Coulomb Gas picture of vortices in the XY model

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Based mostly on Kardar, Statistical Physics of Fields, section 8.2-8.3

1 Introduction

In this tutorial we will discuss an effective picture for vortices statistics in the XY model in 2D. Recall that in this model (2D XY model) a unique kind of phase transition takes place, named Berezinskii-Kosterlitz-Thouless (BKT) phase transition. Both above and below the phase transition there is no long range order in the usual sense, but instead there is a change in the decay of correlations from exponential decay above the transition to power law decay below it. Now we shall briefly describe the context of the 2D XY model and then look at an effective picture of gas of vortices which illustrates the BKT transition.

2 Context

The XY model in 2D is a special case of the O(n) model in d dimensions, for $n = 2$ and $d = 2$. One route to motivate the interest in this case is the following cascade

- Start with the Landau theory, with the Landau Free Energy (LFE)

$$F[\eta] = \alpha(T - T_c)|\eta|^2 + b\left(|\eta|^2\right)^2$$

  which predicts a symmetry breaking phase transition at T_c.

- The LFE is a mean field approximation and the Ginzburg criterion sets its limits of applicability. For $d > 4$ (upper critical dimension) it gives good predictions but for $d < 4$ we pass to the Ginzburg-Landau FE (GLFE)

$$F[\eta(x)] = \int dx \left[|\nabla\eta|^2 + \alpha(T - T_c)|\eta|^2 + b\left(|\eta|^2\right)^2\right]$$

- The GLFE predicts Goldstone modes, or spin waves, below the critical temperature. These modes destroy order for $d \leq 2$ (lower critical dimension): $\left\langle (\Delta\eta)^2 \right\rangle \sim \frac{a^{2-d} - L^{2-d}}{d-2}$ (Eq.(165) in notes).
- This implies $T_c \sim d - 2 \;\rightarrow$ low temperature expansion, for $\epsilon = d - 2 \ll 1$
- Critical temperature (from RG approach): $\frac{2\pi(d-2)}{n-2} + O\left(\epsilon^2\right)$ - self consistent! (for $n > 2$).
- What happens in $d = 2, n = 2$???

3 Mapping to 2D Coulomb Gas

Start with the XY Hamiltonian

$$H = -J \sum_{\langle i,j \rangle} \cos\left(\theta_i - \theta_j\right)$$

In the spin wave (low temperature) approximation

$$H \approx \frac{J}{2} \int \left|\nabla\theta(\mathbf{r})\right|^2 d^2r + const. \tag{1}$$

Our aim is to study the BKT transition using an effective picture of spin waves and vortices (the basic excitations of the theory). The way to do this is to work in the continuous approximation - which is appropriate at low temperatures and far from any vortex core (we will then have a correction due to the vortex core). Denoting $\mathbf{u}(\mathbf{r}) \equiv \nabla\theta(\mathbf{r})$, we can always (for any vector) split $\mathbf{u}$ to longitudinal and transversal parts

$$\begin{aligned} \mathbf{u}(\mathbf{r}) &= \mathbf{u_l}(\mathbf{r}) + \mathbf{u_t}(\mathbf{r}) & (2) \\ \nabla \cdot \mathbf{u_t} &= 0 & (3) \\ \nabla \times \mathbf{u_l} &= 0 & (4) \end{aligned}$$

where $\nabla \times \mathbf{u_t} = \left(\partial_x u_{t,y} - \partial_y u_{t,x}\right)\hat{\mathbf{z}}$. The motivation is that $\mathbf{u_l}$ will account for spin waves and $\mathbf{u_t}$ for the distortion due to vortices. Eq. (4) implies that

$$\mathbf{u_l} = \nabla\phi \tag{5}$$

for some potential (analytic function)$\phi(\mathbf{r})$. Notice that $\nabla \times \mathbf{u_t} = \nabla \times \mathbf{u}$, and hence using Stock's theorem, for any area A

$$\begin{aligned} \int_A \left(\nabla \times \mathbf{u_t}\right) \cdot \left(\hat{\mathbf{z}} d^2r\right) &= \int_A \left(\nabla \times \mathbf{u}\right) \cdot \left(\hat{\mathbf{z}} d^2r\right) \\ &= \oint_{\partial A} \mathbf{u} \cdot d\mathbf{s} \\ &= \oint_{\partial A} \nabla\theta \cdot d\mathbf{s} = 2\pi n \end{aligned}$$

where n is an integer. The last equality is a manifestation of the fact that θ is defined up to $2\pi n$. Hence we can view the integrand in the LHS as

$$\nabla \times \mathbf{u_t} = 2\pi \hat{z} \sum n_i \delta \left(\mathbf{r} - \mathbf{r}_i \right)$$

This can be solved by setting

$$\mathbf{u_t} = -\nabla \times (\Psi \hat{\mathbf{z}}) \tag{6}$$

and remebering that $\nabla\times\nabla\times(\boldsymbol{\Psi}\hat{\mathbf{z}}) = \nabla\times(\partial_y\Psi, -\partial_x\Psi, 0) = -\partial_x^2\Psi - \partial_y^2\Psi = -\Delta\Psi$, hence

$$\Delta\Psi = 2\pi\hat{\mathbf{z}} \sum n_i \delta \left(\mathbf{r} - \mathbf{r}_i \right)$$

which is the potential formed by a set of charges n_i at locations r_i. The solution (in 2D) is

$$\Psi(\mathbf{r}) = \sum_i n_i \ln \left(|\mathbf{r} - \mathbf{r}_i| \right) \tag{7}$$

Rearranging we got

$$u(r) = \nabla\phi - \nabla \times (\Psi \hat{\mathbf{z}}) \tag{8}$$

with Ψ given by Eq.(7). The field degrees of freedome are $\phi(\mathbf{r})$ (spin waves) and $\{n_i, r_i\}$ (charges and locations of vortices). Plugging (8) into the Hamiltonian (1) yields (ommitting the constant term)

$$H = \frac{J}{2} \int \left(|\nabla\phi(\mathbf{r})|^2 - 2\left(\nabla\phi(\mathbf{r})\right) \cdot \nabla \times (\Psi\hat{\mathbf{z}}) + |\nabla \times (\Psi\hat{\mathbf{z}})|^2 \right) d^2 r$$

The second term vanish as using integration by parts

$$\int \nabla\phi(\mathbf{r}) \cdot \nabla \times (\Psi\hat{\mathbf{z}})\, d^2 r = -\int \phi(\mathbf{r})\nabla \cdot \left[\nabla \times (\Psi\hat{\mathbf{z}})\, d^2 \right] r = 0$$

Hence we see that we can write the Hamiltonian as

$$\begin{aligned} H\left(\phi(\mathbf{r}), \{n_i, r_i\}\right) &= H_0\left(\phi\left(\mathbf{r}\right)\right) + H_1\left(\{n_i, r_i\}\right) \\ H_0 &= \frac{J}{2} \int |\nabla\phi(\mathbf{r})|^2 \, d^2 r \\ H_1 &= \frac{J}{2} \int |\nabla \times (\Psi\hat{\mathbf{z}})|^2 \, d^2 r \end{aligned}$$

and the partition function as

$$\begin{aligned} Z &= \int D\phi \int \prod_i d^2\mathbf{r}_i \sum_{\{n_i\}} Exp\left[-\beta H_0\left(\phi\left(\mathbf{r}\right)\right) + \beta H_1\left(\{n_i, \mathbf{r}_i\}\right) \right] \\ &= \left[\int D\phi e^{-\beta H_0} \right] \left[\sum_{\{n_i\}} \int \prod_i d^2\mathbf{r}_i e^{-\beta H_1} \right] \equiv Z_{sw} Z_v \end{aligned}$$

Now H_1 can be simplified using the fact that $|\nabla\times(\Psi\hat{\mathbf{z}})|^2=|\nabla\Psi|^2$ and then using integration by parts

$$\begin{aligned}
H_1 &\equiv \frac{J}{2}\int|\nabla\times(\Psi\hat{\mathbf{z}})|^2\,d^2r\\
&= \frac{J}{2}\int\nabla\Psi\cdot\nabla\Psi d^2r\\
&= \oint_\gamma\Psi\nabla\Psi\cdot d\mathbf{s}-\frac{J}{2}\int\Psi\nabla^2\Psi d^2r\\
&= -J\pi\int\sum_i n_i\ln\left(|\mathbf{r}-\mathbf{r}_i|\right)\sum_j n_j\delta\left(\mathbf{r}-\mathbf{r}_j\right)d^2r\\
&= -J\pi\sum_{i,j}n_in_j\ln\left(|\mathbf{r}_i-\mathbf{r}_j|\right)
\end{aligned}$$

which is a Hamiltonian of a gas (without kinetic energy) of charged particles in 2D interacting through Coloumb interactions. Notice that in order to neglect the term $\oint_\gamma\Psi\nabla\Psi\cdot d\mathbf{s}$ we assumed that the gas is neutral as a whole ($\sum n_i=0$) - other configurations are suppressed (as each charge's contribution goes like $n_i log(L)$). This picture breaks down at $i=j$ where the approximation of continuous phase change is not adequate and the lattice structure is important. For this we have to add the energy of the vortices core, which depends on how exactly we took the continuous limit (which also affects the value of J) but formally we can write

$$H_1=-\sum_i\varepsilon\left(n_i\right)-J\pi\sum_{i\neq j}n_in_j\ln\left(|\mathbf{r}_i-\mathbf{r}_j|\right)$$

4 Analysis of the Coulomb gas picture

The spin waves free energy $F_{sw}=-T\log Z_{sw}$ is analytic and hence a phase transition can come only from the vortex part. The energy $\varepsilon\left(n_i\right)$ is nonlinear in n_i and it is customary to assume that due to this the probable excitations are $n_i=\pm1$. The energy of the vortex core is independent of the sign of the charge and we can thus denote $y_0=e^{-\beta\varepsilon(\pm1)}$. The parition function is then approximated as

$$Z_v\approx\sum_{N=0}^{\infty}y_0^N\int\prod_i^N d^2\mathbf{r}_ie^{K\sum_{i<j}n_in_j\ln(|\mathbf{r}_i-\mathbf{r}_j|)}$$

with $K=2\beta J\pi$, $n_i=\pm1$ and $\sum_i n_i=0$. This is a grand-canonical partition function with fugacity y_0. The general picture is as follows: at low temperature $y_0\to0$ there are no vortices, only spin waves (which have linear excitation spectrum in low temperatures). As temperature increases vortices start to appear in pairs of vortex and anti-vortex, but due to the logarithmic energy cost they are confined together. At the BKT critical temperature a deconfinement transition occurs and the gas becomes a plasma of vortices which screen the interactions of the "charges" (vortices) and cut-off the correlation between the original spins.

To do the analysis more rigourosly, one can work in the grand canonical ensemble and follow a Renormalization Group flow as done in Kardar, section 8.3. Alternatively, we can work in other ensembles and make more heuristic arguments as we shall do now:

4.1 Canonical Ensemble

In the canonical ensemble N is fixed and we need to calculate

$$Z \sim \int \prod_i^N d^2\mathbf{r}_i e^{-K\sum_{i<j} n_i n_j \ln(|\mathbf{r}_i - \mathbf{r}_j|)} = \int \prod_i^N d^2\mathbf{r}_i \prod_{j>i} |\mathbf{r}_i - \mathbf{r}_j|^{-Kn_in_j} \quad (9)$$

We define a center of mass coordinate $\mathbf{R} = \frac{1}{N}\sum \mathbf{r}_i$ and change variables $\tilde{\mathbf{r}}_i = \mathbf{r}_i - \mathbf{R}$ yielding

$$Z \sim V \int \prod_i^{N-1} d^2\mathbf{r}_i \prod_{j>i} |\mathbf{r}_i - \mathbf{r}_j|^{-Kn_in_j} \quad (10)$$

where the V factor arises due to integration over $\mathbf{R}$. To probe the transition, we calculate the contribution of configurations for which $\tilde{\mathbf{r}}_i \to \epsilon \to 0$. The contribution scales with ϵ as

$$Z_\epsilon \sim \epsilon^{2(N-1)-K\sum n_i n_j}$$

Now

$$\sum_{i,j} n_i n_j = N_{++} + N_{--} - N_{+-} \quad (11)$$

where $N_{s,t}$ is the number of vortex pairs out of the $N(N-1)/2$ pairs with signs s and t. Simply counting we get $N_{++} = N_{--} = \frac{1}{2}\frac{N}{2}\left(\frac{N}{2} - 1\right)$ and $N_{+-} = \left(\frac{N}{2}\right)^2 N_{+-} = \left(\frac{N}{2}\right)^2$. Hence

$$\sum_{i,j} n_i n_j = \frac{N}{2} \quad (12)$$

and

$$Z_\epsilon \sim \epsilon^{2(N-1)-KN/2}$$

We see that there is a critical coupling if $K_c = \frac{4(N-1)}{N}$ which in the thermodynamic limit ($N \to \infty$) is $K_c = 4$. For $K < K_c$ (high temperature phase) the exponent of ϵ is positive and hence $Z_\epsilon \to 0$ as $\epsilon \to 0$, while if $K > K_c$ (low temperature phase) these configurations dominate, which means that all of the vortices are confined together (yielding a power low decay of correltions).

4.2 Micro-Canonical Ensemble

Here we shall derive the equation of state of the gas of vortices:

In the micro-canonical ensemble we should calculate the density of states $g(E, A) = \int \delta(E - H[\{\mathbf{r}_i\}]) \prod_i d^2\mathbf{r}_i$. We can rescale $\mathbf{r}_i = L\mathbf{x}_i$ with $A = L^2$

$$
\begin{aligned}
\beta H_1(\{\mathbf{r}_i\}) &= -K \sum_{i,j} n_i n_j \ln(|\mathbf{r}_i - \mathbf{r}_j|) \\
&= -K \sum_{i,j} n_i n_j \ln(|\mathbf{x}_i - \mathbf{x}_j|) - K \sum_{i,j} n_i n_j \ln(L) \\
&= \beta H_1(\{\mathbf{x}_i\}) - \frac{1}{2} K \ln(A) \sum_{i,j} n_i n_j
\end{aligned}
$$

and hence

$$
\begin{aligned}
g(E, A) &= A^N \int \delta\left(E - H[\{\mathbf{x}_i\}] + \frac{1}{2} KT \ln(A) \sum_{i,j} n_i n_j\right) \prod_i d^2\mathbf{x}_i \\
&= A^N g(E', 1) \equiv A^N \tilde{g}(E') \\
E' &= E + \frac{1}{2} KT \ln(A) \sum_{i,j} n_i n_j
\end{aligned}
$$

Using Eq.(12) we find

$$
E' = E - \frac{N}{4} KT \ln(A)
$$

The equation of state can be found in the following way

$$
\begin{aligned}
S(E, A) &= \ln(g(E, A)) = N \ln A + \ln \tilde{g}(E') \\
T = \left(\frac{\partial S}{\partial E}\right)_A^{-1} &= \frac{\tilde{g}(E')}{\partial_E \tilde{g}(E')} \\
P = T \left(\frac{\partial S}{\partial A}\right)_E &= T\left(\frac{N}{A} - \frac{NKT}{4A} \frac{\partial_E \tilde{g}(E')}{\tilde{g}(E')}\right) \\
&= \frac{NT}{A}\left(1 - \frac{K}{4}\right)
\end{aligned}
$$

For $K \to 0$ $(T \to \infty)$ the system becomes an ideal gas of vortices. As $K \to 4$ the pressure vanishes due to confinement of vortices.