VII.B Topological Defects in the XY model

As stated in the previous section, thermal excitation of Goldstone modes destroys spontaneous order in two dimensional models with a broken continuous symmetry. The RG study of the non-linear σ-model 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 same RG procedure appears to suggest a different behavior for $n = 2$. The first indication of unusual behavior for the two dimensional XY model ($n = 2$), appeared in an analysis of high temperature series by Stanley and Kaplan in 1966. The series results strongly suggested the divergence of susceptibility at a finite temperature, seemingly in contradiction with the absence of symmetry breaking. It was indeed this contradiction that led Wigner to explore the possibility of a phase transition without symmetry breaking. The Z_2 lattice gauge theory, discussed in sec.VI.E as the dual of the three dimensional Ising model, realizes such a possibility. The two phases of the Z_2 gauge theory are characterized by different functional forms for the decay of an appropriate correlation function (the Wilson loop). We can similarly examine the asymptotic behavior of the spin-spin correlation functions of the XY model at high and low temperatures.

A high temperature expansion for the correlation function for the XY model on a lattice is constructed from

$$\begin{aligned}\langle \vec{s}_{\mathbf{0}} \cdot \vec{s}_{\mathbf{r}} \rangle = \langle \cos(\theta_{\mathbf{0}} - \theta_{\mathbf{r}}) \rangle &= \frac{1}{Z} \prod_{i=1}^{N} \left(\int_0^{2\pi} \frac{d\theta_i}{2\pi} \right) \cos\left(\theta_{\mathbf{0}} - \theta_{\mathbf{r}}\right) e^{K \sum_{<i,j>} \cos(\theta_i - \theta_j)} \\ &= \frac{1}{Z} \prod_{i=1}^{N} \left(\int_0^{2\pi} \frac{d\theta_i}{2\pi} \right) \cos\left(\theta_{\mathbf{0}} - \theta_{\mathbf{r}}\right) \prod_{<i,j>} \left[1 + K \cos\left(\theta_i - \theta_j\right) + \mathcal{O}\left(K^2\right) \right].\end{aligned} \tag{VII.35}$$

The expansion for the partition function is similar, except for the absence of the factor $\cos(\theta_{\mathbf{0}} - \theta_{\mathbf{r}})$. To the lowest order in K, each bond on the lattice contributes either a factor of one, or $K\cos(\theta_i - \theta_j)$. Since,

$$\int_0^{2\pi} \frac{d\theta_1}{2\pi} \cos\left(\theta_1 - \theta_2\right) = 0, \tag{VII.36}$$

any graph with a single bond emanating from an *internal* site vanishes. For the numerator of eq.(VII.35) to be non-zero, there must be bonds originating from the *external* points at $\mathbf{0}$ and $\mathbf{r}$. Integrating over an *internal* point with two bonds leads to

$$\int_0^{2\pi} \frac{d\theta_2}{2\pi} \cos\left(\theta_1 - \theta_2\right) \cos\left(\theta_2 - \theta_3\right) = \frac{1}{2} \cos\left(\theta_1 - \theta_3\right). \tag{VII.37}$$

The first graph that contributes to eq.(VII.35) is the shortest path (of length r) connecting the points $\mathbf{0}$ and $\mathbf{r}$. Since integrating over the end points gives

$$\int_0^{2\pi} \frac{d\theta_{\mathbf{0}} d\theta_{\mathbf{r}}}{(2\pi)^2} \cos\left(\theta_{\mathbf{0}} - \theta_{\mathbf{r}}\right)^2 = \frac{1}{2}, \tag{VII.38}$$

each bond along the path contributes $(K/2)$. (In constructing graphs for the partition function, there is an additional factor of 2 for every loop.) Thus to lowest order

$$\langle \vec{s}_{\mathbf{0}} \cdot \vec{s}_{\mathbf{r}} \rangle \approx \left(\frac{K}{2}\right)^r = e^{-r/\xi}, \qquad \text{with} \qquad \xi \approx \frac{1}{\ln\left(2/K\right)}, \tag{VII.39}$$

and the disordered high temperature phase is characterized by an exponential decay of correlations. (This is clearly quite generic in all spin systems.)

At low temperatures, the cost of small fluctuations around the ground state is obtained by a quadratic expansion, which gives $K \int d^d\mathbf{x} (\nabla\theta)^2/2$ in the continuum limit. The standard rules of Gaussian integration yield,

$$\langle \vec{s}_{\mathbf{0}} \cdot \vec{s}_{\mathbf{r}} \rangle = \left\langle \Re e^{i(\theta_{\mathbf{0}} - \theta_{\mathbf{r}})} \right\rangle = \Re \exp\left[-\frac{1}{2}\left\langle \left(\theta_{\mathbf{0}} - \theta_{\mathbf{r}}\right)^2 \right\rangle\right]. \tag{VII.40}$$

In two dimensions, the Gaussian fluctuations grow as

$$\frac{1}{2}\left\langle \left(\theta_{\mathbf{0}} - \theta_{\mathbf{r}}\right)^2 \right\rangle = \frac{1}{2\pi K} \ln\left(\frac{r}{a}\right), \tag{VII.41}$$

where a is a short distance cut-off (of the order of the lattice spacing). Hence, at low temperatures,

$$\langle \vec{s}_{\mathbf{0}} \cdot \vec{s}_{\mathbf{r}} \rangle \approx \left(\frac{a}{r}\right)^{\frac{1}{2\pi K}}, \tag{VII.42}$$

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

The distinct asymptotic decays of correlations at high and low temperatures allows for the possibility of a finite temperature phase transition separating the two regimes. However, the arguments put forward above 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. To show that the Gaussian behavior persists at finite 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 was probed in the previous section using the non-linear σ-model. 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 leads to instability towards high temperature behavior.) The low temperature phase of the XY model is said to posses *quasi–long range order*, as opposed to *true long range order* that accompanies a finite magnetization.

What is the mechanism for the disordering of the quasi–long range ordered phase? As the RG study suggests that higher order terms in the gradient expansion are not relevant, we must search for other operators. 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. Kosterlitz and Thouless (1973) suggested that the disordering is caused by *topological defects* that can not be regarded as simple deformations of the ground state. Since the angle describing the orientation of a spin is undefined up to an integer multiple of 2π, it is possible to construct spin configurations for which in going around a closed path the angle rotates by $2\pi n$. The integer n is the *topological charge* enclosed by the path. Because of the discrete nature of this charge, it is impossible to continuously deform to the uniformly ordered state in which the charge is zero. (More generally, topological defects arise in any model with a compact group describing the order parameter.)

The elementary defect, or *vortex*, has unit charge. In completing a circle centered on the defect the orientation of the spin changes by $\pm 2\pi$. 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 a uniform magnitude, and points along the circle (i.e. perpendicular to the radial vector). The magnitude of the distortion is obtained from

$$\oint \nabla\theta \cdot d\vec{s} = \frac{d\theta}{ds}(2\pi r) = 2\pi n, \qquad \Longrightarrow \qquad \frac{d\theta}{ds} = \frac{n}{r}. \tag{VII.43}$$

Since $\nabla\theta$ is a radial vector, it can be written as

$$\nabla\theta = n\left(-\frac{y}{r^2}, +\frac{x}{r^2}, 0\right) = -\frac{n}{r}\hat{r} \times \hat{z} = -n\nabla \times (\hat{z}\ln r)\,. \tag{VII.44}$$

Here, $\hat{r}$ and $\hat{z}$ are unit vectors respectively in the plane and perpendicular to it, and $\vec{a} \times \vec{b}$ indicates the cross product of the two vectors. This (continuum) approximation fails close to the center (core) of the vortex, where the lattice structure is important.

The energy cost of a single vortex of charge n has contributions from the core region, as well as from the relatively uniform distortions away from the center. 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.

$$\begin{aligned}\beta\mathcal{E}_n =&\beta\mathcal{E}_n^0(a) + \frac{K}{2}\int_a d^2\mathbf{x}(\nabla\theta)^2\\ =&\beta\mathcal{E}_n^0(a) + \frac{K}{2}\int_a^L (2\pi r dr)\left(\frac{n}{r}\right)^2 = \beta\mathcal{E}_n^0(a) + \pi K n^2 \ln\left(\frac{L}{a}\right).\end{aligned} \tag{VII.45}$$

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

$$Z_1(n) \approx \left(\frac{L}{a}\right)^2 \exp\left[-\beta\mathcal{E}_n^0(a) - \pi K n^2 \ln\left(\frac{L}{a}\right)\right] = y_n^0(a)\left(\frac{L}{a}\right)^{2-\pi K n^2}, \tag{VII.46}$$

where $(L/a)^2$ 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 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 favor spontaneous formation of vortices. On increasing temperature, the first vortices to appear correspond to $n = \pm 1$ at $K_c = 2/\pi$. Beyond this point there are many vortices in the system, and eq.(VII.46) is no longer useful.

The coupling $K_c = 2/\pi$ is a *lower bound* for the stability of the system to topological defects. This is because pairs (dipoles) of defects may appear at larger couplings. Consider a pair of charges ± 1 at a separation d. The distortions far away from the dipole center, $r \gg d$, can be obtained by superposing those of the individual vortices, and

$$\nabla\theta = \nabla\theta_+ + \nabla\theta_- \approx \vec{d}\cdot\nabla\left(\frac{\hat{r}\times\hat{z}}{r}\right), \tag{VII.47}$$

decays as d/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 thus be visualized as a gas of tightly bound dipoles. The number (and size) of dipoles increases with temperature, and the high temperature state is a plasma of unbound vortices. The distinction between the two regimes can be studied by examining a typical net topological charge, $Q(\ell)$, in a large area of dimension $\ell \gg a$. The average charge in always zero, while fluctuations in the low temperature phase are due to the dipoles straddling the parameter, i.e. $\left\langle Q(\ell)^2 \right\rangle \propto \ell$. In the high temperature state, charges of either sign can appear without restriction and $\left\langle Q(\ell)^2 \right\rangle \propto \ell^2$. (Note the similarity to the distinct behaviors of the Wilson loop in the high and low temperature phases of the Z_2 gauge theory.)

To describe the transition between the two regimes, we need to properly account for the interactions between vortices. The distortion field $\vec{u} \equiv \nabla\theta$, in the presence of a collection of vortices is similar to the velocity of a fluid. In the absence of vorticity, the flow is *potential*, i.e. $\vec{u} = \vec{u}_0 = \nabla\phi$, and $\nabla \times \vec{u}_0 = 0$. The topological charge can be related to $\nabla \times \vec{u}$ by noting that for any closed path,

$$\oint \vec{u} \cdot d\vec{s} = \int (d^2\mathbf{x}\,\hat{z}) \cdot \nabla \times \vec{u} \quad , \tag{VII.48}$$

where the second integral is over the area enclosed by the path. Since the left hand side is an integer multiple of 2π, we can set

$$\nabla \times \vec{u} = 2\pi\hat{z}\sum_i n_i\, \delta^2(\mathbf{x} - \mathbf{x}_i), \tag{VII.49}$$

describing a collection of vortices of charge $\{n_i\}$ at locations $\{\mathbf{x}_i\}$. The solution to eq.(VII.49) can be obtained by setting $\vec{u} = \vec{u}_0 - \nabla \times (\hat{z}\psi)$, leading to

$$\nabla \times \vec{u} = \hat{z}\nabla^2\psi, \qquad \Longrightarrow \qquad \nabla^2\psi = 2\pi\sum_i n_i\, \delta^2(\mathbf{x} - \mathbf{x}_i). \tag{VII.50}$$

Thus ψ behaves like the potential due to a set of charges $\{2\pi n_i\}$. The solution,

$$\psi(\mathbf{x}) = \sum_i n_i\, \ln\left(|\mathbf{x} - \mathbf{x}_i|\right), \tag{VII.51}$$

is simply a superposition of the potentials as in eq.(VII.44).

Any two dimensional distortion can thus be written as

$$\vec{u} = \vec{u}_0 + \vec{u}_1 = \nabla\phi - \nabla \times (\hat{z}\psi), \tag{VII.52}$$

and the corresponding "kinetic energy", $\beta\mathcal{H} = K\int d^2\mathbf{x}\,|\vec{u}|^2/2$, decomposed as

$$\beta\mathcal{H} = \int d^2\mathbf{x}\,\left[(\nabla\phi)^2 - 2\nabla\phi \cdot \nabla \times (\hat{z}\psi) + (\nabla \times \hat{z}\psi)^2\right]. \tag{VII.53}$$

The second term vanishes, since following an integration by parts,

$$-\int d^2\mathbf{x}\,\nabla\phi\cdot\nabla\times(\hat{z}\psi)=\int d^2\mathbf{x}\,\phi\nabla\cdot(\nabla\times\hat{z}\psi)\,, \tag{VII.54}$$

and $\nabla\cdot\nabla\times\vec{u}=0$ for any vector. The third term in eq.(VII.53) can be simplified by noting that $\nabla\psi=(\partial_x\psi,\partial_y\psi,0)$, and $\nabla\times(\hat{z}\psi)=(-\partial_y\psi,\partial_x\psi,0)$, are orthogonal vectors of equal length. Hence

$$\beta\mathcal{H}_1\equiv\frac{K}{2}\int d^2\mathbf{x}\,\left(\nabla\times\hat{z}\psi\right)^2=\frac{K}{2}\int d^2\mathbf{x}\,\left(\nabla\psi\right)^2=-\frac{K}{2}\int d^2\mathbf{x}\,\psi\nabla^2\psi, \tag{VII.55}$$

where the second identity follows an integration by parts. Equations (VII.50) and (VII.51) now result in

$$\begin{aligned}\beta\mathcal{H}_1=&-\frac{K}{2}\int d^2\mathbf{x}\left(\sum_i n_i\,\ln\left(|\mathbf{x}-\mathbf{x}_i|\right)\right)\left(2\pi\sum_j n_j\,\delta^2(\mathbf{x}-\mathbf{x}_j)\right)\\=&-2\pi^2K\sum_{i,j}n_in_j\,C(\mathbf{x}_i-\mathbf{x}_j),\end{aligned} \tag{VII.56}$$

where $C(\mathbf{x})=\ln(|\mathbf{x}|)/2\pi$ is the two dimensional Coulomb potential. There is a difficulty with the above result for $i=j$ due to the divergence of the logarithm at small arguments. This is a consequence of the breakdown of the continuum treatment at short distances. The self-interaction of a vortex is simply its core energy $\beta\mathcal{E}^0_n$, and

$$\beta\mathcal{H}_1=\sum_i\beta\mathcal{E}^0_{n_i}-4\pi^2K\sum_{i<j}n_in_jC(\mathbf{x}_i-\mathbf{x}_j). \tag{VII.57}$$

The configuration space of the XY model close to zero temperature can thus be partitioned into different topological segments. The degrees of freedom in each segment are the charges $\{n_i\}$, and locations $\{\mathbf{x}_i\}$, of the *vortices*, in addition to the field $\phi(\mathbf{x})$ describing *spin waves*. The partition function of the model can thus be approximated as

$$\begin{aligned}Z=&\prod_i\int_0^{2\pi}\frac{d\theta_i}{2\pi}\,\exp\left[K\sum_{<i,j>}\cos(\theta_i-\theta_j)\right]\\\propto&\int\mathcal{D}\phi(\mathbf{x})\,e^{-\frac{K}{2}\int d^2\mathbf{x}\,(\nabla\phi)^2}\sum_{\{n_i\}}\int d^2\mathbf{x}_i\,e^{-\sum_i\beta\mathcal{E}^0_{n_i}+4\pi^2K\sum_{i<j}n_in_jC(\mathbf{x}_i-\mathbf{x}_j)}\\\equiv&\,Z_{\text{s.w.}}Z_Q\quad,\end{aligned} \tag{VII.58}$$

where $Z_{\text{s.w.}}$ is the Gaussian partition function of spin waves, and Z_Q is the contribution of vortices. The latter describes a grand canonical gas of charged particles, interacting via the two dimensional Coulomb interaction. In calculating the Hamiltonian $\beta\mathcal{H}_1$ in eq.(VII.55), we performed an integration by parts. The surface integral that was ignored in the process in fact grows with system size as $(\sum_i n_i)\ln L$. Thus only configurations that are overall neutral are included in calculating Z_Q. We further simplify the problem by considering only the elementary excitations with $n_i = \pm 1$, which are most likely at low temperatures due to their lower energy. Setting $y_0 \equiv \exp\left[-\beta\mathcal{E}^0_{\pm 1}\right]$,

$$Z_Q = \sum_{N=0}^{\infty} y_0^N \int \prod_{i=1}^{N} d^2\mathbf{x}_i \, \exp\left[4\pi^2 K \sum_{i<j} q_i q_j C(\mathbf{x}_i - \mathbf{x}_j)\right], \tag{VII.59}$$

where $q_i = \pm 1$, and $\sum_i q_i = 0$.