(\mathbf{x},\mathbf{x}')$ due to screening from internal charges

$$\beta V(\mathbf{x}-\mathbf{x}')=4\pi^2C(\mathbf{x}-\mathbf{x}')\left[K-4\pi^3K^2y^2\int_a^\infty r^3\,e^{-4\pi^2KC(r)}dr\right]. \tag{5.31}$$

Hence, if dipoles ranging from a to ba are removed from the theory, K needs to be reduced by the following amount if we are to obtain the same *physical* potential from the partition function

$$\begin{aligned} \delta K &= -4\pi^3K^2y^2\int_a^{ba} r^3\,e^{-4\pi^2KC(r)}dr \\ &= -4\pi^3K^2y^2a^4\delta l, \end{aligned} \tag{5.32}$$

where $b=e^l$.

Restoring the original cutoff by $\mathbf{x}=b\mathbf{x}'$:

To complete the RG transformation and restore the cutoff on vortex separation, we simply rescale space by

$$\begin{aligned} \mathbf{x} &= b\mathbf{x}', \\ |\mathbf{x}_i-\mathbf{x}_j|>ba &\;\rightarrow\; |\mathbf{x}_i'-\mathbf{x}_j'|>a. \end{aligned} \tag{5.33}$$

In the above partition function $d^2\mathbf{x}_i = b^2 d^2\mathbf{x}'_i$ and $C(\mathbf{x}_i - \mathbf{x}_j) = C((\mathbf{x}'_i - \mathbf{x}'_j)/b) = C(\mathbf{x}'_i - \mathbf{x}'_j) + \frac{1}{2\pi}\ln b$. Both can be absorbed into the fugacity. Note that overall charge neutrality leads to

$$2\pi^2 K \sum_{i\neq j} q_i q_j \frac{1}{2\pi}\ln b = \pi K \ln b \left[\left(\sum_i q_i\right)^2 - \sum_i q_i^2\right] = -N\pi K \ln b. \tag{5.34}$$

We thus conclude that the following replacement of the partition function can be made

$$\begin{aligned} \mathcal{Z} &= \sum_{N=0}^{\infty} \frac{y^N}{((N/2)!)^2} \int \prod_{i=1}^{N} d^2\mathbf{x}_i \, e^{-2\pi^2 K \sum_{i\neq j} q_i q_j C(\mathbf{x}_i - \mathbf{x}_j)} \\ &\to \sum_{N=0}^{\infty} \frac{y'^N}{((N/2)!)^2} \int \prod_{i=1}^{N} d^2\mathbf{x}'_i \, e^{-2\pi^2 K' \sum_{i\neq j} q_i q_j C(\mathbf{x}'_i - \mathbf{x}'_j)}, \end{aligned} \tag{5.35}$$

where $y' = yb^{2-\pi K}$, $K' = K - \delta K$ and the cutoff on vortex separation is a. The corresponding RG equations in the $\{K, y\}$ parameter space are

$$\boxed{\begin{aligned} \frac{dK}{dl} &= -4\pi^3 K^2 a^4 y^2 + \mathcal{O}(y^4), \\ \frac{dy}{dl} &= (2 - \pi K)y + \mathcal{O}(y^3). \end{aligned}} \tag{5.36}$$

5.3.3 Analysis of the RG Flow for the XY Model

Making the following substitution

$$\begin{aligned} K^{-1} - \pi/2 &\to x, \\ ya^2 &\to y, \end{aligned} \tag{5.37}$$

it is straightforward to show that the RG flow proceeds along hyperbolas

$$x^2 - \pi^4 y^2 = c \tag{5.38}$$

parametrised by a constant c. Fig. 5.3.3 shows the resulting RG flows in $\{x, y\}$ space.

The constant c parametrises the transition; close to the critical temperature T_c, we can write

$$c = x^2 - \pi^4 y^2 = b^2(T_c - T), \tag{5.39}$$

where $x = T - \frac{\pi}{2}$, $\ln y \propto \frac{1}{T}$ and b is a constant of the order of unity. This relation allows us to derive several of the XY model's critical properties. In particular for $c > 0$, (i.e., below the critical temperature), the RG flow terminates on the line of fixed points

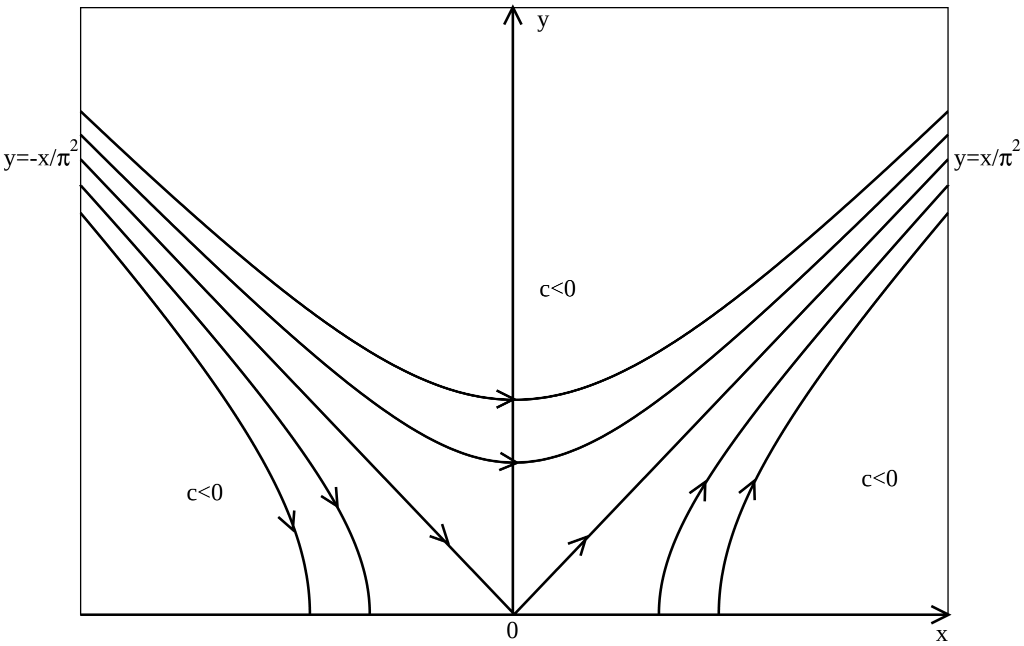

Figure 5.4: RG flow for the XY model in the Coulomb gas description limit.

formed by the negative x-axis. The effective theory below T_C is Gaussian. This is because fugacity vanishes on the line of fixed points, which means that short-distance fluctuations parametrised by E, i.e., vortex cores, in the original XY model are quenched – we are in the zero vortex sector. The effective K, which parametrises the cost of long-distance fluctuations of the original XY model is given by its fixed point K value

$$K = \frac{2}{\pi} - \frac{4}{\pi^2} \lim_{l\to\infty} x = \frac{2}{\pi} + \frac{4b}{\pi^2}\sqrt{T_c - T} \tag{5.40}$$

For $T > T_C$, K flows to zero and y flows to 1 ($E = 0$), i.e., the theory flows away from the dilute Coulomb gas limit towards the high-temperature phase with finite correlations. This is the *Debye plasma phase* where vortices, separated by distances larger than the correlation length, are completely screened from each other.

Divergence of the correlation length at $T = T_c$:

We consider an RG trajectory for $T - T_C \ll 1$, starting at $x(0) = 0$ and terminating at $x(l) = 1$, where $\xi(l) \sim a$. Substituting for y, using Eq. (5.39), into the RG flow equation for x we obtain

$$\frac{dx}{dl} = 4\pi^3 y^2 = \frac{4}{\pi}\left(x^2 + b^2(T - T_c)\right), \tag{5.41}$$

Integrating we obtain

$$\begin{aligned}\int_0^1 \frac{dx}{x^2 + b^2(T - T_c)} &= \int_0^l \frac{4dl}{\pi}, \\ \frac{1}{b^2\sqrt{T - T_C}} \arctan\left(\frac{1}{b^2\sqrt{T - T_C}}\right) &= \frac{4l}{\pi}.\end{aligned} \tag{5.42}$$

Approximating $\arctan\left(\frac{1}{b^2\sqrt{T-T_C}}\right)$ by $\pi/2$ close to the critical temperature, we obtain

$$l = \frac{\pi^2}{8b^2\sqrt{T-T_C}} \tag{5.43}$$

and

$$\xi(0) = \xi(l)e^l \sim a e^{\frac{\pi^2}{8b^2\sqrt{T-T_C}}} \tag{5.44}$$

for the divergence of the correlation length at the critical point.

5.3.4 Debye Plasma Phase

For $T > T_c$, the Coulomb gas model flows to the limit where $E \to 0$. We now look more closely at the Coulomb gas Hamiltonian in this limit

$$\beta H = E\sum_i q_i^2 - 2\pi^2 K \sum_{i\neq j} q_i q_j C_2\left(\frac{\mathbf{x}_i - \mathbf{x}_j}{a}\right). \tag{5.45}$$

For $E \to 0$ vortices proliferate and the sum over q_i in the partition function can be replaced by an integral

$$\mathcal{Z}_{\mathrm{Db}} = \int \mathcal{D}q(\mathbf{x}) \int \mathcal{D}\Psi(\mathbf{x})\, e^{\int d^2\mathbf{x}\left(-Eq(\mathbf{x})^2 + i\Psi(\mathbf{x})q(\mathbf{x})\right)} e^{-\frac{1}{4\pi^2 K}\int d^2\mathbf{x}\Psi(\mathbf{x})\nabla^2\Psi(\mathbf{x})}, \tag{5.46}$$

where a Hubbard-Stratonovich field $\Psi(\mathbf{x})$ has been introduced. Integrating out the vortex charges $q(\mathbf{x})$, we obtain

$$\mathcal{Z}_{\Psi} = \int \mathcal{D}\Psi(\mathbf{x})\, e^{-\int d^2\mathbf{x}\Psi(\mathbf{x})\left(\frac{1}{4E} + \frac{1}{4\pi^2 K}\nabla^2\right)\Psi(\mathbf{x})}. \tag{5.47}$$

The interaction between two static unit charges of opposite sign introduced into the system at positions $\mathbf{x}$ and $\mathbf{x}'$ is given by the following correlator

$$\begin{aligned} e^{-\beta V(\mathbf{y}-\mathbf{y}')} &= \langle e^{i\Psi(\mathbf{y}) - i\Psi(\mathbf{y}')}\rangle_{\mathcal{Z}_\Psi}, \\ \beta V(\mathbf{y}-\mathbf{y}') &= \langle \Psi(\mathbf{y})\Psi(\mathbf{y}'))\rangle_{\mathcal{Z}_\Psi} - \langle \Psi(0)^2\rangle_{\mathcal{Z}_\Psi} = e^{-|\mathbf{y}-\mathbf{y}'|/\xi} C(|\mathbf{y}-\mathbf{y}'|), \end{aligned} \tag{5.48}$$

where $\xi = \sqrt{\frac{E}{\pi^2 K}}$ is the Debye screening length and the potential energy has the form of the 2D Ornstein-Zernike correlator that we have encountered earlier.

5.4 3D Coulomb Gas

In 3D the Coulomb gas Hamiltonian takes the following form

$$\beta H = E\sum_i q_i^2 - K\sum_{i\neq j} q_i q_j \left(\frac{a}{|\mathbf{x}_i - \mathbf{x}_j|} - 1\right), \tag{5.49}$$

where position vectors $\mathbf{x}_i$ span three-dimensional space and a is the cutoff on the separation of charges. A simple application of the RG scheme used for the 2D Coulomb gas model (see Problem Set 2) shows that the there is no stable Coulomb phase. E always flow to zero towards the Debye phase fixed point. The fact that the 3D Coulomb gas is always in the Debye phase has important ramifications for 3D lattice gauge theories, which as we will see in the next chapter can be mapped onto 2D quantum electrodynamics.

3D Lattice Gauge Theory Hamiltonian: A 3D lattice gauge theory has the following Hamiltonian

$$\beta H = -K \sum_{\mathrm{P}} \cos\left(\mathrm{curl}_{\mathrm{P}}\theta\right), \tag{5.50}$$

where the variables θ live, say, on the links of a 3D simple cubic lattice, e.g., θ_{ij} lives on the link between the ith and the jth sites. The curl is taken around each face of the cubic units making up the lattice; e.g., for face P with corners at sites $i = 1, 2, 3, 4$, we have

$$\mathrm{curl}_{\mathrm{P}}\theta = \theta_1 - \theta_2 + \theta_3 - \theta_4. \tag{5.51}$$

Gaussian Limit: In the large K limit, the low energy fluctuations will be long-wavelength and, as usual, we can take the continuum Gaussian approximation

$$\begin{aligned}
&\theta_{ij} = \mathbf{A}\cdot\mathbf{e}_{ij} \\
&\mathrm{curl}_{\mathrm{P}}\theta = (\nabla\times\mathbf{A})\cdot\hat{\mathbf{n}} \\
&\beta H = \frac{K}{2}\int d^3\mathbf{r}\,(\nabla\times\mathbf{A})^2 = \frac{K}{2}\int d^3\mathbf{r}\,\mathbf{B}^2,
\end{aligned} \tag{5.52}$$

where $\mathbf{e}_{ij}$ is the vector joining lattice sites i and j, $\hat{\mathbf{n}}$ is the unit vector normal to face P and $\mathbf{B} = \nabla\times\mathbf{A}$ is the magnetic field. The connection with Maxwellian electromagnetism is now clear.

Just as before, higher order gradient terms are irrelevant and we need to look for topological defects to determine the RG flow around the $K = \infty$ fixed point.

Magnetic Monopoles: Just like $\nabla\theta$ was only measured modulo 2π for the XY model, the magnetic field $(\nabla\times\mathbf{A})$ is now only measured modulo 2π. This is because the Hamiltonian is periodic (compact gauge theory) and the energy cost of a magnetic field which is an integer multiple of 2π is zero. Let us therefore consider a pair of magnetic monopoles of charge $\pm 2\pi$. Since the magnetic field has no divergence, these have to be connected by a magnetic field line of strength 2π, known as the Dirac string. Thus for monopoles at positions $\mathbf{x}$ and $\mathbf{x}'$ the divergenceless magnetifc field configuration is given by

$$\mathbf{B}(\mathbf{r}) = \frac{(\mathbf{r}-\mathbf{x})}{2|\mathbf{r}-\mathbf{x}|^3} - \frac{(\mathbf{r}-\mathbf{x}')}{2|\mathbf{r}-\mathbf{x}'|^3} + 2\pi\Theta(z)\delta(x)\delta(y)\hat{\mathbf{e}}_z, \tag{5.53}$$

where the monopoles are separated by a distance d in the z-direction, $\mathbf{x}-\mathbf{x}' = d\hat{\mathbf{e}}_z$, and $\Theta(z) = 1$ for $\mathbf{x}'\cdot\hat{\mathbf{e}}_z < z < \mathbf{x}\cdot\hat{\mathbf{e}}_z$ and vanishes otherwise.

Because the Hamiltonian is periodic in $\mathbf{B}$, this string contributes no energy, regardless of its length (i.e., has zero tension) and can be simply neglected. The only interaction between the magnetic monopoles is now the usual 3D Coulomb attraction, obtained by integrating $\frac{K}{2}\mathbf{B}^2$ over all space.

Magnetic Monopole Gas: The defects in the lattice gauge theory form a 3D Coulomb gas. But this is always in the Debye phase! This means that magnetic monopoles proliferate and screen any externally placed static monopoles. The Gaussian expansion of the 3D lattice gauge theory is unstable and we do not obtain ordinary Maxwellian electromagnetism for any finite K. What is more, the proliferation of magnetic monopoles (large fluctuations of the magnetic field) means that in the corresponding 2D quantum electrodynamics the conjugate electric field is confined to narrow tubes (small fluctuations of the conjugate variable by Heisenberg uncertainty principle) and externally placed static electric charges feel a force that increases linearly with their separation. This is somewhat akin to quark confinement that takes place in Yang-Mills theory.

Chapter 6

Quantum Phase Transitions

The aim of this chapter is to introduce the Feynman path integral as a useful tool in deriving the Ginzburg-Landau action for a quantum Hamiltonian. We then look at finite-size corrections to RG scaling in order to demonstrate the key ideas behind quantum-classical crossover.

6.1 Path Integral Representation of a Quantum Partition Function

We will be looking at N-body quantum Hamiltonians of the form

$$\hat{H} = \sum_{i=1}^{N} \frac{\hat{\mathbf{p}}_i^2}{2m} + \hat{V}(\hat{\mathbf{x}}_1, \hat{\mathbf{x}}_2, ..., \hat{\mathbf{x}}_N), \tag{6.1}$$

where $\hat{V}(\hat{\mathbf{x}}_1, \hat{\mathbf{x}}_2, ..., \hat{\mathbf{x}}_N)$ is a many-body potential that generically includes external forces, as well as interactions between particles. $\hat{\mathbf{p}}_i$ and $\hat{\mathbf{x}}_i$ are the momentum and position operators of the ith particle and satisfy the usual commutation relations

$$[\hat{x}_\mu, \hat{p}_\nu] = i\delta_{\mu\nu}, \tag{6.2}$$

where μ, ν label the d Cartesian components of the operators, and d is the dimensionality. Note that operators corresponding to different particles commute.

The partition function for the Hamiltonian in Eq. 6.1 can be written down in a path integral form using a prescription originally due to Feynman:

$$\mathcal{Z} = \int \left(\prod_{i=1}^{N} d^d\mathbf{x}_i \right) \langle \mathbf{x}_1, \mathbf{x}_2, ..., \mathbf{x}_N | e^{-\beta \hat{H}} | \mathbf{x}_1, \mathbf{x}_2, ..., \mathbf{x}_N \rangle. \tag{6.3}$$

To simplify the notation, we will use the following shorthand for both $\mathbf{x}$ and $\mathbf{p}$:

$$\begin{aligned} X &\equiv \mathbf{x}_1, \mathbf{x}_2, ..., \mathbf{x}_N \\ dX &\equiv \left(\prod_{i=1}^{N} d^d \mathbf{x}_i \right), \\ X^2 &\equiv \sum_{i=1}^{N} \mathbf{x}^2, \\ X \cdot P &\equiv \sum_{i=1}^{N} \mathbf{x}_i \cdot \mathbf{p}_i \,. \end{aligned}$$

We insert the following resolution of the identity in $N_\tau - 1$ places in the partition function indicated below:

$$\mathbf{1} = \int dX |X\rangle\langle X| \tag{6.4}$$

$$\mathcal{Z} = \int dX \langle X| e^{-\frac{\beta}{N_\tau}\hat{H}} \mathbf{1} e^{-\frac{\beta}{N_\tau}\hat{H}} \mathbf{1} e^{-\frac{\beta}{N_\tau}\hat{H}} ... e^{-\frac{\beta}{N_\tau}\hat{H}} |X\rangle. \tag{6.5}$$

As $N_\tau \to \infty$, we can expand the exponentials to obtain

$$\begin{aligned} \mathcal{Z} = \int \left(\prod_{i=1}^{N_\tau} dX_i \right) \langle X_1| \mathbf{1} \left(1 - \epsilon\hat{H}\right) |X_2\rangle \langle X_2| \mathbf{1} \left(1 - \epsilon\hat{H}\right) |X_3\rangle \times \\ \langle X_3| \mathbf{1} \left(1 - \epsilon\hat{H}\right) |X_4\rangle \times ... \times \langle X_{N_\tau}| \mathbf{1} \left(1 - \epsilon\hat{H}\right) |X_1\rangle, \end{aligned} \tag{6.6}$$

where $\epsilon = \frac{\beta}{N_\tau}$ and the variable X corresponding to the $(i-1)$th resolution of the identity has been indexed as X_i. We now insert the resolution of the identity in momentum space $\mathbf{1} = \int dP |P\rangle\langle P|$ in N_τ places indicated above to obtain

$$\begin{aligned} \mathcal{Z} = \int \left(\prod_{i=1}^{N_\tau} dX_i \right) \int \left(\prod_{i=1}^{N_\tau} dP_i \right) \langle X_1|P_1\rangle\langle P_1| \left(1 - \epsilon\hat{H}\right) |X_2\rangle \times \\ \langle X_2|P_2\rangle\langle P_2| \left(1 - \epsilon\hat{H}\right) |X_3\rangle \times ... \times \langle X_{N_\tau}|P_{N_\tau}\rangle\langle P_{N_\tau}| \left(1 - \epsilon\hat{H}\right) |X_1\rangle. \end{aligned} \tag{6.7}$$

Using the fact that

$$\begin{aligned} \langle X_i|P_j\rangle &= e^{iX_i\cdot P_j}, \\ \langle P_i| \left(1 - \epsilon\hat{H}\right) |X_{i+1}\rangle &= \left[1 - \epsilon\left(\frac{P_i^2}{2m} + V(X_{i+1})\right)\right] e^{-iP_i\cdot X_{i+1}} \\ &= e^{-\epsilon\left(\frac{P_i^2}{2m} + V(X_{i+1})\right)} e^{-iP_i\cdot X_{i+1}}, \end{aligned} \tag{6.8}$$

we obtain the following expression for the partition function valid in the limit $N_\tau \to \infty$:

$$\boxed{\mathcal{Z} = \int \left(\prod_{i=1}^{N_\tau} dX_i\right) \int \left(\prod_{i=1}^{N_\tau} dP_i\right) e^{-i\sum_{i=1}^{N_\tau} P_i\cdot(X_{i+1}-X_i)-\epsilon\sum_{i=1}^{N_\tau}\left(\frac{P_i^2}{2m}+V(X_i)\right)},} \tag{6.9}$$

where $X_{N_\tau+1} = X_1$. The partition function is particularly useful in the continuum limit $X_i \to X(\tau)$, with $\tau = (i-1)\epsilon$, where it becomes a functional integral,

$$\boxed{\mathcal{Z} = \int_{X(\beta)=X(0)} \mathcal{D}X(\tau) \int \mathcal{D}P(\tau) e^{-\int_0^\beta d\tau\left(iP(\tau)\cdot\partial_\tau X(\tau)+\frac{P^2}{2m}+V[X(\tau)]\right)}.} \tag{6.10}$$

Only terms to first order in ϵ have been kept. Integrating out the momentum fields $P(\tau)$, we obtain the following partition function and a corresponding real action

$$\boxed{\begin{aligned} \mathcal{Z} &= \int_{\mathbf{x}_i(\beta)=\mathbf{x}_i(0)} \mathcal{D}\mathbf{x}_i(\tau) e^{-H[\mathbf{x}_i(\tau)]}, \\ H[\mathbf{x}_i(\tau)] &= \int_0^\beta d\tau \left[\sum_{i=1}^{N} \frac{m|\partial_\tau \mathbf{x}_i|^2}{2} + V[\mathbf{x}_i(\tau)]\right]. \end{aligned}} \tag{6.11}$$

From the form of the partition function above, we see that a d-dimensional quantum system at zero temperature $\beta = \infty$ can be mapped onto a $d+1$-dimensional classical system whose energy is given by the classical Hamiltonian and where the extra dimension is spanned by the imaginary time coordinate τ.

A d-dimensional quantum system at finite temperature β^{-1} can be mapped onto a $(d+1)$- dimensional classical system with the extra dimension now being of finite length β.

We now turn to analysing particular choices of many-body quantum Hamiltonians that are both illustrative and ubiquitous in condensed matter systems.

Key correspondences of the Quantum-Classical mapping

Correspondence	**Quantum**	**Classical**
Hamiltonian $\hat{H} \leftrightarrow \beta H$	$\hat{H} = \sum_i \frac{\hat{p}_i^2}{2M} + V\left[\hat{x}_i\right]$, where $[\hat{x}_i, \hat{p}_j] = i\delta_{ij}$	$\beta H = \int_0^\beta \mathrm{d}\tau \left[\sum_i \frac{M}{2} \left(\frac{\partial m_i(\tau)}{\partial \tau} \right)^2 + V\left[m_i(\tau)\right] \right]$
Order Parameter $\hat{x}_i \leftrightarrow m_i(\tau)$	$\hat{x}_i$	$m_i(\tau)$
Partition function $\mathcal{Z}_\mathrm{Q} = \mathcal{Z}_\mathrm{C}$	$\mathcal{Z}_\mathrm{Q} = \sum_n \langle n \vert e^{-\beta \hat{H}} \vert n \rangle$	$\mathcal{Z}_\mathrm{C} = \int_{m_i(0)=m_i(\beta)} \mathcal{D}m_i(\tau)\, e^{-\beta H[m_i(\tau)]}$
Expectation Value $\langle \hat{x}_i \rangle = \langle m_i(0) \rangle$	$\langle \hat{x}_i \rangle = \frac{1}{\mathcal{Z}_\mathrm{Q}} \sum_n \langle n \vert e^{-\beta \hat{H}} \hat{x}_i \vert n \rangle$	$\langle m_i(0) \rangle = \frac{1}{\mathcal{Z}_\mathrm{C}} \int_{m_i(0)=m_i(\beta)} \mathcal{D}m_i(\tau)\, m_i(0) e^{-\beta H[m_i(\tau)]}$
Correlator $\langle e^{\hat{H}\tau} \hat{x}_j e^{-\hat{H}\tau} \hat{x}_i \rangle = \langle m_j(\tau) m_i(0) \rangle$, where $\tau > 0$	$\langle e^{\hat{H}\tau} \hat{x}_j e^{-\hat{H}\tau} \hat{x}_i \rangle =$ $\frac{1}{\mathcal{Z}_\mathrm{Q}} \sum_n \langle n \vert e^{-\beta \hat{H}} e^{\hat{H}\tau} \hat{x}_j e^{-\hat{H}\tau} \hat{x}_i \vert n \rangle$	$\langle m_j(\tau) m_i(0) \rangle =$ $\frac{1}{\mathcal{Z}_\mathrm{C}} \int_{m_i(0)=m_i(\beta)} \mathcal{D}m_i(\tau)\, m_j(\tau) m_i(0) e^{-\beta H[m_i(\tau)]}$

Notes:

- At zero temperature ($\beta = \infty$), the τ dimension becomes of infinite extent in the classical picture, and we are integrating over the whole τ-space $\int_0^\beta \mathrm{d}\tau \to \int_{-\infty}^{\infty} \mathrm{d}\tau$. In the quantum picture, the zero-temperature expectation values are taken with respect to the ground state of $\hat{H}$, e.g., $\langle \hat{x}_i \rangle = \frac{1}{\mathcal{Z}_\mathrm{Q}} \langle \mathrm{g.s.} \vert \hat{x}_i \vert \mathrm{g.s.} \rangle$, where $\mathcal{Z}_\mathrm{Q} = \langle \mathrm{g.s.} \vert \mathrm{g.s.} \rangle$.
- In the continuum limit, as usual, the lattice sums are replaced with integrals $\sum_i \to \int \mathrm{d}^d\mathbf{r}/a^d$ and the Kronecker delta with the Dirac delta-function. The commutator $[\hat{x}_i, \hat{p}_j] = i\delta_{ij}$ is replaced with $[\hat{x}(\mathbf{r}), \hat{p}(\mathbf{r}')] = ia^d \delta(\mathbf{r} - \mathbf{r}')$.
- We have assumed translational invariance in τ-space
- Note that the UV cutoff for the imaginary time dimension is $\Lambda_\tau = \infty$. When doing momentum-shell RG this allows us to rescale ω without changing the cutoff.

6.2 O(2) Quantum Rotors

Let us begin by considering the case of a particle constrained to move on a ring of unit radius, centred on the z-axis. The particle represents the motion of a 2d rotor of inertia m. The 2-dimensional rotor is also known as the O(2) rotor because its possible orientations, described by the unit vector $\mathbf{x} = (\cos\phi, \sin\phi)$, are generated by the O(2) group. The kinetic energy operator of the quantum rotor is given by $\frac{\hat{L}^2}{2m}$, where $\hat{L} = -\mathrm{i}\frac{\partial}{\partial_\phi}$ is the z angular momentum operator, i.e., it is the kinetic energy operator of a particle constrained to move on a ring.

We will consider a system of interacting quantum rotors on a d-dimensional simple cubic lattice. The rotors interact with their nearest neighbours via a potential of the form $\hat{V}(\hat{\mathbf{x}}_i, \hat{\mathbf{x}}_j) = -g\hat{\mathbf{x}}_i \cdot \hat{\mathbf{x}}_j$. The O(2) quantum rotor Hamiltonian can be written as

$$\boxed{\hat{H}_{\mathrm{O}(2)} = \sum_i \frac{\hat{L}_i^2}{2m} - g\sum_{\langle ij\rangle} \hat{\mathbf{x}}_i \cdot \hat{\mathbf{x}}_j,} \tag{6.12}$$

where $\langle ij\rangle$ indicates that the sum is taken over nearest neighbours only.

Quantum Phase Transition: Defined as non-analytic behaviour of the ground state energy of the infinite system. This is therefore a phase transition that takes place at zero temperature.

Ground state: The Hamiltonian has a qualitatively different ground state in the large $mg \gg 1$ and low $mg \ll 1$ limits and from this we can infer the presence of a *quantum* phase transition at some intermediate value of mg. In the former limit, the potential energy term dominates and rotor alignment is favoured. The second term can be expanded in the rotor azimuthal angle $\hat{\phi}$. The fluctuations will be small and of long-wavelength with a gapless excitation spectrum. The Hamiltonian can be approximated by a series of simple Harmonic oscillators

$$\hat{H} \overset{mg\gg 1}{\approx} \sum_{\mathbf{k}} \left[\frac{1}{2m}\hat{L}_{\mathbf{k}}\hat{L}_{-\mathbf{k}} + \frac{1}{2}g|\mathbf{k}|^2\hat{\phi}_{\mathbf{k}}\hat{\phi}_{-\mathbf{k}}\right], \tag{6.13}$$

where $\hat{\phi}_{\mathbf{k}} = \frac{1}{\sqrt{N}}\sum_i \hat{\phi}_i e^{\mathrm{i}ki}$ and $\hat{L}_{\mathbf{k}} = \frac{1}{\sqrt{N}}\sum_i \hat{L}_i e^{\mathrm{i}ki}$ are the Fourier transforms of the operators $\hat{\phi}_i$ and $\hat{L}_i$ respectively. Comparison with the simple harmonic oscillator Hamiltonian shows that the excitation spectrum is given by $\sqrt{\frac{g}{m}}|\mathbf{k}|$.

In the low $mg \ll 1$ limit, the former term dominates and the ground state is given by the zero angular momentum sector for all rotors. The second term can be treated as a perturbation which gives a small (in mg) mixing of states. There is therefore an energy gap between the ground state and the first excited state in this phase. We will now look in more detail at the stability of these phases and the transition between them by exploiting the quantum-classical mapping.

The above Hamiltonian is equivalent to the one in Eq. (6.1), provided we choose an additional external potential in Eq. (6.1) that constrains the motion of each particle to a ring. We can therefore immediately write down the corresponding partition function using Eq. (6.11):

$$\boxed{\begin{aligned} \mathcal{Z}_{\mathrm{O}(2)} &= \int\limits_{\phi_i(\beta)-\phi_i(0)=2\pi n} \mathcal{D}\phi_i(\tau) e^{-H[\phi_i(\tau)]}, \\ H[\phi_i(\tau)] &= \int_0^\beta d\tau \left[\sum_{i=1}^{N} \frac{m(\partial_\tau \phi_i)^2}{2} - g \sum_{\langle ij \rangle} \cos(\phi_i - \phi_j) \right], \end{aligned}} \tag{6.14}$$

where ϕ_i is the azimuthal angle of the ith rotor and is allowed to wind by a multiple of 2π for the periodic boundary conditions along imaginary time τ.

Ginzburg-Landau Action: We proceed to derive the coarse-grained Ginzburg-Landau action for the O(2) quantum rotor Hamiltonian. Its form can be deduced from general symmetries. However, in dimensions $d = 3$ and higher of the Hamiltonian in Eq. (6.12) ($d = 4$ of the corresponding classical action in Eq. (6.14)), where as we will see mean-field behaviour holds well, one might be interested in the bare parameters of the Ginzburg-Landau action. The derivation here mirrors the one for the Ising model.

Step 1 — Hubbard-Stratonovich decoupling introduces the order parameter:

$$\begin{aligned} \mathcal{Z}_{\mathrm{O}(2)} &= \mathcal{N} \int\limits_{\phi_i(\beta)-\phi_i(0)=2\pi n} \mathcal{D}\phi_i(\tau) \mathcal{D}\left(\Psi_i(\tau), \Psi_i^*(\tau)\right) e^{-S[\phi_i(\tau), \Psi_i(\tau)]}, \\ S[\phi_i(\tau), \Psi_i(\tau)] &= \int_0^\beta d\tau \sum_i \left\{ \frac{m}{2}(\partial_\tau \phi_i)^2 + \left[e^{i\phi_i(\tau)}\Psi_i(\tau) + e^{-i\phi_i(\tau)}\Psi_i^*(\tau)\right] \right. \\ &\qquad \left. + \sum_j \Psi_i^*(\tau) G_{ij}^{-1} \Psi_j(\tau) \right\}, \end{aligned} \tag{6.15}$$

where $G_{ij} = \frac{g}{2}$ for nearest neighbours and vanishes otherwise. $\mathcal{N}$ is a normalisation constant and the integration measure $\mathcal{D}\left(\Psi_i(\tau), \Psi_i^*(\tau)\right)$ shows that we are integrating over the real and imaginary parts of the order parameter.

> **Exercise for the Reader:**
> Show by completing the square that integrating out the order parameter $\Psi_i(\tau)$ gives the partion function in Eq. (6.14). Find the required normalisation constant $\mathcal{N}$. *Hint: $\Psi_i(\tau)$ and $\Psi_i^*(\tau)$ can be transformed independently.*

Step 2 — Expansion in the order parameter:

$$\mathcal{Z}_{\mathrm{O}(2)} \approx \mathcal{N}\mathcal{Z}_\phi \int \mathcal{D}\left(\Psi_i(\tau), \Psi_i^*(\tau)\right) \Big[1 + \sum_i \int d\tau d\tau' \Psi_i(\tau)\Psi_i^*(\tau') \langle e^{i\phi_i(\tau) - i\phi_i(\tau')}\rangle_{S[\phi_i(\tau)]}$$
$$+ \frac{12}{4!}\sum_{i\neq j}\int d\tau_1 d\tau_2 d\tau_3 d\tau_4 \langle e^{i\phi_i(\tau_1) - i\phi_i(\tau_2) + i\phi_j(\tau_3) - i\phi_j(\tau_4)}\rangle_{S[\phi_i(\tau)]}\Psi_i(\tau_1)\Psi_i^*(\tau_2)\Psi_j(\tau_3)\Psi_j^*(\tau_4)$$
$$+ \frac{6}{4!}\sum_i \int d\tau_1 d\tau_2 d\tau_3 d\tau_4 \langle e^{i\phi_i(\tau_1) - i\phi_i(\tau_2) + i\phi_i(\tau_3) - i\phi_i(\tau_4)}\rangle_{S[\phi_i(\tau)]}\Psi_i(\tau_1)\Psi_i^*(\tau_2)\Psi_i(\tau_3)\Psi_i^*(\tau_4)\Big]$$
$$\times \exp\left[-\int_0^\beta d\tau \sum_{i,j} \Psi_i^*(\tau) G_{ij}^{-1} \Psi_j(\tau)\right], \quad (6.16)$$

where

$$\mathcal{Z}_\phi \equiv \int_{\phi_i(\beta)-\phi_i(0)=2\pi n} \mathcal{D}\phi_i(\tau) e^{-\int_0^\beta \sum_i \frac{m}{2}(\partial_\tau \phi_i)^2},$$
$$\langle e^{i\phi_j(\tau_1) - i\phi_j(\tau_2)}\rangle_{S[\phi_i(\tau)]} \equiv \frac{1}{\mathcal{Z}_\phi}\int_{\phi_i(\beta)-\phi_i(0)=2\pi n} \mathcal{D}\phi_i(\tau) e^{-\int_0^\beta d\tau \sum_i \frac{m}{2}(\partial_\tau\phi_i)^2} e^{i\phi_j(\tau_1) - i\phi_j(\tau_2)}$$

and similarly for the other averages with respect to $S[\phi_i(\tau)]$. We have truncated the expansion at the fourth order in $\Psi_i(\tau)$. Note that terms that are not invariant under a phase rotation $\phi(\tau) \to \phi(\tau) + \chi$, where χ is constant in time, have zero expectation value and are not included.

Step 3 — Integrating out the original field:

We are interested in the zero-temperature transition where $\beta \to \infty$ and the boundary conditions $\phi_i(\beta) - \phi_i(0) = 2\pi n$ can be neglected. In this case, simple Gaussian integration gives $\langle \phi(\tau)\phi(\tau')\rangle_{S[\phi_i(\tau)]} = \frac{1}{2m}|\tau - \tau'|$ and $\langle e^{i\phi(\tau) - i\phi(\tau')}\rangle_{S[\phi_i(\tau)]} = e^{-\frac{1}{2m}|\tau - \tau'|}$. We can thus write down the quadratic term in Eq. 6.16 as

$$\begin{aligned}
\int d\tau_1 d\tau_2\, \Psi_i(\tau_1)\Psi_i^*(\tau_2)\langle e^{i\phi_i(\tau_1) - i\phi_i(\tau_2)}\rangle &= \int d\tau_1 d\tau_2\, \Psi_i(\tau_1)\Psi_i^*(\tau_2) e^{-\frac{1}{2m}|\tau_2 - \tau_1|} \\
&= \int d\tau du\, \Psi_i(\tau - \frac{u}{2})\Psi_i^*(\tau + \frac{u}{2})\, e^{-|u|/2m} \\
&\approx \int d\tau du\, \left[\Psi_i(\tau) - \frac{u}{2}\partial_\tau \Psi_i(\tau) + \frac{u}{8}\partial_\tau^2 \Psi_i(\tau)\right] \\
&\qquad \left[\Psi_i^*(\tau) + \frac{u}{2}\partial_\tau \Psi_i^*(\tau) + \frac{u}{8}\partial_\tau^2 \Psi_i^*(\tau)\right]\, e^{-|u|/2m} \\
&= \int d\tau du\, \left[|\Psi_i(\tau)|^2 - \frac{u^2}{2}|\partial_\tau \Psi_i(\tau)|^2\right] e^{-|u|/2m} \\
&= \int d\tau\, \left[4m|\Psi_i(\tau)|^2 - 16m^3|\partial_\tau \Psi_i(\tau)|^2\right], \quad (6.17)
\end{aligned}$$

where irrelevant higher order derivatives have been neglected, and we performed integrations by parts and discarded the vanishing boundary terms.

To obtain the coefficients of the quartic terms we need to evaluate the 4-point correlator. In the case $i \neq j$, the four-point correlator reduces to a product of 2-point correlators $\langle e^{i\phi_i(\tau_1)-i\phi_i(\tau_2)}\rangle_{S[\phi_i(\tau)]}\langle e^{i\phi_j(\tau_3)-i\phi_j(\tau_4)}\rangle_{S[\phi_i(\tau)]}$, and we obtain

$$
\begin{aligned}
&\frac{1}{2}\sum_{i\neq j}\int d\tau_1 d\tau_2 d\tau_3 d\tau_4 \,\langle e^{i\phi_i(\tau_1)-i\phi_i(\tau_2)}\rangle\langle e^{i\phi_j(\tau_3)-i\phi_j(\tau_4)}\rangle\Psi_i(\tau_1)\Psi_i^*(\tau_2)\Psi_j(\tau_3)\Psi_j^*(\tau_4) \\
&= \frac{1}{2}\sum_{i\neq j}\left(\int d\tau(4m)|\Psi_i(\tau)|^2\right)\left(\int d\tau(4m)|\Psi_j(\tau)|^2\right), \qquad (6.18)
\end{aligned}
$$

where we have used the result of Eq. 6.17 and neglected irrelevant terms of the order of $\Psi^3(\partial\Psi/\partial\tau)$.

The case $i = j$ requires a bit more thought. Here, it is very insightful to map the 4-point path-integral correlator to the expectation value of a quantum operator, although the following can also be derived by Gaussian integration, which the reader is encouraged to do. The derivation of the path integral representation of the quantum partition function in Eq. (6.14) can be straightforwardly extended to find a path integral representation of imaginary time quantum correlators. In general, for an n-point correlator, we have

$$
\boxed{
\begin{aligned}
&\langle A_n(\tau_n)...A_1(\tau_1)\rangle_S \equiv \sum_n \langle n|e^{-\beta\hat{H}}\hat{\mathcal{T}}\left[\hat{A}_n(\tau_n)...\hat{A}_1(\tau_1)\right]|n\rangle, \\
&\hat{A}(\tau) := e^{\hat{H}\tau}\hat{A}e^{-\hat{H}\tau},
\end{aligned}
} \qquad (6.19)
$$

where $\hat{\mathcal{T}}$ is a time-ordering operator that puts the operators in order of increasing time, starting from the right, $|n\rangle$ are any orthonormal basis vectors and S is the classical action corresponding to the quantum Hamiltonian $\hat{H}$. We can thus write down the 4-point correlator as

$$
\begin{aligned}
&\langle e^{i\phi_i(\tau_4)-i\phi_i(\tau_3)+i\phi_i(\tau_2)-i\phi_i(\tau_1)}\rangle_{S[\phi_i(\tau)]} \equiv \langle 0|\hat{\mathcal{T}}\left[e^{i\hat{\phi}_i(\tau_4)}e^{-i\hat{\phi}_i(\tau_3)}e^{i\hat{\phi}_i(\tau_2)}e^{-i\hat{\phi}_i(\tau_1)}\right]|0\rangle, \\
&e^{i\hat{\phi}_i(\tau)} = e^{\hat{H}_0\tau}e^{i\hat{\phi}_i}e^{-\hat{H}_0\tau}, \qquad (6.20)
\end{aligned}
$$

where $\hat{H}_0 = \sum_i \frac{\hat{L}_z^2}{2m}$ and $|0\rangle$ is its zero angular momentum ($m_l = 0$) ground state. The operators $e^{\pm\phi_i}$ increase or decrease m_l, the z component of angular momentum on site i respectively, by an integer unit. Thus $e^{\pm i\hat{\phi}(\tau)}$ increases/decreases m_l by 1 at time τ. This corresponds to an excitation of the ground state. If we let $m_l(\tau)$ be the angular momentum at time τ, the 4-point correlator can be expressed as follows

$$
\langle e^{i\phi_i(\tau_4)-i\phi_i(\tau_3)+i\phi_i(\tau_2)-i\phi_i(\tau_1)}\rangle_{S[\phi_i(\tau)]} = \exp\left[\frac{1}{2m}\int d\tau\, m_l(\tau)^2\right], \qquad (6.21)
$$

where $m_l(0) = m_l(\beta) = 0$ and the Boltzmann weight measures the energy cost of the excitations.

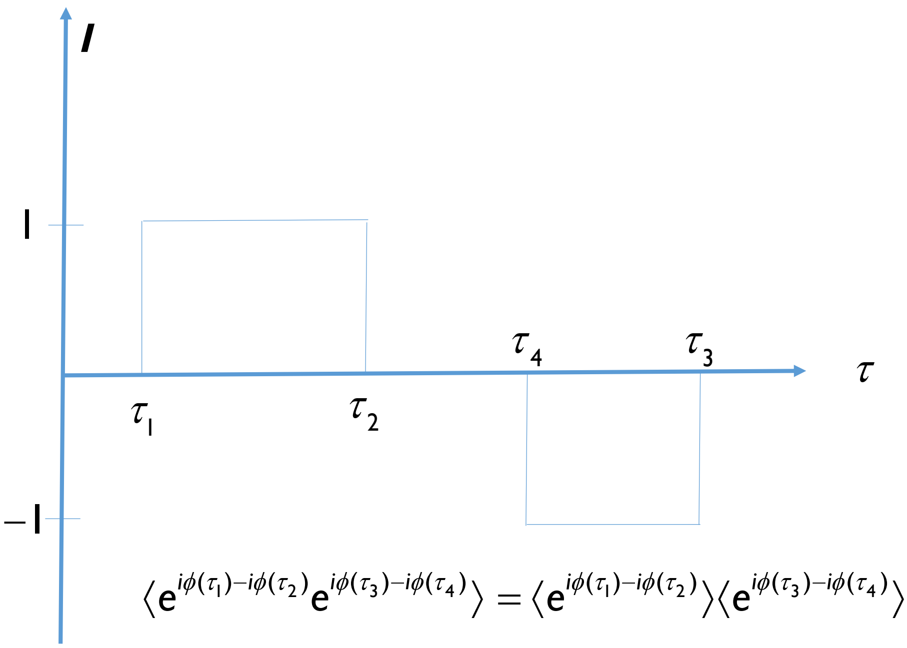

Figure 6.1: The 4-point correlator reduces to a product of 2-point correlators if the $|m_l| \leq 1$ for all imaginary time.

The configurations that we sum over in the penultimate line of Eq. 6.16 fall into two categories:

- (a) $|m_l(\tau)| \leq 1$, $\forall \tau$.

  In this case the 4-point correlator can always be expressed as a product of two *non-overlapping* 2-point correlators. See Fig. 6.1 for an example. The two $|m_l| = 1$ excitations (one for each 2-point correlator) can be translated freely in time with no change in the energy cost as long as they do not overlap.

  To sum over all configurations, we take the ordering $\tau_{1,2} < \tau_{3,4}$ without loss of generality. Remember that the raising operators act at times τ_1 and τ_3 and the lowering operators at times τ_2 and τ_4. There are 2^2 equivalent orderings that preserve the constraint $|m_l(\tau)| \leq 1$, $\forall \tau$ obtained by the independent interchanges

$\tau_1 \leftrightarrow \tau_3$ and $\tau_2 \leftrightarrow \tau_4$:

$$
\begin{aligned}
&\frac{2^2}{4}\int\limits_{\tau_{1,2}<\tau_{3,4}} d\tau_1 d\tau_2 d\tau_3 d\tau_4\, \Psi_i(\tau_1)\Psi_i^*(\tau_2)\Psi_i(\tau_3)\Psi_i^*(\tau_4)\langle e^{i\phi_i(\tau_1)-i\phi_i(\tau_2)+i\phi_i(\tau_3)-i\phi_i(\tau_4)}\rangle = \\
&\int\limits_{t_2-t_1>\frac{|u_1|+|u_2|}{2}} du_1 du_2 dt_1 dt_2\, \Psi_i(t_1-\frac{u_1}{2})\Psi_i^*(t_1+\frac{u_1}{2})\Psi_i(t_2-\frac{u_2}{2})\Psi_i^*(t_2+\frac{u_2}{2}) \\
&\qquad \times e^{-|u_1|/2m-|u_2|/2m} \\
&\approx \int\limits_{t_2-t_1>\frac{|u_1|+|u_2|}{2}} du_1 du_2 dt_1 dt_2\, |\Psi_i(t_1)|^2|\Psi_i(t_2)|^2 e^{-|u_1|/2m-|u_2|/2m} \\
&= \int\limits_{u>\frac{|u_1|+|u_2|}{2}} du_1 du_2 d\tau du\, |\Psi_i(\tau-\frac{u}{2})|^2|\Psi_i(\tau+\frac{u}{2})|^2 e^{-|u_1|/2m-|u_2|/2m} \\
&= \frac{1}{2}\int du_1 du_2 d\tau du\, |\Psi_i(\tau-\frac{u}{2})|^2|\Psi_i(\tau+\frac{u}{2})|^2 e^{-|u_1|/2m-|u_2|/2m} \\
&-\frac{1}{2}\int\limits_{|u|<\frac{|u_1|+|u_2|}{2}} du_1 du_2 d\tau du\, |\Psi_i(\tau-\frac{u}{2})|^2|\Psi_i(\tau+\frac{u}{2})|^2 e^{-|u_1|/2m-|u_2|/2m} \\
&\approx \frac{1}{2}\int dt_1 dt_2\, |\Psi_i(t_1)|^2|\Psi_i(t_2)|^2(4m)^2 \\
&-\frac{1}{2}\int du_1 du_2 d\tau\, |\Psi_i(\tau)|^4\left(|u_1|+|u_2|\right) e^{-|u_1|/2m-|u_2|/2m} \\
&\approx \frac{1}{2}\left(\int d\tau\, 4m|\Psi_i(\tau)|^2\right)^2 - 32m^3\int d\tau\, |\Psi_i(\tau)|^4, \qquad (6.22)
\end{aligned}
$$

where $t_1 = (\tau_1+\tau_2)/2$, $u_1 = (\tau_2-\tau_1)$, $t_2 = (\tau_3+\tau_4)/2$, $u_2 = (\tau_4-\tau_3)$ and $\tau = (t_1+t_2)/2$, $u = (t_2-t_1)$. Irrelevant terms of the order of $\Psi^3(\partial\Psi/\partial\tau)$ have been neglected.

- (b) $|m_l(\tau)| = 2$ for some non-zero time.

If the angular momentum is raised (or lowered) twice before it is lowered (or raised) twice $|m_l| = 2$ for some non-zero time, which carries an increased energy cost. Such configurations cannot be expressed as products of 2-point correlators, but are energetically supressed and do not play a vital role in the quantum phase transition. See Fig. 6.2 for an example.

Again to sum over the relevant configurations, we take the ordering $\tau_{1,3} < \tau_{2,4}$. There are two equivalent orderings, obtained by the simultaneous interchange of

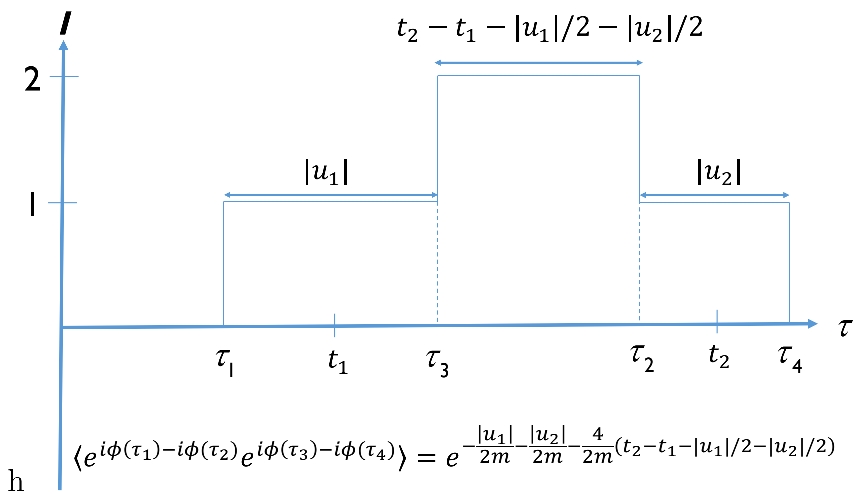

Figure 6.2: The 4-point correlator does not reduce to a product of 2-point correlators if $|m_l| = 2$ for non-zero imaginary time.

$\tau_1 \leftrightarrow \tau_2$ and $\tau_3 \leftrightarrow \tau_4$:

$$
\begin{aligned}
&\frac{2}{4}\int\limits_{\tau_{1,3}<\tau_{2,4}} d\tau_1 d\tau_2 d\tau_3 d\tau_4\ \Psi_i(\tau_1)\Psi_i^*(\tau_2)\Psi_i(\tau_3)\Psi_i^*(\tau_4)\langle e^{i\phi_i(\tau_1)-i\phi_i(\tau_2)+i\phi_i(\tau_3)-i\phi_i(\tau_4)}\rangle \\
&= \frac{1}{2}\int\limits_{t_2-t_1>\frac{|u_1|+|u_2|}{2}} du_1 du_2 dt_1 dt_2\ \Psi_i(t_1-\frac{u_1}{2})\Psi_i(t_1+\frac{u_1}{2})\Psi_i^*(t_2-\frac{u_2}{2})\Psi_i^*(t_2+\frac{u_2}{2}) \\
&\times \exp\left[-\frac{|u_1|}{2m}-\frac{|u_2|}{2m}-\frac{2}{m}\left((t_2-t_1)-\frac{|u_1|}{2}-\frac{|u_2|}{2}\right)\right] \\
&\approx \frac{1}{2}\int d\tau\ |\Psi_i(\tau)|^4 \int\limits_{u>\frac{|u_1|+|u_2|}{2}} du_1 du_2 du\ e^{-2u/m+|u_1|/2m+|u_2|/2m} \\
&= \frac{1}{4}\int d\tau\ |\Psi_i(\tau)|^4 \int du_1 du_2 du\ e^{-2|u|/m-|u_1|/2m-|u_2|/2m} = 4m^3 \int d\tau\ |\Psi_i(\tau)|^4\,,
\end{aligned}
$$

where $t_1 = (\tau_1+\tau_3)/2$, $u_1 = (\tau_3-\tau_1)$, $t_2 = (\tau_2+\tau_4)/2$, $u_2 = (\tau_4-\tau_2)$ and $\tau = (t_1+t_2)/2$, $u = (t_2-t_1)$. Irrelevant terms of the order of $\Psi^3(\partial\Psi/\partial\tau)$ have been neglected.

Putting everything together, we can write down

$$\mathcal{Z}_{\mathrm{O}(2)} \approx \mathcal{N}\mathcal{Z}_\phi \int \mathcal{D}\left(\Psi_i(\tau), \Psi_i^*(\tau)\right) \Bigg[1 + \sum_i \int d\tau \left(4m|\Psi_i(\tau)|^2 - 16m^3|\partial_\tau \Psi_i(\tau)|^2\right) \\ + \frac{1}{2}\left(\sum_i \int d\tau 4m|\Psi_i(\tau)|^2\right)^2 - 28m^3 \sum_i \int d\tau |\Psi_i(\tau)|^4 \Bigg] e^{-\int_0^\beta \sum_{i,j} \Psi_i^*(\tau) G_{ij}^{-1} \Psi_j(\tau)}. \tag{6.23}$$

Step 4 – Re-expontiation:

Firstly note that in Fourier space the matrix G is diagonal:

$$G_{\mathbf{q},\mathbf{q}'} = \frac{1}{N}\sum_{ij} e^{i\mathbf{q}\cdot\mathbf{x}_i - i\mathbf{q}'\cdot\mathbf{x}_j} G_{ij} = \delta_{\mathbf{q}+\mathbf{q}'} \sum_{\mu=1,\ldots,d} 2g\cos(q_\mu a) = 2g\delta_{\mathbf{q}+\mathbf{q}'}\left[d - |\mathbf{q}|^2\frac{a^2}{2} + \mathcal{O}(|\mathbf{q}|^4)\right], \tag{6.24}$$

and its inverse is given by

$$G^{-1}_{\mathbf{q},\mathbf{q}'} = \delta_{\mathbf{q}+\mathbf{q}'}(2gd)^{-1}\left[1 + \frac{a^2}{2d}|\mathbf{q}|^2 + \mathcal{O}(|\mathbf{q}|^4)\right]. \tag{6.25}$$

Since we are interested in the coarse-grained long-wavelength properties of the system we will only keep the first two terms in the expansion for $G^{-1}_{\mathbf{q},\mathbf{q}'}$.

Coarse-graining the summation over lattice sites $\Psi_i(\tau) \to \Psi(\mathbf{r},\tau)$, $\sum_i \to \int \frac{d^d\mathbf{r}}{a^d}$ and re-expontiating the terms in the square brackets we obtain the final expression for the O(2) quantum rotor Ginzburg-Landau action:

$$\boxed{\begin{aligned} &\mathcal{Z}_{\mathrm{O}(2)} \approx \mathcal{N}\mathcal{Z}_\phi \int \mathcal{D}\left(\Psi(\mathbf{r},\tau), \Psi^*(\mathbf{r},\tau)\right) e^{-S[\Psi(\mathbf{r},\tau)]}, \\ &S[\Psi(\mathbf{r},\tau)] = \int \frac{d^d\mathbf{r}}{a^d} d\tau \Big[t|\Psi(\mathbf{r},\tau)|^2 + \frac{a^2}{4gd^2}|\nabla\Psi(\mathbf{r},\tau)|^2 \\ &\qquad +16m^3|\partial_\tau\Psi(\mathbf{r},\tau)|^2 + 28m^3|\Psi(\mathbf{r},\tau)|^4 \Big] \\ &\qquad -\frac{1}{2}\left(\int \frac{d^d\mathbf{r}}{a^d} d\tau 4m|\Psi(\mathbf{r},\tau)|^2\right)^2, \end{aligned}} \tag{6.26}$$

where $t = (\frac{1}{2gd} - 4m)$. Note that the $t = 0$ corresponds to the zero-temperature transition, where $g = \frac{1}{8md}$, and $t = -4m$ corresponds to the classical limit, where $g = \infty$. The above derivation makes it clear that proliferation of virtual (in imaginary time) particle-hole excitations $m_l = \pm 1$ drives the quantum phase transition from the gapped phase to the ordered phase. The stability of the Ginzburg-Landau action is ensured by the quartic term, which originates from hardcore repulsion between particle-hole pairs. Virtual particle-hole proliferation is also the mechanism behind the quantum phase transition in the Bose-Hubbard model and there it results in boson condensation. The two are in fact in the same $O(2)$ universality class.

Dynamical Exponent: The Ginzburg-Landau action for the quantum O(2) rotor is isotropic in spacetime, which can be explicitly shown by rescaling time and space $\mathbf{r} \to \frac{a}{2\sqrt{g}\,d}\mathbf{r}$, $\tau \to \tau 4m^{3/2}$. (In fact the theory is also relativistic with a speed of light equal to unity after rescaling). The correlations in time and space will therefore diverge with the same exponent at the critical point $t = 0$,

$$\xi \sim \xi_\tau \sim \frac{1}{|t|^\nu}. \tag{6.27}$$

This is however generally not the case as question 2 on the second example sheet demonstrates. In general,

$$\boxed{\begin{aligned} \xi &\sim \frac{1}{|t|^\nu}, \\ \xi_\tau &\sim \frac{1}{|t|^{z\nu}}, \end{aligned}} \tag{6.28}$$

where z is known as the dynamical exponent. For $O(N)$ quantum rotor systems, $z = 1$.

Energy Gap: A finite energy gap (in the thermodynamic limit, namely as system size tends to infinity) between the lowest excitation and the ground state results in a finite correlation length in imaginary time ξ_τ for ground state expectation values. From Eq. (6.19) expressed in the energy eigenstates basis $|n\rangle$ and at zero temperature, we obtain

$$\begin{aligned} \langle A(\tau)B(\tau')\rangle_{S[\phi_i(\tau)]} &\equiv \sum_n \langle 0|\hat{A}|n\rangle e^{-|\tau-\tau'|E_n/\hbar}\langle n|\hat{B}|0\rangle \\ &\overset{|\tau-\tau'|\to\infty}{\to} \langle 0|\hat{A}|1\rangle e^{-|\tau-\tau'|E_1/\hbar}\langle 1|\hat{B}|0\rangle, \end{aligned} \tag{6.29}$$

where without loss of generality $E_0 = 0$ and E_1 is the energy gap to the first excited state, which dominates the sum in the limit $|\tau - \tau'|$. We thus conclude that the imaginary time correlation length ξ_τ is related to the energy gap to the first excited state as follows:

$$\boxed{\xi_\tau = \frac{\hbar}{E_1}.} \tag{6.30}$$

6.3 † O(3) Quantum Rotors

We now consider the case of a particle constrained to move on a sphere of unit radius. The particle represents the motion of a 3D rotor of inertia m. The kinetic energy operator of the quantum rotor is given by the kinetic energy operator of a particle constrained to move on a sphere, i.e., $\frac{\hat{\mathbf{L}}^2}{2m}$, where $\hat{\mathbf{L}}$ is the usual angular momentum operator. The

3-dimensional rotor is also known as an O(3) rotor because its possible orientations, described by the unit vector $\mathbf{x}$, are generated by the O(3) group.

As before, we will consider a system of interacting quantum rotors on a d-dimensional simple cubic lattice. The rotors interact with their nearest neighbours via a potential of the form $g\hat{\mathbf{x}}_i \cdot \hat{\mathbf{x}}_j$. The O(3) quantum rotor Hamiltonian can be written as follows

$$\boxed{\hat{H}_{\mathrm{O}(3)} = \sum_i \frac{\hat{\mathbf{L}}_i^2}{2m} - g \sum_{<ij>} \hat{\mathbf{x}}_i \cdot \hat{\mathbf{x}}_j \,.} \tag{6.31}$$

As before, naive expansions lead to the conclusion that there are two zero-temperature phases (i.e., two qualitatively different ground states): an ordered one with gapless excitations, where $\langle \hat{\mathbf{x}} \rangle \neq \mathbf{0}$, at large mg; and a disordered one with gapped excitations, where $\langle \hat{\mathbf{x}} \rangle = \mathbf{0}$, at small mg.

As before, the above Hamiltonian is equivalent to the one in Eq. (6.1), provided we choose an additional external potential in Eq. (6.1) that constrains the motion of each particle to a sphere and gives rise to a functional delta function in the partition function. It then follows from Eq. (6.11) that the O(3) quantum rotor partition function is given by

$$\boxed{\begin{aligned} \mathcal{Z}_{\mathrm{O}(3)} &= \int\limits_{\mathbf{x}_i(\beta)=\mathbf{x}_i(0)} \mathcal{D}\mathbf{x}_i(\tau)\, \delta\left(\mathbf{x}^2 - 1\right) e^{-H[\mathbf{x}_i(\tau)]}, \\ H[\mathbf{x}_i(\tau)] &= \int_0^\beta d\tau \left[\sum_{i=1}^{N} \frac{m(\partial_\tau \mathbf{x}_i)^2}{2} - g \sum_{<ij>} \mathbf{x}_i . \mathbf{x}_j \right] . \end{aligned}} \tag{6.32}$$

Weak coupling limit and the non-linear σ model: As before, we could proceed to derive the Ginzburg-Landau action or simply write it down on a phenomenological basis with undetermined parameters. However, we shall be mostly interested in the properties of the model in the limit $mg \gg 1$, also known as the weak coupling limit. The reasons behind this name will soon become apparent. When $mg \gg 1$, the fluctuations in $\mathbf{x}_i(\tau)$ will involve only long wavelength modes which can be treated in a continuum approximation. Accordingly, we can make the replacement

$$\begin{aligned} -g \sum_{<ij>} \mathbf{x}_i(\tau) \cdot \mathbf{x}_j(\tau) &= \frac{g}{2} \sum_{<ij>} \left[\mathbf{x}_i(\tau) - \mathbf{x}_j(\tau)\right]^2 + \text{const.} \\ &\to \frac{g}{2} \int \frac{d^d \mathbf{r}}{a^{d-2}} |\nabla \mathbf{S}(\mathbf{r}, \tau)|^2, \end{aligned} \tag{6.33}$$

where we have replaced the lattice variables $\mathbf{x}_i(\tau)$ with the continuous vector field $\mathbf{S}(\mathbf{r}, \tau)$. Rescaling time and space $\tau \to \tau\sqrt{\frac{m}{2}}$, $\mathbf{r} \to \mathbf{r}\sqrt{\frac{ga}{2}}$, we obtain the non-linear σ model:

$$\boxed{\begin{aligned} \mathcal{Z} &= \int \mathcal{D}\mathbf{S}(\mathbf{r}, \tau) \delta(\mathbf{S}\left(\mathbf{r}, \tau\right)^2 - 1) e^{-S[\mathbf{S}(\mathbf{r}, \tau)]}, \\ S[\mathbf{S}(\mathbf{r}, \tau)] &= \frac{1}{f} \int \frac{d^d \mathbf{r} d\tau}{a^d} \partial_\mu \mathbf{S}(\mathbf{r}, \tau) \partial^\mu \mathbf{S}(\mathbf{r}, \tau), \end{aligned}} \tag{6.34}$$

where the dimensionful coupling $f = (\frac{4}{g^d a^d m})^{\frac{1}{2}}$. In the weak-coupling limit $mg \gg 1$ the variations in $\mathbf{S}(\mathbf{r},\tau)$ around a globally uniform configuration will be small and we can expand the non-linear σ model action as

$$\begin{aligned}
S[\mathbf{S}(\mathbf{r},\tau)] &= \frac{1}{f}\int \frac{d^d\mathbf{r}d\tau}{a^d}\left(\mathbf{e}_\theta\partial_\mu\theta + \mathbf{e}_\phi\sin\theta\partial_\mu\phi\right)\cdot\left(\mathbf{e}_\theta\partial_\mu\theta + \mathbf{e}_\phi\sin\theta\partial_\mu\phi\right)\\
&\overset{\theta\to\frac{\pi}{2}+\theta}{=} \frac{1}{f}\int \frac{d^d\mathbf{r}d\tau}{a^d}\left[\partial_\mu\theta\partial^\mu\theta + \partial_\mu\phi\partial^\mu\phi - \frac{1}{2}\theta^2\partial_\mu\phi\partial^\mu\phi + \mathcal{O}(\theta^4\phi^2)\right]\\
&\overset{\substack{\theta\to\sqrt{f}\theta\\ \phi\to\sqrt{f}\phi}}{=} \int \frac{d^d\mathbf{q}d\tau}{(2\pi)^d a^d}\left[|\partial_\tau\theta(\mathbf{q})|^2 + |\partial_\tau\phi(\mathbf{q})|^2 + |\mathbf{q}|^2\left(|\theta(\mathbf{q})|^2 + |\phi(\mathbf{q})|^2\right)\right]
\end{aligned} \tag{6.35}$$

where $\theta(\mathbf{r},\tau)$ and $\phi(\mathbf{r},\tau)$ are the spherical polar angles of the spin vector $\mathbf{S}(\mathbf{r},\tau)$, and $\theta = \pi/2$, $\phi = 0$ in the globally uniform configuration around which we are expanding.

Comparison with Eq. (6.11) shows that in the weak-coupling limit the original Hamiltonian can be approximated by a sum of simple harmonic oscillators, one for each mode $\mathbf{q}$ and an interaction that is proportional to the coupling f. In quantum field theory language the excitation of the $\mathbf{q}$-mode simple harmonic oscillator corresponds to creating particles with momentum $\hbar\mathbf{q}$, energy $2|\mathbf{q}|$ and the weak interaction that scales with f is responsible for particle-particle scattering.

$$\begin{aligned}
\hat{H} &= \int \frac{d^d\mathbf{q}}{(2\pi)^d}\left[\hat{\pi}_\theta(\mathbf{q})\hat{\pi}_\theta(-\mathbf{q}) + \hat{\pi}_\phi(\mathbf{q})\hat{\pi}_\phi(-\mathbf{q}) + |\mathbf{q}|^2\left(\hat{\theta}(\mathbf{q})\hat{\theta}(-\mathbf{q}) + \hat{\phi}(\mathbf{q})\hat{\phi}(-\mathbf{q})\right)\right],\\
&\quad +\mathcal{O}(f)
\end{aligned} \tag{6.36}$$

with the canonical commutation relations $[\hat{\pi}_\theta(\mathbf{q}), \hat{\theta}(\mathbf{k})] = \delta_{\mathbf{k}+\mathbf{q}}$ and $[\hat{\pi}_\phi(\mathbf{q}), \hat{\phi}(\mathbf{k})] = \delta_{\mathbf{k}+\mathbf{q}}$.

Exercise for the Reader:
Show that the above Hamiltonian does indeed host gapless excitations with energy proportional to $|\mathbf{q}|$.

Haldane Gap: Our analysis of the previous chapter showed that in $d = 2$, the Gaussian $f = 0$ fixed point ($T = 0$ of the corresponding classical model) of the $N = 3$ non-linear sigma model is unstable and the model flows towards the phase with a finite correlation length which close to $f = 0$ varies as follows (isotropically along rescaled τ and $\mathbf{r}$):

$$\xi \sim a e^{\frac{2\pi}{f}}. \tag{6.37}$$

Thus the energy gap Δ of the corresponding quantum O(3) rotor chain ($d = 1$) is given by

$$\Delta = \frac{1}{\xi} \sim e^{-\frac{2\pi}{f}}. \tag{6.38}$$

The energy gap Δ is known as the Haldane gap in the context of Heisenberg antiferromagnetic chains with integer spins, which map onto the one-dimensional quantum O(3) rotor chains.

Asymptotic Freedom: Following on from our investigation of the 2-dimensional classical non-linear sigma model in the previous Chapter, where we showed that high-momentum correlators are given by a quadratic theory with an effective coupling that vanishes logarithmically as $p \to \infty$, we conclude that the high-momentum, large-energy excitations of the above *quantum field Hamiltonian* interact weakly at large momenta. (At low momenta the interactions are strong since the running coupling grows.) The particles, represented by these excitations, are thus *free* at large momenta and energies. This is known as *asymptotic freedom*. A similar phenomenon occurs in quantum chromodynamics (QCD), where the quarks interact strongly at small energies and are confined to form hadrons but behave as free particles at large energies.

6.4 Finite-Size Scaling

In this section we look at finite-size corrections to the critical properties of the d-dimensional Ising model with the following Ginzburg-Landau action,

$$S[\Psi(\mathbf{x})] = \int d^d\mathbf{x} \left[(\nabla\Psi(\mathbf{x}))^2 + t\Psi^2(\mathbf{x}) + u\Psi(\mathbf{x})^4 - h\Psi(\mathbf{x}) \right] , \tag{6.39}$$

although the scalings that we derive are applicable to most critical systems. We consider a system of finite extent, i.e., length L along each dimension. An RG transformation involves the rescaling of each dimension

$$\begin{aligned} \mathbf{x} &= b\mathbf{x}', \\ L &= bL'. \end{aligned} \tag{6.40}$$

We therefore conclude that the inverse system size L^{-1} is a relevant RG variable with eigenvalue $y_{L^{-1}} = 1$

$$\boxed{\begin{aligned} &L'^{-1} = bL^{-1}, \\ &y_{L^{-1}} = 1. \end{aligned}} \tag{6.41}$$

The free energy density changes by a scaling factor (homogeneously) under an RG transformation

$$f\left(t, h, L^{-1}\right) = b^{-d} f\left(b^{y_t} t, b^{y_h} h, bL^{-1}\right) \tag{6.42}$$

where we only need to include relevant variables sufficiently close to the critical point. It follows that the singular part of the susceptibility has the following form

$$\begin{aligned} \chi \sim \frac{\partial^2 f}{\partial h^2}_{h=0} &= b^{2y_h - d} f\left(b^{y_t} t, bL^{-1}\right) \\ &\overset{b^{y_t}t=1}{=} t^{\frac{d-2y_h}{y_t}} \Phi(t^{-\frac{1}{y_t}} L^{-1}) \\ &= t^{-\gamma} \Phi(t^{-\nu} L^{-1}) \\ &= L^{\frac{\gamma}{\nu}} \Psi(\xi L^{-1}), \end{aligned} \tag{6.43}$$

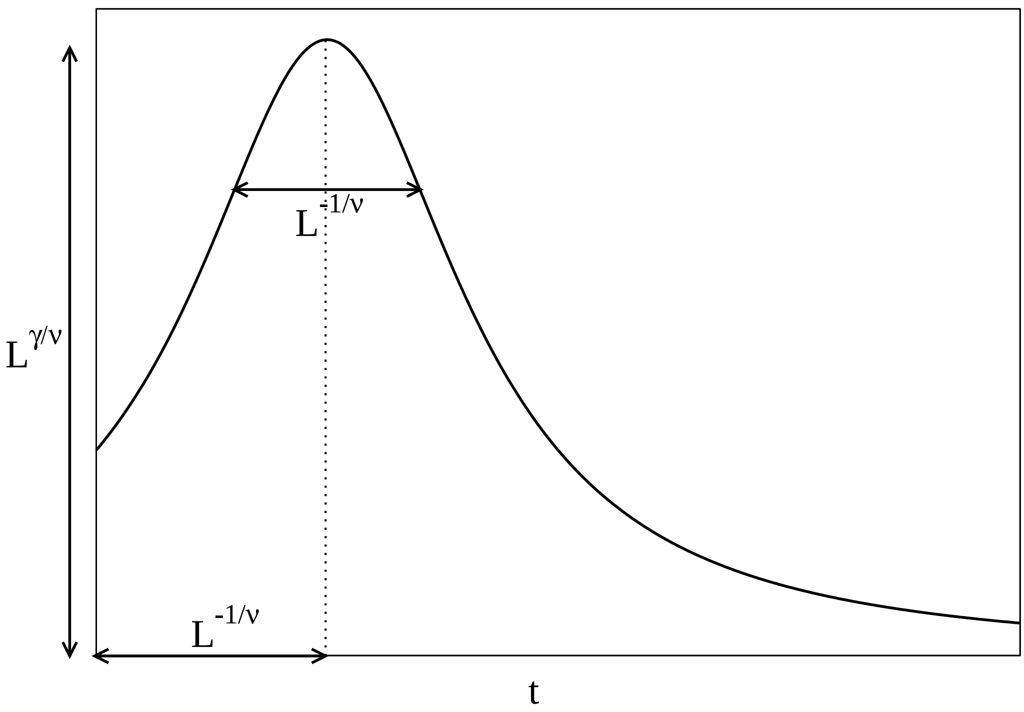

Figure 6.3: Scaling of susceptibility with system size.

where the homogenous function $\Psi(x)$ is a finite function of the order of unity since the susceptibility of a finite system cannot have any singularities. $\Psi(x) \to x^{\frac{\gamma}{\nu}}$ as $x \to 0$ restores the correct universal behaviour in the thermodynamic limit. There is therefore a smooth crossover to the thermodynamic limit behaviour when $\xi L^{-1} \sim \mathcal{O}(1)$, i.e., at a crossover temperature

$$\boxed{t_X = L^{-\frac{1}{\nu}}.} \tag{6.44}$$

The susceptibility of a finite system is still expected to have a finite maximum in the vicinity of the transition point. The function $\Psi(x)$ has a maximum at some value $x \sim \mathcal{O}(1)$ and with a width $\Delta x \sim \mathcal{O}(1)$. We therefore conclude that for finite systems the susceptibility has a maximum at $t \sim L^{-\frac{1}{\nu}}$ with a width $\Delta t \sim L^{-\frac{1}{\nu}}$ and an amplitude that scales as $L^{\frac{\gamma}{\nu}}$. Fig. 6.3 illustrates the main points.

6.5 Quantum Critical Behaviour

We will focus on the d-dimensional quantum O(2) rotor system with the following Hamiltonian (Eq. (6.12))

$$\boxed{\hat{H}_{\mathrm{O}(2)} = \sum_i \frac{\hat{L}_z^2}{2m} - g \sum_{<ij>} \hat{\mathbf{x}}_i \cdot \hat{\mathbf{x}}_j,} \tag{6.45}$$

and a corresponding classical partition function (Eq. (6.14))

$$\boxed{\begin{aligned} \mathcal{Z}_{\mathrm{O}(2)} &= \int\limits_{\phi_i(\beta)-\phi_i(0)=2\pi n} \mathcal{D}\phi_i(\tau) e^{-H[\phi_i(\tau)]}, \\ H[\phi_i(\tau)] &= \int_0^\beta d\tau \left[\sum_{i=1}^N \frac{m(\partial_\tau \phi_i)^2}{2} - g \sum_{<ij>} \cos(\phi_i - \phi_j) \right]. \end{aligned}} \tag{6.46}$$

We take $d > 2$ so that the O(2) rotor system orders at finite temperature. The partition function of the d dimensional quantum system can be written as the partition function of a corresponding $(d+1)$-dimensional classical system. The zero-temperature ($\beta = \infty$) quantum transition maps onto the classical $(d+1)$-dimensional fixed point F_{d+1} with a relevant scaling variable $t = (\frac{1}{g} - 4m)$. The exponents controlling RG flow around this fixed point belong to the $(d+1)$-dimensional $n = 2$ universality class.

We have seen (by deriving the relevant Ginzburg-Landau action) that in the vicinity of the quantum critical point F_{d+1}, where the correlation length diverges along the spatial and imaginary time directions, a continuum field-theory picture is valid. The imaginary time dimension enters on the same footing as the spatial dimensions and controls the size of the system. Now, if the quantum system is at a finite-temperature T the extra dimension of the corresponding classical system becomes finite with a length $L = \beta$. Therefore, temperature $T = L^{-1}$ is a relevant RG variable around the F_{d+1} fixed point with eigenvalue $y_T = 1$. Fig. 6.4 shows the RG flow around the F_{d+1} fixed point – the quantum critical point.

The axis $t = -4m$ ($g = \infty$) corresponds to classical d-dimensional O(2) rotors and contains the usual stable low and high temperature fixed points corresponding to the ordered and disorderd phases respectively (see the high/low temperature expansions in Chapter 4). These are separated by the d-dimensional fixed point F_d at $T = T_c$. The exponents controlling RG flow around F_{d+1} belong to the $n = 2$, d-dimensional universality class. Note that t is an irrelevant RG variable at this point, because fluctuations of $\phi_i(\tau)$ along the imaginary time direction τ are gapped out. $\omega = \frac{2\pi}{\beta}$ is the lowest allowed frequency and $2\pi^2 m T_c \sim 2\pi^2 m g \gg 1$ is the energy cost of this mode ($T_c \sim g$). Also note that the stable Gaussian fixed point at $t = -4m$, $T = 0$, is a terminating point for all RG trajectories inside the ordered phase.

Quantum-Classical Crossover: We now employ the finite-size scaling arguments of the preceding section to discuss quantum-classical crossover in the vicinity of the quantum critical point F_{d+1}. Using Eq. (6.43) with $L^{-1} = T$ we can express the singular part of the susceptibility in the vicinity of the quantum critical point as

$$\boxed{\chi = T^{-\frac{\gamma}{\nu}} \Psi(T\xi),} \tag{6.47}$$

where γ and ν are the critical exponents associated with the F_{d+1} fixed point. Note that, $\Psi(x) \to x^{\frac{\gamma}{\nu}}$ recovers the correct zero-temperature limit. However, unlike the case of a system of finite extent in all directions, the susceptibility and the function $\Psi(x)$ do not have to be finite for non-zero T. In fact, we expect a singularity in Ψ associated with crossing the ordered-disordered phase boundary at some value $T\xi = b \sim \mathcal{O}(1)$. This singularity will be controlled by the critical exponents associated with the F_d fixed point γ' and ν'. We can therefore write

$$\boxed{\chi = T^{-\frac{\gamma}{\nu}} (T\xi - b)^{\gamma'} \quad \text{for } T\xi \sim b.} \tag{6.48}$$

The transition temperature scales like $T_c = bt^{\nu}$ in the vicinity of the critical point. Note that the susceptibility is controlled by the above classical F_d singular behaviour for $T\xi \sim b$. This condition maps out the wedge marked in Fig. 6.4 which gets narrower as we approach the quantum critical point. The characteristic cross-over temperature associated with passing between classical $T\xi \sim b$ and quantum $T\xi \ll 1$ behaviour is given by $T_X \sim t^{\nu}$.

For $T\xi \gg 1$ finite-size effects dominate, and we enter the *quantum critical* region. $\Psi(x) \sim \mathcal{O}(1)$ as $x \to \infty$ so that $\chi \sim T^{-\frac{\gamma}{\nu}}$ in the quantum critical region.

In terms of RG flow, the free energy density at a particular point in parameter space is dominated by the singular behaviour of fixed point F if the RG trajectory that starts there spends a long 'RG time' in the vicinity of the point F. Because RG flow is slow in the vicinity of the fixed point, it suffices for the trajectory to pass close to the fixed point. The trajectories in the classical region all pass close to the F_d fixed point, which means that the free energy here is dominated by the singular behaviour associated with F_d critical exponents.

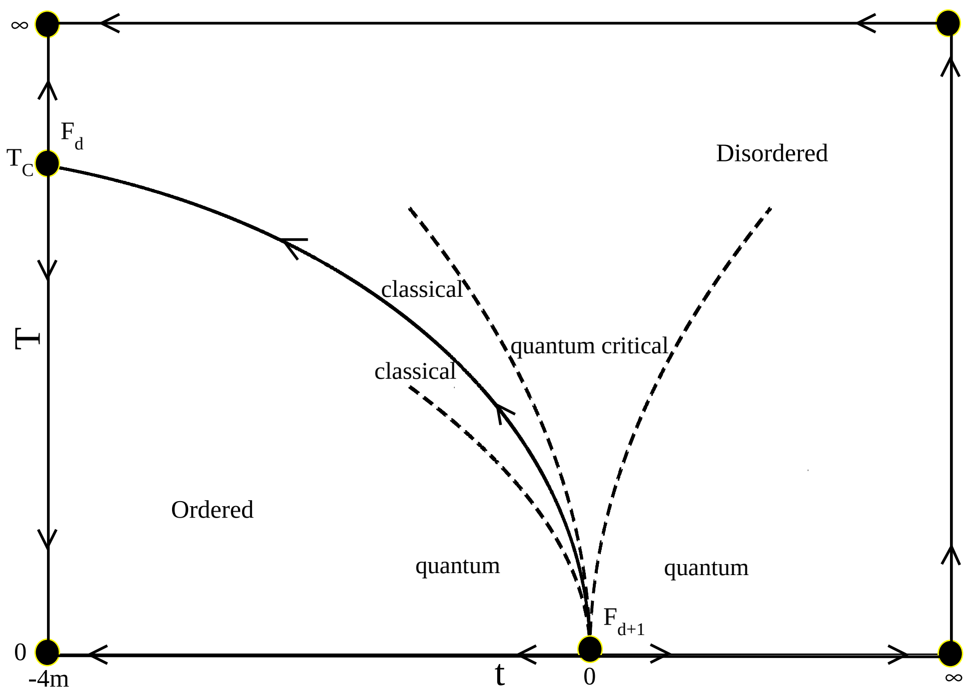

Figure 6.4: RG flow around the quantum critical point. Understanding quantum critical behaviour is one of the finest applications of RG scaling.