Topological Defects in Two-Dimensional Crystals

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Abstract

Crystal lattices break continuous translational symmetry, and thus they exhibit Goldstone modes, namely phonons. In three or more dimensions, long range order is robust, but crystals in two or fewer dimensions do not possess long range order (at $T > 0$) because long-wavelength phonons destroy long-range correlations. In precisely two dimensions, crystals exhibit *quasi-long range order*, with spatial correlations that decay as a power law in distance, and they still exhibit solid-like properties like nonzero elastic shear moduli. However, as the temperature is increased from 0, two-dimensional crystals exhibit *topological* excitations that destroy local translational order. This paper is meant to be a rudimentary introduction to the phenomena of topological defects in two-dimensional lattices.

1 Topological Excitations in the XY Model

One of the simplest and most well-studied two-dimensional system that exhibits a phase transition is the XY model for planar magnetism. The model consists of a latice of spins that can take on continuous values (S_x, S_y) such that $|\mathbf{S}| \leq 1$. The ferromagnetic model energetically penalizes neighboring spins that are misaligned. If only nearest neighbor couplings are considered, then the Hamiltonian is

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j = -J \sum_{\langle i,j \rangle} |\mathbf{S}_i| \, |\mathbf{S}_j| \cos(\theta_i - \theta_j). \tag{1}$$

The ground state of the system is where all spins have magnitude 1 and point along the same direction. This phase breaks global rotational invariance, so, by Goldstone's theorem, we should expect an elementary excitation associated with this broken symmetry. This is the spin-wave, which is a spatial modulation in the spins' orientations. The lowest order approximation expands the cosine term to the first nontrivial term and posits that $|\mathbf{S}_i| = 1$:

$$\mathcal{H} = -\frac{J}{2k_B T} \sum_{\langle i,j \rangle} (\theta_i - \theta_j)^2. \tag{2}$$

This low-temperature approximation is solvable by moving to Fourier space. I report here the results from José et al. [1], where the authors calculate the spin-spin correlation function for a square lattice and large separation distances:

$$\langle \mathbf{S_i} \cdot \mathbf{S_j} \rangle = \mathrm{Re}\left[\left\langle e^{i(\theta_i - \theta_j)} \right\rangle \right] \sim r_{ij}^{-\eta(T)}, \qquad \eta(T) = \frac{k_B T}{2\pi J}. \tag{3}$$

Here, r_{ij} is the separation distance between the spins, and η is a non-universal exponent that depends on the temperature and the spin coupling J, with a more detailed calculation available in the appendix. This result is consistent with the Mermin-Wagner theorem [2], which states for continuous spin system in two or fewer dimensions, there is no long range order (LRO). LRO would manifest as a constant-valued correlation function for all values of r_{ij}. In one dimension, the situation is even worse, where the correlation function decays exponentially for all temperatures.

From this low-temperature approximation, it seems that the correlations decay faster and faster for all temperatures, but it is reasonable to expect that other important physics that were thrown away in the quadratic approximation will come into effect as the temperature increases. The most important consequence is that the quadratic approximation violates the periodicity symmetry of the spin variable θ_i. The system is clearly invariant under $\theta_i \to \theta_i + 2\pi n_i$, where n_i is an integer-valued field on the lattice, which is implicitly preserved in the cosine Hamiltonian. The quadratic approximation ignores *vortex configurations*, where a continuous closed path traced through the system finds that the spin

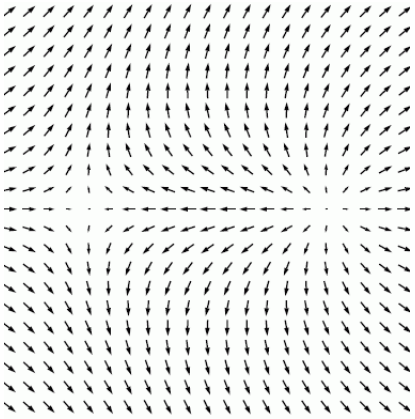

Figure 1: The left defect is a vortex with winding number 1, and the right defect is an antivortex, or a vortex with winding number -1. Image credit to `http://www.ibiblio.org/e-notes/Perc/xy.htm`

variable has changed by an integer multiple of 2π. An illustration of such defects are shown in Figure 1.

The work of Kosterlitz, Thouless, and Berezinskii showed that there is a non-zero temperature where the correlation function switches from power-law decay to exponential decay [3]. Though the spin waves are responsible for the lack of long-range order, it is the vortices that are responsible for the phase transition. Below T_C, vortices are bound tightly in pairs of zero vorticity. This is because a bare vortex costs an amount of energy proportional to the log of the system size, so only vorticity-zero configurations are thermodynamically probable in the thermodynamic limit when the system size goes to infinity. Above T_C, vortices unbind and move freely about and destroy local order.

Vortices become important at higher temperatures where the low-temperature expansion is invalid, because the low-temperature expansion ignores the topology of the *order parameter space.* The thermodynamic ground state of the XY system is degenerate: the spins point along a preferred direction, and so the average spin is a 2-d vector on the unit circle, as shown schematically in Figure 2. A path in this order parameter space can wind around the space zero times, once, twice, etc., and all of these paths must be accounted for in any representation of the Hamiltonian. Berezinskii's solution was to amend the lattice Hamiltonian by including a new integer-valued field [4]:

$$\mathcal{H} = -\frac{J}{2}\sum_{\langle i,j\rangle}\left(\theta_i - \theta_j - 2\pi n_{ij}\right)^2, \quad n_{ij} \in \mathbb{Z}. \tag{4}$$

However, a more common approach is to use a continuum model to estimate from macroscopic elastic constants (the Lamé coefficients) the energy cost of having a vortex in the system. Then the Hamiltonian is broken up into a nonsingular spin-wave part and a contribution from the quantized vortices. I outline here Chaikin and Lubensky's derivation [5]. In the continuum limit, the Hamiltonian of the system is

$$\mathcal{H} = -\frac{J}{2}\sum_{\langle i,j\rangle}\cos\left(\theta_i - \theta_j\right) \to \frac{J}{2}\int d^2\mathbf{r}\,\left(\nabla\theta\right)^2. \tag{5}$$

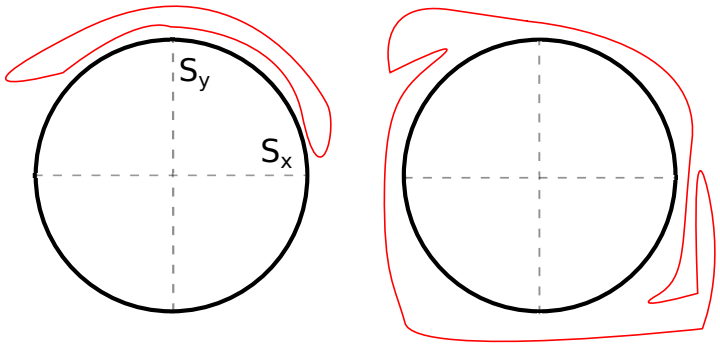

Figure 2: The order parameter **S** lives on the unit disk (black). If a closed path is drawn in the system, the variable **S** changes and traces out a path in this order parameter space (red). The diagram on the left represents the loop in order parameter space where the loop in real space does not encircle a vortex. The loop on the right, however, represents a path in real space that encircles a vortex core of unit strength.

This is also a quadratic order approximation, so we need to put the vortices back in by hand. Taking a functional derivative, we find that the condition that minimizes the energy is Laplace's equation: $\nabla^2\theta(\mathbf{r}) = 0$. If we want to stick a single vortex with strength (winding number) k into the system, we impose the winding condition $\oint d\ell \cdot \nabla\theta = 2\pi k$ around the origin (we can put the vortex anywhere, so may as well be the origin). The solution is given by $\theta(\mathbf{r}) = k\phi$, where ϕ is the polar angle in two dimensions. We have that $\nabla\phi = \frac{1}{r}\hat{r}$, so the energy of the isolated vortex is

$$E_k = \frac{J}{2}\int d^2\mathbf{r}\left(\frac{k^2}{r^2}\right) = \pi J k^2 \int_\alpha^R \frac{rdr}{r^2} = \pi J k^2 \log\frac{R}{\alpha}. \tag{6}$$

The energy of the vortex will hit an infrared divergence unless we cut off the size of the system to the scale R, and the integral has an ultraviolet cutoff α which is the core radius of the vortex. This justifies the earlier claim that isolated vortices don't occur with any probability in the thermodynamic limit. The energy of a pair of vortices is calculated by linearly superimposing solutions to Laplace's equation and finding the energy with vortices of strength k_1 and k_2 separated by a distance r. Simply stating the result:

$$E_{k_1,k_2} = \pi J\left(k_1 + k_2\right)^2 \log\frac{R}{\alpha} + 2\pi J k_1 k_2 \log\frac{r}{\alpha}. \tag{7}$$

There is still the divergent term that goes as $\log R$, but if $k_1 + k_2 = 0$, that is, if the system has no net vorticity, then the energy is finite. It's an interesting point that this Hamiltonian is the same as that of a 2-dimensional Coulomb gas, which isn't surprising because this energy was obtained by solving Laplace's equation in two dimensions with point singularities. Vortices of opposite sign are drawn together while vortices of like sign are pushed apart. There is also a core energy E_c which Chaikin and Lubensky calculate by treating α as a variational parameter. The core energy should go as α^2, because it should be proportional to the area of the vortex. Thus the total energy should obey

$$\frac{\partial E_v}{\partial\alpha} = \frac{\partial}{\partial\alpha}\left(E_k + E_c\right) = \frac{\partial}{\partial\alpha}\left(E_k + \alpha^2 E_{c,0}\right) = 0, \quad \rightarrow \quad \frac{\pi J k^2}{\alpha} = 2E_{c,0}\alpha.$$

$$\alpha^2 = \frac{\pi J k^2}{2E_{c,0}}, \quad E_c = \frac{\pi J k^2}{2}. \tag{8}$$

This is the cost of having a vortex of strength k, so the final Hamiltonian, with vortices included, is

$$\mathcal{H} = \frac{J}{2}\int d^2\mathbf{r}\ (\nabla\theta)^2 + 2\pi J \sum_{i<j} k_i k_j \log\frac{r_{ij}}{\alpha} + \frac{\pi J}{2}\sum_i k_i^2. \tag{9}$$

Here, all of the multi-valued nature of the field $\theta(\mathbf{r})$ has been removed and placed into the vortex terms. From this point, there are a few techniques to perform renormalization group calculations of fixed points for this Hamiltonian, but the purpose of introducing the XY model was to give a solid and physically intuitive picture that transfers very easily to two-dimensional crystals.

2 Crystals and Hexatics in 2D Solids

The story for a two-dimensional crystal proceeds along a similar route to the XY model. There is a quadratic Hamiltonian which is good to lowest order, but the lowest order approximation neglects topological excitations that arise because of the topological structure of the order parameter space. The relevant topological defects in a two-dimensional system are *dislocations* which disrupt translational order and *disclinations* that disrupt orientational order.

I will present relevant specific calculations from Nelson [6] and José [7]. The calculations here, because they occur for a two-dimensional order parameter $\mathbf{u}$, are more tedious, but have the same spirit as the XY calculations. The relevant order parameter here is the phonon field, usually denoted by $\mathbf{u}(\mathbf{r})$. If the ground state of a crystal system is defined by a set of real-space lattice vectors $\mathbf{a}_1$ and $\mathbf{a}_2$, then the position of every atom of the lattice can be indexed with a set of lattice vectors $\mathbf{R}_i = m_i\mathbf{a}_1 + n_i\mathbf{a}_2$. From this ground state, we perturb the system slightly, so the true position of the atoms are a small displacement $\mathbf{u}(\mathbf{r}_i)$ from their assigned lattice position $\mathbf{R}$. As long as $\mathbf{u}$ is small compared to the lattice vectors $\mathbf{a}$, a harmonic approximation (on any periodic lattice) will lead to the usual continuum elastic free energy:

$$\mathcal{H} = \frac{1}{2}\int d^2\mathbf{r}\ \left(2\mu u_{ij}^2(\mathbf{r}) + \lambda u_{ii}^2\mathbf{r}\right), \qquad u_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial r_j} + \frac{\partial u_j}{\partial r_i}\right). \tag{10}$$

The Hamiltonian can be written as a function of the symmetrized strain tensor, u_{ij}, which is a derivative of the strain field, or phonon field. Small perturbations in this field represent phonons, which, like spin waves, are the Goldstone modes responsible for the destruction of long-range order. And just as there was trouble because the spin-wave Hamiltonian only depended on differences in neighboring phases, the elastic Hamiltonian only depends on derivatives of the strain field, not the strain field itself. This is easy to understand: if $\mathbf{u}(\mathbf{r}) = \mathbf{u}_0$ a constant, then every atom in the lattice is shifted by the same amount, which should leave the energy of the system invariant. This is the same as the global phase symmetry

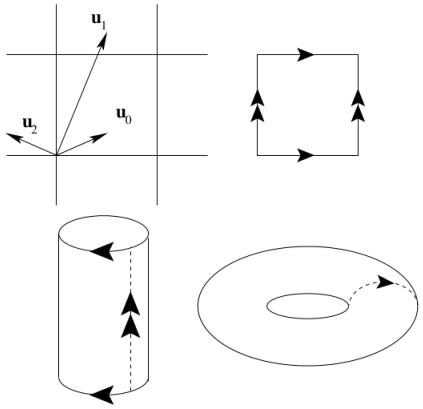

Figure 3: The order parameter space for the phonon field on a square lattice. Top left: different expressions of $\mathbf{u}$ are related by crystal lattice vector translation. Top right: $\mathbf{u}$ needs to be confined to a periodic square, that is, the unit cell. Bottom: gluing together the ends identified by periodicity, it becomes clear that the order paramter $\mathbf{u}$ lives on a torus. Figure credit to Sethna [8].

of the XY model. But whereas the XY model possesses the symmetry of $\theta \to \theta + 2\pi n$, the crystal model possesses the symmetry $\mathbf{u} \to \mathbf{u} + m\mathbf{a}_1 + n\mathbf{a}_2$, where $m, n \in \mathbb{Z}$. The order parameter space of the XY ground state was a circle, but the order paramter space of the two-dimensional crystal is a *torus*, with *two dimensions* of periodicity, as shown in Figure 3.

The order parameter $\mathbf{u}$ can wind nontrivially along two axes, so we need a vector winding number to classify dislocations. These are the Burgers vectors, and they are integer multiples of the underlying real-space lattice vectors, just as the winding number in the XY system was an integer multiple of 2π, the angular periodicity. Some examples of dislocations and their corresponding Burgers vectors are shown in Figure 4.

Now a proper Hamiltonian is needed that takes into account the topological structure of the order parameter $\mathbf{u}$. The field $\mathbf{u}$ is divided into a part that trivially traverses the order parameter space, which is labeled ϕ and a part composed of dislocation energies [9].

$$\mathcal{H} = \frac{1}{2}\int d^2\mathbf{r}\,\left(2\mu\phi_{ij}^2(\mathbf{r}) + \lambda\phi_{ii}^2(\mathbf{r})\right) - \frac{K}{4\pi}\sum_{i<j} b_\mu(\mathbf{r}_i)b_\nu(\mathbf{r}_j)\left(\delta_{\mu\nu}\log\frac{|\mathbf{r}_i-\mathbf{r}_j|}{\alpha} - \frac{(\mathbf{r}_i-\mathbf{r}_j)_\mu(\mathbf{r}_i-\mathbf{r}_j)_\nu}{|\mathbf{r}_i-\mathbf{r}_j|^2}\right) + E_C\sum_i |\mathbf{b}(\mathbf{r}_i)|^2\,. \quad (11)$$

Here, the constant $K = \frac{4\mu(\mu+\lambda)}{2\mu+\lambda}$, and E_C is the core energy of the dislocations. This Hamiltonian bears a resemblance to the XY Hamiltonian with vortices, except that the interaction energies of the defects depend on their directions. Still, there is a tendency for dislocations that are pointing along the same direction to repel from each other, and there is a logarithmic potential well that binds two dislocations of opposite Burgers vector together. The set of possible Burgers vectors is also subject to the condition $\sum_i \mathbf{b}_i = 0$, just like in the XY model.

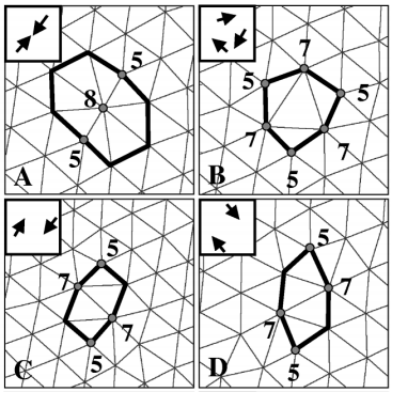

Figure 4: Shown here are bound dislocations, and in the top left corners, the Burgers vectors associated with the dislocations.

It's clear that the spontaneous generation of dislocation pairs will destroy local order. When the temperature becomes high enough, dislocation pairs will unbind and roam freely around the sample. Just like the unbinding of vortex-antivortex pairs leads to exponential correlation decay, dislocation pair unbinding leads to exponential translational order decay. This correlation function below the unbinding transition temperature is

$$\left\langle e^{i\mathbf{G}\cdot(\mathbf{u}(\mathbf{r})-\mathbf{u}(0))}\right\rangle \sim r^{-\eta(T)}, \qquad \eta(T) = \frac{k_B T\,|\mathbf{G}|^2}{4\pi}\frac{3\mu+\lambda}{\mu(2\mu+\lambda)}.$$

Here, $\mathbf{G}$ is any reciprocal lattice vector. The correlation decay exponent depends on nonuniversal parameters like the temperature and elastic coupling strengths λ and μ, just as it did in the XY model, but there with J.

From this point, the next step would be to calculate the renormalized elastic constants λ_R and μ_R, as the presence of free dislocations give the crystal an avenue by which to relieve applied stress. In this way, dislocations are said to reduce the elasticity of materials. To recreate or explain sufficiently the renormalization group calculation is beyond my ability, but the results due to Kosterlitz and Thouless (taken from [7]) show that the ratio K flows to a universal value as the melting temperature is approached:

$$K_R(T_m^-) = \frac{1}{k_B T_m}\frac{4\mu_R(\mu_R+\lambda_R)}{2\mu_R+\lambda_R} \to 16\pi. \tag{12}$$

Here, the temperature T_m is the temperature at which the system changes from power-law translational correlations to exponentially decaying translational correlations.

The work of Nelson and Halperin [9], and Young [10] extended the work of Kosterlitz and Thouless by considering *bond orientational order*. Though the presence of dislocations disrupt translational order (Figure 5), they do not disrupt the six-fold orientational order. Any path around a dislocation produces zero winding of the bond order. The defects responsible for destroying bond orientational order are *disclinations*. Two bare disclinations are shown in Figure 5. A disclination core is marked by a lattice

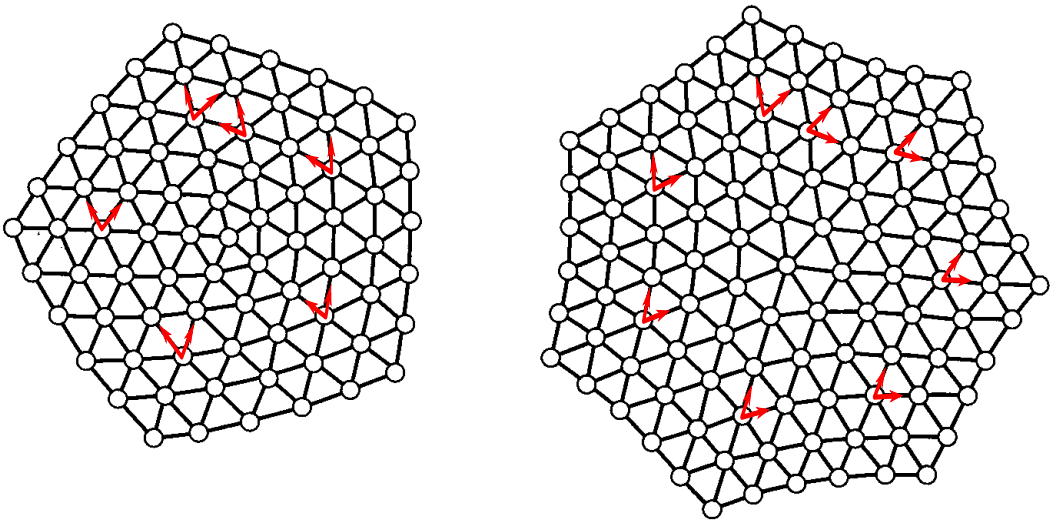

Figure 5: Illustrations of bare disclinations in a triangular lattice. Any path around the defect core (a site that has more or less than six bonds) produces a nonzero winding of the bond orientation. The left shows a $+\pi/3$ disclination, and the right shows a $-\pi/3$ disclination. Figure due to Chaikin and Lubensky [5], arrows added for clarity.

site that has more or fewer than 6 bonds. Looking closely at Figure 4, a dislocation defect is really a bound state of two oppositely charged disclination defects.

The Hamiltonian involving the bond orientational order is identical to the XY Hamiltonian, but instead of the fundamental relevant winding numbers being ± 1, the bond-orientation winding numbers of interest are $\pm 1/6$.

The correlation function of interest in this regime of interest is the bond-orientational correlation function, or the hexatic correlation function:

$$\psi_6(\mathbf{r}) = e^{6i\theta(\mathbf{r})}, \quad \langle \psi_6(\mathbf{r})\psi_6^*(0)\rangle \sim r^{-\eta_6(T)}. \tag{13}$$

This algebraic decay of bond-orientation correlations in a regime where the translational correlations decay exponentially defines the *hexatic phase*. This is a liquid-like phase that retains quasi-long range orientational order without a definite crystal lattice. From here, because of the identification with the XY model Hamiltonian, Nelson, Halperin, and Young deduced that the transition from the hexatic phase to the true liquid phase takes place by dislocations unbinding into their composite disclination pairs which move around the sample and destroy local orientational order. The true fluid phase occurs above this second transition temperature and is defined by exponentially decaying bond-orientation and translational correlations [9, 10].

3 Conclusion

The XY model provided the first system where topological defects in the order paramter were shown to participate crucially near the critical point. Two-dimensional melting of crystal lattices provides another model with more detail that follows the spirit of the XY model calculations. Kosterlitz and Thouless's early work on the XY model showed that the transition from quasi-long ranged order to disorder was mediated by unbinding of topological defects. Nelson, Young and Halperin showed later that topological defects in crystals became unbound and mediated the transition from quasi-long range translational and then orientational order. The basic theory finds applications in superfluid helium films, where topological defects are vortices of superfluid flow, in liquid crystals, where the topological defects are also dislocations and disclinations, and several other systems [5].

4 Appendix: Calculation of η in the XY Model without Vortices

This appendix is a detailed calculation of the critical exponent η in the XY model, mostly to prove to myself that I can perform this calculation. The Hamiltonian corresponding to our spin variables θ_i on a square lattice of spacing a in the quadratic approximation is

$$\mathcal{H} = \frac{J}{2} \sum_{\langle i,j \rangle} (\theta_i - \theta_j)^2 \to \frac{J}{2} \int d^2\mathbf{r} \, (\nabla\theta(\mathbf{r}))^2 \,. \tag{14}$$

We can apply the Fourier transform:

$$\theta(\mathbf{r}) = \frac{1}{(2\pi)^2} \int d^2\mathbf{k} \, e^{-i\mathbf{k}\cdot\mathbf{r}} \tilde{\theta}(\mathbf{k}), \qquad \mathcal{H} = \frac{J}{2} \int \frac{d^2\mathbf{k}}{(2\pi)^2} \, k^2 \left|\tilde{\theta}(\mathbf{k})\right|^2 . \tag{15}$$

Here, the integral over $\mathbf{k}$ is the square Brillouin zone $k_x, k_y \in [-\pi/a, \pi/a]$. The canonical partition function is then

$$Z = \int \mathcal{D}\theta \, \exp\left(-\frac{\beta J}{2} \int \frac{d^2\mathbf{k}}{(2\pi)^2} \, k^2 \left|\tilde{\theta}\right|^2 \right). \tag{16}$$

This is a Gaussian functional integral which is calculable exactly. If we add a term that is linear in $\tilde{\theta}$ that is coupled to some other function $\tilde{h}(\mathbf{k})$, then the partition function is

$$Z(\tilde{h}) = \int \mathcal{D}\theta \, \exp\left(\frac{1}{2\pi} \int \frac{d^2\mathbf{k}}{(2\pi)^2} \, \left(-\frac{\beta J k^2}{2} \left|\tilde{\theta}\right|^2 + \tilde{h}\tilde{\theta}^* \right) \right). \tag{17}$$

We can complete the square to compute this Gaussian integral:

$$-\frac{\beta Jk^2}{2}\left|\tilde{\theta}\right|^2+\tilde{h}\tilde{\theta}^*=-\frac{1}{2}\left(\beta Jk^2\left|\tilde{\theta}\right|^2-2\tilde{h}\tilde{\theta}^*-\frac{1}{\beta Jk^2}\left|\tilde{h}\right|^2\right)+\frac{1}{2\beta Jk^2}\left|\tilde{h}\right|^2$$
$$=-\frac{\beta Jk^2}{2}\left|\tilde{\theta}-\frac{a}{k\sqrt{\beta J}}\tilde{h}\right|^2+\frac{1}{2\beta Jk^2}\left|\tilde{h}\right|^2. \quad (18)$$

The functional integral integrates over all possible configurations of $\tilde{\theta}(\mathbf{k})$, so the shift by a function of $\mathbf{k}$ does not affect the functional integral. What remains is an exponential function of $\tilde{h}$:

$$Z(\tilde{h})=Z(\tilde{h}=0)\exp\left(\int\frac{d^2\mathbf{k}}{(2\pi)^2}\,\frac{1}{2\beta Jk^2}\left|\tilde{h}\right|^2\right). \quad (19)$$

This is useful now because we are interested in calculating the correlation function

$$\langle\mathbf{S}(\mathbf{r})\cdot\mathbf{S}(0)\rangle=\left\langle e^{i(\theta(\mathbf{r})-\theta(0))}\right\rangle=\frac{1}{Z(\tilde{h}=0)}\int\mathcal{D}\theta e^{-\beta\mathcal{H}+i\theta(\mathbf{r})-i\theta(0)}.$$

Here, we can right away substitute the linear function $h(\mathbf{r}')=i\left(\delta(\mathbf{r}'-\mathbf{r})-\delta(\mathbf{r}')\right)$ which is easily expressed in Fourier space:

$$\tilde{h}(\mathbf{k})=\frac{i}{(2\pi)^2}\left(e^{i\mathbf{k}\cdot\mathbf{r}}-1\right). \quad (20)$$

So the correlation function is then

$$\left\langle e^{i(\theta(\mathbf{r})-\theta(0))}\right\rangle=\frac{Z(\tilde{h}=0)}{Z(\tilde{h}=0)}\exp\left(\int\frac{d^2\mathbf{k}}{(2\pi)^2}\,\frac{1}{2\beta Jk^2}\left(2-2\cos\left(\mathbf{k}\cdot\mathbf{r}\right)\right)\right). \quad (21)$$

The integral over the Brillouin zone in the exponent is very difficult to solve analytically, but for large r, Mathematica gives that the leading order term is logarithmic in r, and the coefficient of the $\log r$ term is $\frac{1}{2\pi\beta J}$:

$$\left\langle e^{i(\theta(\mathbf{r})-\theta(0))}\right\rangle=e^{\text{const.}-\eta(T)\log(r/a)}=C_0\left(\frac{r}{a}\right)^{-\eta(T)},\quad \eta(T)=\frac{k_BT}{2\pi J}. \quad (22)$$

This gives the power-law decay in the absence of vortices which is a good approximation at low temperatures.

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