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)).

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

[1]

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 interact ferromagnetically with their neighbours.

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

At zero temperature 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 (c.f. section 2.4)

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

John Michael Kosterlitz and David James Thouless: co-recipients of the 2000 Lars Onsager Prize "for the introduction of the theory of topological phase transitions, as well as their subsequent quantitative predictions by means of early and ingenious applications of the renormalization group, and advancing the understanding of electron localization and the behavior of spin glasses".

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 2.4 which predicted the absence of long-range order in $d \leq 2$. Arguing that this result implies a critical temperature $T_c \sim O(d-2)$, Polyakov (Phys. Lett. **59**B, 79 (1975)) developed a perturbative RG expansion close to two-dimensions.[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 $\epsilon = (d-2) \to 0$. However, the RG also indicates that the behaviour for $n = 2$ is in some sense marginal.

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.

5.2 Topological Defects in the XY-Model

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

[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.

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. (2.9)

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

in the continuum limit. 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 2.4 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 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 the Goldstone modes. The *relevance* of these interactions can be discussed within the framework of perturbative RG (see Problem Set 2). The conclusion is that the zero

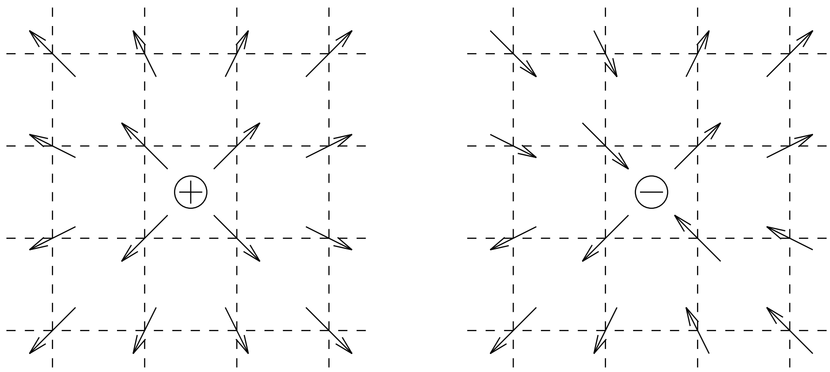

Figure 5.1: Spin configurations of the two-dimensional XY-model showing vortices of charge ± 1.

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 leads 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.

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,

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

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.

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.

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

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

$$\mathcal{Z}_1(n) \approx \left(\frac{L}{a}\right)^2 \exp\left[-\beta E_n^0(a) - \pi K n^2 \ln\left(\frac{L}{a}\right)\right], \qquad (5.1)$$

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. (5.1) 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 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.

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

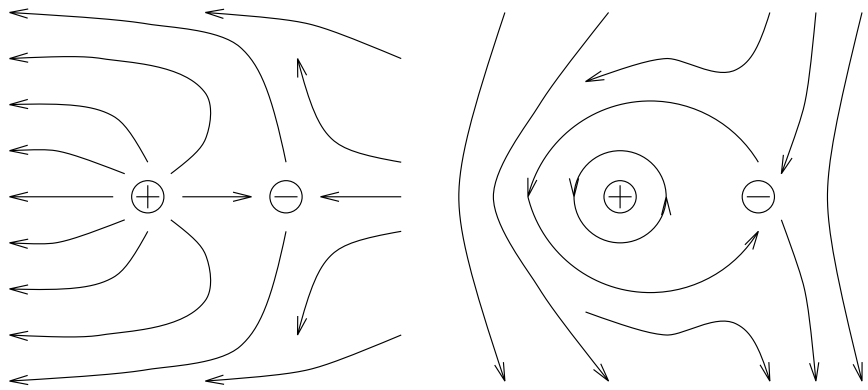

Figure 5.2: Spin configurations of vortex/antivortex pairs.

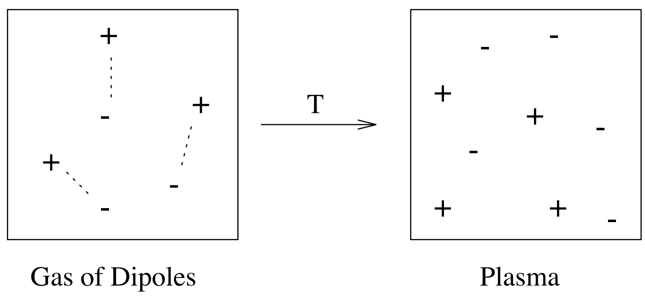

Figure 5.3: Schematic diagram showing the deconfinement of vortex pairs.