Vortices and the Berezinskii-Kosterlitz-Thouless Transition

In the 2d XY model, powerlaw correlations arise in the low temperature region. This exotic phase is destroyed by vortices leading to the Berezinskii-Kosterlitz-Thouless phase transition. We derive an effective Hamiltonian describing the thermodynamics of vortices, which takes the form of a two-component Coulomb plasma.

Demise of the quasi long-range order

FIG. 1: Vortices created by air turbulence of a jet airplane.

The state of matter we have identified is as close as XY spins can get to order in $d = 2$, and is called "quasi long-range order" (QLRO). We do not have broken symmetry or long range correlations, but the correlations still decay very slowly with distance. We have a situation which can be described as a critical state, especially having in mind that the coupling constant g does not acquire any singular corrections at due to spin-wave interactions. It does not flow, and in the RG language we have a "line of fixed points". The situation will

become even more clear after we perform an appropriate RG analysis of the Berezinskii-Kosterlitz-Thouless transition.

An interesting aspect of this scenario is that spin wave theory alone does not provide a mechanism for the destruction of QLRO no matter how high is the temperature. This possibility seems clearly at odds from what we expect, since at high temperatures ($T \gg J$), we expect exponentially decaying correlations and short range order only. It is likely that our analysis has overlooked something important. But what? To understand what is missing let us think about the cost of different spin configurations. It is clear that at temperatures $T \ll J$ nearby spins should nearly line-up. Does this mean that we can have only spin wave excitations? Not really.

FIG. 2: The "Big Red Spot" on Jupiter is a gigantic hurricane-like storm (votex), that lasts for centuries, and is larger then the entire planet Earth.

As first realized by Berezinskii (1971), and then examined in detail by Kosterlitz and Thouless (1973), in the $d = 2$ XY model we can identify *vortex* configurations where the spins field is "smooth" everywhere except in a small region of space. These "topological defects" have a property that once present in the system, they immediately eliminate the slowly decaying correlations in the spin phase $\theta(\mathbf{x})$. We can be more precise and define the "topological charge" of a vortex. To do this, we calculate the change of phase along a closed loop enclosing the vortex core (see figure). Because all physical quantities (e.g. the energy) is a periodic function of the spin phase θ with period 2π, the topological charge must be an

integer $n = 0, \pm 1, \pm 2 ...$(this is very similar as in the quantization of the angular momentum in elementary quantum mechanics).

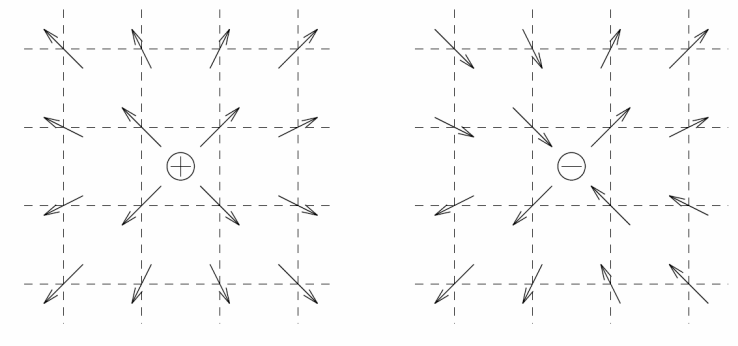

FIG. 3: Vortex configurations characterized by topological charge $n = +1$ (left) and $n = -1$ (right).

Clearly, since the presence of a vortex "rotates" the phase over large distances, randomly placed vortices will completely "scramble" the phase, leading to short range order. In contrast, if a vortex and an antivortex pair are close to each other, the phase accumulated over a loop enclosing both of them vanishes. Thus, vortices may or may not destroy QLRO, depending how they are distributed in the system. But before we address this subtle question, let us first calculate the energy cost to create an isolated vortex, in order to estimate their concentration at finite temperature. To do this, for the moment we ignore the "background" smooth spin-wave distortions, since they cannot play an important role in removing QLRO.

Consider a vortex with topological number n (see figure). For the spin configuration to be single valued (just as the wavefunction phase in quantum mechanics), the accumulated phase has to be an integer multiple of 2π as we go around the vortex. If we consider a circular trajectory of radius R, then $\nabla\theta(R)$ depends only on R, and we find

$$\oint d\theta = \oint d\mathbf{s} \cdot \nabla\theta = 2\pi R \nabla\theta(R) = 2\pi n.$$

We conclude that $\nabla\theta(R) = n/R$. We can immediately calculate the energy of an isolated vortex

$$\begin{aligned} \beta E_n &= \beta E_n^o + \frac{1}{2g} \int d\mathbf{x} \ \left(\nabla\theta(\mathbf{x})\right)^2 \\ &= \beta E_n^o + \frac{n^2}{2g} \int_a^L \frac{dR}{R} \\ &= \beta E_n^o + \frac{n^2 \pi}{g} \ln(L/a). \end{aligned}$$

Clearly, the vortices with $n = \pm 1$ cost least energy, and will thus be most abundant. In doing this calculation we have taken into account the fact that the continuum approximation breaks down around the vortex center. To correct for this, we have added a (finite) correction corresponding to the energy E_n^o of a vortex core.

Berezinskii-Kosterlitz-Thouless transition

We are now in a position to present a rough heuristic argument (Kosterlitz and Thouless, 1973) to estimate how many vortices are present at a given temperature, we have to compare the energy cost for creating a vortex, from the entropy gain associated with many different positions it can be placed.

The entropy of creating a single vortex, is

$$\begin{aligned} S_n &= \ln(\#\text{ of possible positions of the vortex center}) \\ &= 2\ln(L/a). \end{aligned}$$

Thus, the free energy of creating a $n = \pm 1$ vortex is

$$\beta F_{\pm 1} = \beta E_{\pm 1}^o + \frac{\pi}{g}\ln(L/a) - 2\ln(L/a).$$

As we can see from this expression, the first term is a finite number, whereas the last two both diverge logarithmically in the thermodynamic limit $L \longrightarrow \infty$. The entropy will win and a finite concentration of free vortices will be created provided that

$$g > g_c = \frac{\pi}{2}.$$

We therefore expect the vortices to proliferate above the Kosterlitz-Thouless temperature $T_{KT} \sim g_c$, and the QLRO state to be destroyed. At the critical point, the anomalous dimension takes a universal value

$$\eta(T_{KT}) = \frac{g_c}{2\pi} = \frac{1}{4},$$

just as in the $d = 2$ Ising model (presumably a coincidence). These hand-waving predictions about the vortex-unbinding BKT transition have been confirmed by more rigorous RG calculations, which we examine in the following.

Coulomb Gas Representation

The first step in developing a theory that describes the thermodynamics of vortices is writing down an effective Hamiltonian describing their energetics. We need to determine the energy of an arbitrary configuration containing a given number of vortices. The situation at hand is very similar to the structure of the velocity field $\mathbf{v}(\mathbf{x})$ in turbulent fluids (see Figs. 1 and 2), where vortex configurations are superimposed on a smooth background, and we can use the same mathematical tricks.

Very generally, an arbitrary vector field $\mathbf{v}(\mathbf{x})$ can be *uniquely* decomposed as a sum of two terms, one being a smooth "potential" component, and the other describing "vortex" configurations by writing

$$\mathbf{v}(\mathbf{x}) = \mathbf{E}(\mathbf{x}) + \mathbf{H}(\mathbf{x}),$$

with $\nabla \times \mathbf{E}(\mathbf{x}) = 0$, and $\nabla \cdot \mathbf{H}(\mathbf{x}) = 0$. Our choice of notation, where we used symbols $\mathbf{E}$ and $\mathbf{H}$ for the respective components is not arbitrary. This was chosen to emphasize the close mathematical analogy with yet another problem well known to us, that of static electric and magnetic fields. As we recall from electrodynamics (or even classical mechanics), any "irrotational" vector field satisfying $\nabla \times \mathbf{E}(\mathbf{x}) = 0$ can be viewed as a "potential" field, which can be represented as $\mathbf{E}(\mathbf{x}) = -\nabla\phi(\mathbf{x})$, since $\nabla \times \nabla\phi(\mathbf{x}) \equiv 0$. This component is vorticity free, since by Stokes theorem

$$\oint d\mathbf{s} \cdot \mathbf{E}(\mathbf{x}) = \int d\mathbf{S} \cdot \nabla \times \mathbf{E}(\mathbf{x}) = 0.$$

In contrast, any "source-free" vector field satisfying $\nabla \cdot \mathbf{H}(\mathbf{x}) = 0$ can be derived from a vector potential as $\mathbf{H}(\mathbf{x}) = \nabla \times \mathbf{A}(\mathbf{x})$. This uniquely determines the potential provided we fix a gauge (e.g. the Landau gauge $\nabla \cdot \mathbf{A}(\mathbf{x}) = 0$).

In our case, the votex-free component $\nabla\theta_{sw}(\mathbf{x})$ corresponds to spin waves, and as such plays no role at the BKT transition, which is dominated by vortices. We concentrate on the component describing vortices, and calculate the corresponding "vortex" component of the phase gradient, which can be represented as

$$\nabla\theta_v(\mathbf{x}) = \nabla \times \mathbf{A}(\mathbf{x}).$$

To calculate the vortex contribution to the free energy, we need to calculate $\mathbf{A}(\mathbf{x})$ for a given configuration of vortices. In standard magnetostatics, the Maxwell's equations require

$$\nabla \times \mathbf{H}(\mathbf{x}) = \mathbf{J}(\mathbf{x}),$$

where the "source" $\mathbf{J}(\mathbf{x}) = \frac{4\pi}{c}\mathbf{j}(\mathbf{x})$, and $\mathbf{j}(\mathbf{x})$ is the electrical current density. In terms of the vector potential

$$\nabla \times \mathbf{H}(\mathbf{x}) = \nabla \times (\nabla \times \mathbf{A}(\mathbf{x})) = \nabla\cdot(\nabla \mathbf{A}(\mathbf{x})) - \nabla^2 \mathbf{A}(\mathbf{x}),$$

and using the Landau gauge, we find

$$-\nabla^2 \mathbf{A}(\mathbf{x}) = \mathbf{J}(\mathbf{x}).$$

Each component of $\mathbf{A}(\mathbf{x})$ satisfies a Poisson-like equation, and a formal solution takes the form

$$\mathbf{A}(\mathbf{x}) = \int d^d\mathbf{x}\, G(\mathbf{x}-\mathbf{x}')\mathbf{J}(\mathbf{x}'),$$

with $G(\mathbf{x})$ being the Green's function of the Laplace operator $-\nabla^2$, with a Fourier transform $G(k) = 1/k^2$.

Our vector field $\nabla\theta_v(\mathbf{x})$ lives in a two-dimensional space, and its components are also confined to the XY plane. Therefore the vector potential points along the z-axis, i.e. $\mathbf{A}(\mathbf{x}) = A(\mathbf{x})\mathbf{e}_z$, and the Green's function is

$$G(\mathbf{x}) = \int d^2k\, \frac{e^{i\mathbf{k}\mathbf{x}}}{k^2} = \frac{1}{2\pi}\ln|\mathbf{x}|\,.$$

In contrast to standard electrodynamics, the "source" $\mathbf{J}(\mathbf{x})$ is not arbitrary, but needs to be determined from the positions of the vortices. To find it, consider an arbitrary loop C enclosing vortices located at positions $\mathbf{x} = \mathbf{x}_i$, with respective topological charges n_i. The total phase accumulated by going around this loop is

$$\sum_{i=1}^{N} 2\pi n_i = \oint d\mathbf{s}\cdot\nabla\theta_v(\mathbf{x}) = \int_C d\mathbf{S}\cdot\nabla\times\nabla\theta_v(\mathbf{x}) = \int_C d\mathbf{S}\cdot\nabla\times(\nabla\times\mathbf{A}(\mathbf{x})) = -\int_C dS\cdot\nabla^2 A(\mathbf{x}).$$

We conclude that

$$-\nabla^2 A(\mathbf{x}) = 2\pi\sum_{i=1}^{N} n_i\delta(\mathbf{x}-\mathbf{x}_i).$$

Thus the potential produced by these N vortices is

$$A(\mathbf{x}) = -\sum_{i=1}^{N} n_i \ln|\mathbf{x}-\mathbf{x}_i|\,.$$

We can now obtain the energy of the vortices

$$\begin{aligned}\beta E_{vort} &= \frac{1}{2g}\int d\mathbf{x}\,(\nabla\theta_v(\mathbf{x}))^2 \\ &= \frac{1}{2g}\int d\mathbf{x}\;(\nabla\times\mathbf{A}(\mathbf{x}))^2 = \frac{1}{2g}\int d\mathbf{x}\;(\nabla A(\mathbf{x}))^2 = -\frac{1}{2g}\int d\mathbf{x}\,A(\mathbf{x})\nabla^2 A(\mathbf{x}) \\ &= -\frac{1}{2g}\int d\mathbf{x}\;\left[-\sum_{i=1}^{N} n_i \ln|\mathbf{x}-\mathbf{x}_i|\right]\left[-2\pi\sum_{i=1}^{N} n_i\delta(\mathbf{x}-\mathbf{x}_j)\right] \\ &= -\frac{\pi}{g}\sum_{i,j=1}^{N} n_i n_j \ln|\mathbf{x}_i-\mathbf{x}_j|\,.\end{aligned}$$

In obtaining this result we performed an integration by part. The corresponding surface term diverges with system size, unless only the configurations that respect charge neutrality are retained

$$\sum_i n_i = 0.$$

Note also that the the $i=j$ term appears to lead to a divergence, which is simply an artefact of the continuum approximation, and which should be replaced by a finite core energy of a vortex. In addition, the vortices with $n_i = \pm 1$ provide the dominant contribution near the BKT transition, and to leading order only those are retained. Finally

$$\beta E_{vort} = \sum_i \beta E_o n_i^2 - \frac{2\pi}{g}\sum_{i<j} n_i \ln(\mathbf{x}_i-\mathbf{x}_j)\,n_j.$$

Mott Metal-insulator transition in the Coulomb gas

This expression for the energy of vortices in the XY model is identical to the Coulomb energy of a two-dimensional system of charged particles with chemical potential E_o, which are interacting through a two-dimensional Coulomb potential $V_c(\mathbf{x}) = \frac{1}{2\pi}\ln|\mathbf{x}|$. As we can see from this expression, vortices with equal "charge" repel each other, while those with opposite charge attract. As a result, they tend to form vortex-antivortex pairs at low temperatures, but dissociate at $T > T_{KT}$.

Very similar processes take place in many different systems where pairs of opposite charges bind at low temperature to form neutral atoms or molecules. An interesting example is the structure of the mantle inside planet Jupiter, which is formed mostly of hydrogen. The outer layer is formed of molecular hydrogen (H_2 molecules), which is an insulating fluid. Deeper

below the surface the pressure is so high that hydrogen molecules dissociate and one finds metallic liquid hydrogen.

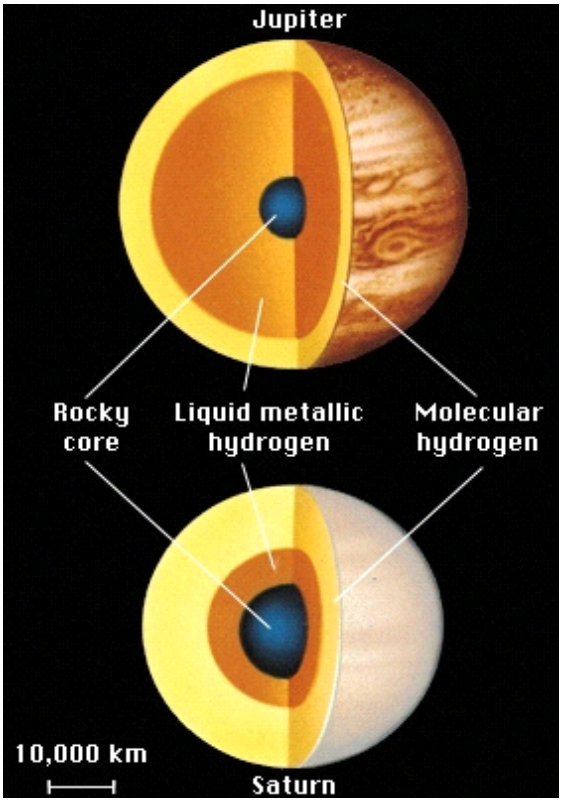

FIG. 4: Interior structure of planets Jupiter and Saturn. Because of large content of metallic liquid hydroge, Jupiter has a huge magnetosphere.

This phase is actually one that contains the largest fraction of Jupiter's mass. The two phases do not differ by any broken symmetry. The only important difference is in the conducting properties, i.e. in form of dielectric screening. In the metallic phase the effective Coulomb potential is screened, i.e. takes the "Yukawa" form

$$V_{eff}(R) \sim \exp\{-R/\xi\},$$

where ξ is the screening (Debye) length. In the molecular (insulating) phase, there are no free charges to do the screening, and the Coulomb potential remains long-ranged

$$V_{eff}(R) \sim 1/\varepsilon R,$$

where ε is the dielectric constant of the molecular liquid, which is finite. Of course, since in this three dimensional situation the interaction between charges is not logarithmic, the

argument of Kosterlitz and Thouless does not apply, and one finds a first order phase transition.

This behavior is very similar to that of vortices in the XY model. Note, though, that in that case free vortices destroy phase correlations of the spin field, so the spin correlations become short ranged. In contrast, at $T < T_{KT}$, the vortices are bound in pairs, and the spin correlations remain "quasi long-ranged", i.e. have powerlaw decay. This is an example of duality, which we shall explore in more detail in the next lecture, when we discuss the mapping of the XY model to the roughening problem and the Sine-Gordon model.

The structure of the Kosterlitz-Thouless phase transition can be established in detail by performing a RG analysis of the Coulomb gas model, as was first done by Kosterlitz and Thouless. When written in this form, the problem looks quite different then the field theories we are used to, and it is not obvious how such a RG calculation can be done. Indeed, the original calculation presented a real-space RG formulation that appears quite different then the momentum shell approach of Wilson. This approach was based on a similar calculation carried out earlier by Anderson, Yuval and Hamann (1971) for the Kondo problem, where the same RG equations are found. We will not follow that rounte here. Instead, we will map the XY model to the its dual Sine-Gordon model, where standard momentum shell RG can be used to derive the same results.