Proseminar Phase Transitions

Berezinkii-Kosterlitz-Thouless Transition

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Outline

- **Introduction**
- **The partition function**
- **Effective interaction**
- **Renormalization group**

Two-dimensional XY model

$O(n)$ model:

- d-dimensional lattice
- n-dimensional (classical) unit vector $\mathbf{S}_x$ at each site
- Spin-spin interaction between nearest neighbors

$$V(\mathbf{S}_x, \mathbf{S}_y) = -J\,\mathbf{S}_x \cdot \mathbf{S}_y = -J\ \cos(\theta_x - \theta_y) = V(\theta_x - \theta_y),$$

exhibiting $O(n)$ symmetry

Two-dimensional XY model:

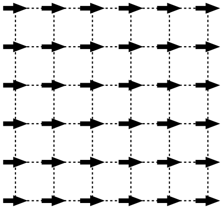
- $d = n = 2$

Absence of symmetry breaking in two dimensions

- Ground state: all spins aligned
- Three and higher dimensions:
  Ferromagnetic phase
- Less than three dimensions:
  No ferromagnetic phase due to fluctuations

  (*Mermin-Wagner theorem*;
  possibly hand-waiving explanation later)
- Nonetheless: Phase transition without symmetry breaking

  (*Kosterlitz-Thouless transition*)

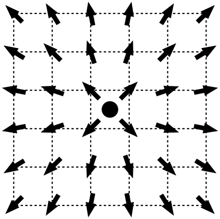


Vortices

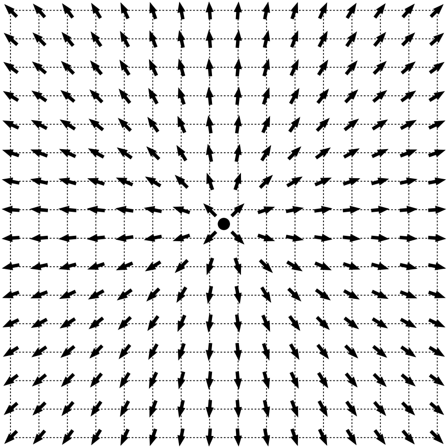
- Adding angles between neighboring spins around a closed loop $\gamma \subset \mathbb{Z}^2$ on lattice:

$$\sum_{xy \in \gamma} \psi_{xy} = 2\pi m, \quad m \in \mathbb{Z}$$

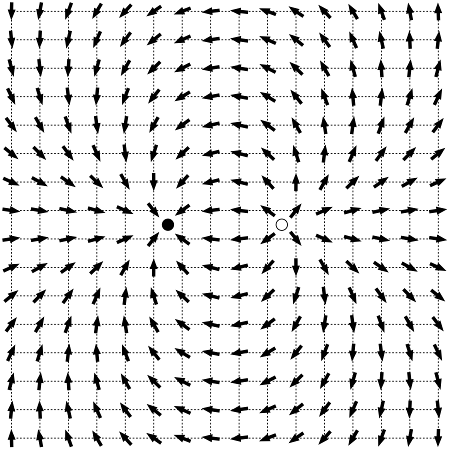
Definition: A *vortex* with vorticity m is a square of the lattice such that the sum of angles around the boundary is $2\pi m$.



A single vortex of charge $k = +1$



Two vortices of charges $k = +1$ and $k = -1$

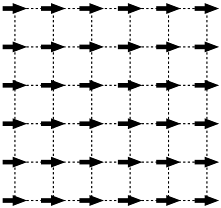


Gaussian approximation

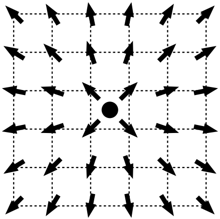
- Gaussian approximation:

$$V(\theta_i, \theta_j) = \frac{J}{2}(\theta_i - \theta_j)^2$$

- Prediction of spin-waves
- Fails to predict vortices because it is not periodic while the original potential is!



An isolated vortex



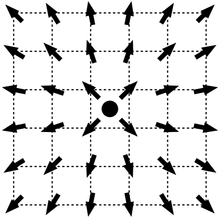
Most simple realization of a vortex:

$$\phi(x, y) = \arctan\left(\frac{y}{x}\right)$$

Energy of the configuration:

$$-J \sum_{\langle x,y \rangle} \cos(\theta_x - \theta_y)$$

An isolated vortex



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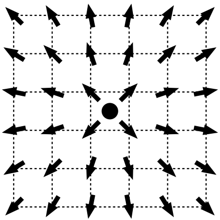

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Energy of the configuration:

$$-J \sum_{\langle x,y \rangle} \cos(\theta_x - \theta_y) \;\longrightarrow\; -J \int_\Lambda \left(1 - \frac{1}{2}(\nabla\phi)^2\right) \,\mathrm{d}^2 x$$

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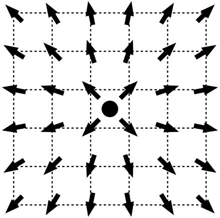

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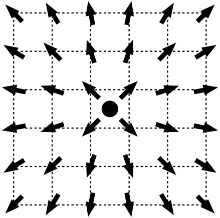

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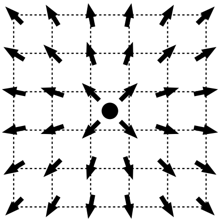
Energy of an isolated vortex in this approximation:

$$\frac{J}{2} \int_{S_L \setminus S_a} (\nabla\phi)^2 \, \mathrm{d}^2 x$$

An isolated vortex



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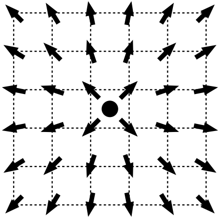
Energy of an isolated vortex in this approximation:

$$\frac{J}{2} \int_{S_L \setminus S_a} \left(\begin{pmatrix} -y/r^2 \\ x/r^2 \end{pmatrix} \right)^2 \mathrm{d}^2 x$$

An isolated vortex



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Energy of an isolated vortex in this approximation:

$$\frac{J}{2}\int_{S_L\setminus S_a}\left(\frac{1}{r}\right)^2\,\mathrm{d}^2x = \frac{J}{2}\int_0^{2\pi}\mathrm{d}\phi\int_a^L\left(\frac{1}{r}\right)^2 r\,\mathrm{d}r = J\pi\log\left(\frac{L}{a}\right)$$

[Note: ϕ is not differentiable on $\mathbb{R}^+$, but this is a Lebesque null set.]

Free Energy argument

Assumption: We add one vortex to a spin configuration

- Number of sites a single vortex could occupy is $\left(\frac{L}{a}\right)^2$:

$$S = 2\log\left(\frac{L}{a}\right)$$

- The Free Energy of one vortex can thus be estimated to be

$$F = U - TS = \log\left(\frac{L}{a}\right)(J\pi - 2T)$$

- Vortex is favorable if $F < 0$:
  - $T > \frac{J\pi}{2}$: $F < 0$
  - $T < \frac{J\pi}{2}$: $F > 0$

  The result resembles the one we will obtain in the RG analysis.

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Summary

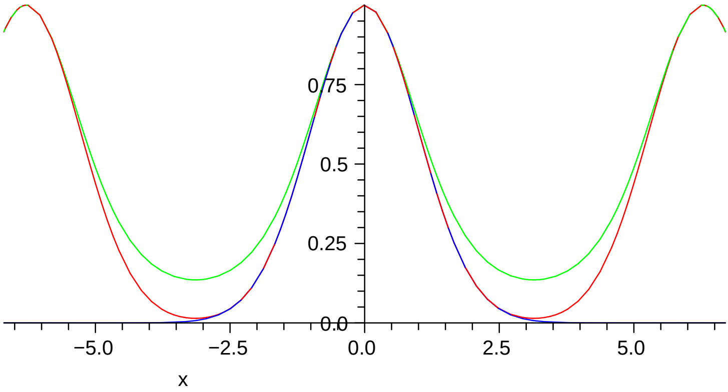
Summary:

- Gaussian model is not periodic, hence does not allow vortex configurations!
- We have seen the qualitative reason for vortices, but this does not include the knowledge of the proper partition function.

How can we obtain the partition function?

- Villain model: By means of Fourier transformation, the partition function can be rewritten in such a way as to predict the formation of vortices directly!

Villain approximation



The original partition function of the model

$$Z_K = \int_{-\pi}^{\pi} \cdots \int_{-\pi}^{\pi} \prod_{x \in \Lambda} \mathrm{d}\theta_x \sum_{xy} e^{K \cos(\theta_x - \theta_y)}, \quad K := \beta J$$

Decoupling of spin-waves and Coulomb gas

Partition function of the Villain model:

$$Z_K = \underbrace{\left(\int_{-\infty}^{\infty} \dots \int_{-\infty}^{\infty} \prod_{x \in \Lambda} \mathrm{d}\phi_x \; e^{-\frac{1}{2K} \sum_{xy} [\phi_x - \phi_y]^2)} \right)}_{Z_K^{\mathrm{SW}}} \cdot \underbrace{\left(\sum_n e^{2\pi^2 K \sum_{xy} n_x C(x-y) n_y} \right)}_{Z_K^{\mathrm{V}}} \quad (1)$$

Generalized Villain model

- The construction of a renormalization group for the Coulomb gas requires the introduction of an energy cost E_c for the creation of a vortex (chemical potential):

$$e^{-\beta E} \quad \longrightarrow \quad e^{-\beta(E+N\cdot E_c)}$$

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with the *fugacity*

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Generalized partition function:

$$Z_K^{\mathrm{V}} = \sum_n {y_0}^{N(n)} \, e^{2\pi^2 K \sum_{xy} n_x C(x-y) n_y}$$

Physical picture

- At low temperatures, particles of opposite charge form closely bound pairs, effectively screening the bare potential.

  Insulator, corresponding to a finite dielectric constant.
- At high temperatures, the pairs unbind and a transition to a plasma takes place

  Metal, corresponding to a vanishing dielectric constant.

Ensemble of none or two charges

Goal: Perturbative calculation of dielectric constant.

Physical assumption: Dominant contribution to the partition function is given by the configurations with none or two charges of opposite sign:

$$Z_K = \sum_n {y_0}^{N(n)} \, e^{2\pi^2 K \sum_{y,y'} n_y C(y-y')_{yy'} n'_y}$$

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$$
\begin{aligned}
Z_K &= \sum_n {y_0}^{N(n)} \; e^{2\pi^2 K \sum_{y,y'} n_y C(y-y')_{yy'} n'_y} \\
&= 1 + {y_0}^2 \sum_{y,y'} e^{-2\pi^2 K C(y-y')} + \mathcal{O}({y_0}^4)
\end{aligned}
$$

Energy cost of two additional charges

Physical assumption: The effective interaction between two *external* test charges can now be understood to be the following:

- The additional reduced energy (βH) when the two charges are added to a given configuration n is

$$E(x, x'; n) = 2\pi K(+1)C(x - x')(-1) + 2\pi KD(x, x'; n)$$

where

$$D(x, x'; n) = \sum_y (+1)C(x - y)n_y + \sum_y (-1)C(x' - y)n_y$$

is the interaction term between the external and the internal charges.

Effective Boltzmann factor

Define the effective Boltzmann factor as

$$e^{-\beta V(x-x')} \quad = \quad \langle e^{-E(x,x';n)} \rangle$$

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$$\begin{aligned} e^{-\beta V(x-x')} &= \langle e^{-E(x,x';n)} \rangle \\ &= \frac{e^{-2\pi^2 KC(x-x')} + \sum_{y,y'} e^{-2\pi^2 KC(y-y')} e^{-E(x,x';y,y')} + \mathcal{O}(y_0^4)}{1 + {y_0}^2 \sum_{y,y'} e^{-2\pi^2 KC(y-y')} + \mathcal{O}({y_0}^4)} \end{aligned}$$

Effective Boltzmann factor

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\end{aligned}
$$

After a number of approximations:

$$
e^{-\beta V(x-x')} = e^{-2\pi^2 K_{\text{eff}} C(x-x')},
$$

with

$$
K_{\text{eff}} = K - 2\pi^3 K^2 {y_0}^2 a^{2\pi K} \int_a^{\infty} \mathrm{d}r \; r^{3-2\pi K} + \mathcal{O}({y_0}^4)
$$

Kosterlitz recursion relations

The effective coupling constant can be restated as:

$$K_{\mathrm{eff}} = K - 4\pi^3 K^2 y^2 \int_a^\infty \mathrm{d}r \; r^{3-2\pi K} + \mathcal{O}(y^4)$$

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$$K_{\text{eff}} = K - 4\pi^3 K^2 y^2 \underbrace{\int_a^\infty \mathrm{d}r\, r^{3-2\pi K}}_{\text{diverges for } K<\frac{2}{\pi} \text{ – the high temperature regime}} + \mathcal{O}(y^4)$$

- Even though the integral actually diverges, we can still obtain information on the scaling behavior.

Kosterlitz recursion relations

The effective coupling constant can be restated as:

$$K_{\text{eff}} = K - 4\pi^3 K^2 y^2 \left[\int_a^{a(1+l)} \mathrm{d}r \; r^{3-2\pi K} + \int_{a(1+l)}^{\infty} \mathrm{d}r \; r^{3-2\pi K} \right] + \mathcal{O}(y^4)$$

- Split integral into a finite and a divergent part.

Kosterlitz recursion relations

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$$K_{\mathrm{eff}} = \left[K - 4\pi^3 K^2 y^2 \int_a^{a(1+l)} \mathrm{d}r \; r^{3-2\pi K} \right] - 4\pi^3 K^2 y'^2 \int_{a(1+l)}^{\infty} \mathrm{d}r \; r^{3-2\pi K} + \mathcal{O}$$

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with

$$K' := K - 4\pi^3 K^2 y^2 \int_a^{a(1+l)} \mathrm{d}r \; r^{3-2\pi K}$$

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Kosterlitz recursion relations

We have thus seen that the coupling constants are transformed by

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Iteratation of this transformation in the limit $l \to 0$:

$$\begin{aligned} \frac{\mathrm{d}K}{\mathrm{d}l} &= -4\pi^3 K^2 y^2 + \mathcal{O}(y^4) \\ \frac{\mathrm{d}y}{\mathrm{d}l} &= (2-\pi K)y + \mathcal{O}(y^3) \end{aligned}$$

(Kosterlitz recursion relations)

Kosterlitz recursion relations

New variables in the vicinity of $(K, y) = (\frac{2}{\pi}, 0)$

$$\begin{aligned} X &:= \frac{1}{4}(2 - \pi K) \\ Y &:= \pi^2 y \\ L &:= 2l, \end{aligned}$$

simplify recursion relations

$$\begin{aligned} \frac{\mathrm{d}X}{\mathrm{d}L} &= 2Y^2 + \mathcal{O}((X+Y)^4) \\ \frac{\mathrm{d}Y}{\mathrm{d}L} &= 2XY + \mathcal{O}((X+Y)^3). \end{aligned}$$

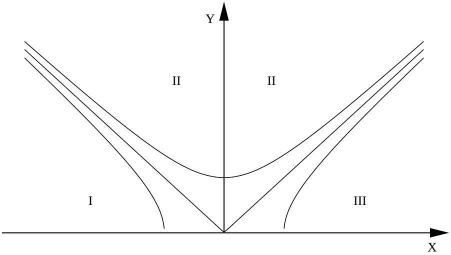
Note:

- $K \propto T^{-1}$, thus small T correspond to small X and vice versa

Renormalization group flow

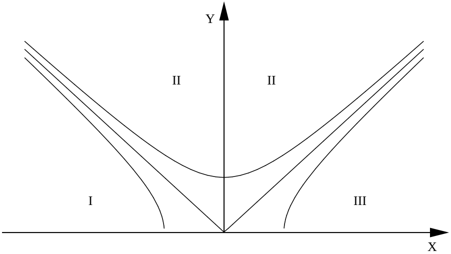
Solutions: Hyperbolae $h_\alpha : L \mapsto (X(L), Y(L))$, $\alpha \in \mathbb{R}$,

$$X(L)^2 - Y(L)^2 = \alpha$$



region I: low temperatures
flows terminate on fixed line
region II: $\alpha > 0$
flows tend to infinity

Renormalization group flow



$$\frac{\mathrm{d}X}{\mathrm{d}L} = 2Y^2 + \mathcal{O}((X+Y)^4)$$
$$\frac{\mathrm{d}Y}{\mathrm{d}L} = 2XY + \mathcal{O}((X+Y)^3)$$

- Fixed line $Y = 0$ is attractor of flows starting at $X < 0$
- Critical point $(X, Y) = (0, 0)$
- Same result as in Free Energy analysis, except that K_c is the *renormalized* coupling constant here!

Screening length

Recall: a is rescaled by $a \to a(1+l)$, meaning $\frac{\mathrm{d}}{\mathrm{d}l}a = a$, thus

$$a(l) = a\exp(l).$$

Assume that screening length scales as

$$\frac{\lambda(0)}{a} = \frac{\lambda(l)}{a\exp(l)} \quad \text{i.e.} \quad \lambda(0) \sim a\exp(l)$$

because we also assume that $\lambda(l) \sim a$.

Screening length

Approaching the critical point from above: Approximate $\alpha < 0$ linearly by

$$\alpha = -b^2(T - T_C), \quad b > 0.$$

Use $X(L)^2 - Y(L)^2 = \alpha$ to integrate the recursion relations:

$$L - L_0 = \frac{1}{2\sqrt{|\alpha|}}\left[\arctan\left(\frac{X(L)}{\sqrt{|\alpha|}}\right) - \arctan\left(\frac{X(L_0)}{\sqrt{|\alpha|}}\right)\right]$$

Close to critical trajectory ($X(L) \approx 1$, $X(L_0) < 0$):

$$L \approx \frac{\pi}{2\sqrt{|\alpha|}} \approx \frac{\pi}{2b\sqrt{T - T_C}}$$

Screening length

Hence:

$$\lambda \sim a \exp(l) \approx a \exp\left(\frac{\pi}{4b\sqrt{T - T_C}}\right).$$

Essential singularity at $T = T_C$
[i.e. $(T_C - T)^n \xi \to \infty$ as $T \to T_C$ for any $n \in \mathbb{N}$]

Experimental realization: Superfluid He^4 films

Heuristic explaination: $\psi = A(x)e^{iS(x)}$

$$H = \int \mathrm{d}x \, \bar{\psi} \left(-\frac{\hbar^2 \nabla^2}{2m} \right) \psi \sim \frac{\hbar^2 |A|^2}{2m} \int \mathrm{d}x \, (\nabla S(x))^2$$

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- K corresponds to superfluid density, which can be measured (i.e. moment of inertia of torsional oscillator)

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