

§2. Symmetry breaking and phase transitions

* Mermin-Wagner theorem (cont'd)

Correlation function:

$$C(\vec{R}_j - \vec{R}_l) = \frac{I^2}{Z} \int \mathcal{D}\theta(\tau) \cos(\theta_j - \theta_l) e^{-S}$$

$$\approx \frac{I^2}{Z_0} \int \mathcal{D}\theta_0 \frac{1}{2} \left[e^{i(\theta_0_j - \theta_0_l)} + e^{-i(\theta_0_j - \theta_0_l)} \right] e^{-S_0}$$

$$\frac{1}{Z_0} \int \mathcal{D}\theta_0 e^{i(\theta_0_j - \theta_0_l)} e^{-S_0}$$

$$= \frac{1}{Z_0} \int \mathcal{D}\theta_0 e^{\frac{i}{\sqrt{N}} \sum_{\vec{k}, i\omega_n} \theta(\vec{k}, i\omega_n) (e^{i\vec{k} \cdot \vec{R}_j} - e^{i\vec{k} \cdot \vec{R}_l}) - \sum_{\vec{k}, i\omega_n} \theta^* \frac{c}{2} (\omega_n^2 + \omega_{\vec{k}}^2) \theta}$$

$$= \frac{1}{Z_0} \int \mathcal{D}\theta_0 e^{-\sum_{\vec{k}, i\omega_n} \left[\theta^* - \frac{i}{\sqrt{N}} \frac{e^{i\vec{k} \cdot \vec{R}_j} - e^{i\vec{k} \cdot \vec{R}_l}}{c(\omega_n^2 + \omega_{\vec{k}}^2)} \right] \frac{c}{2} (\omega_n^2 + \omega_{\vec{k}}^2) \left[\theta - \frac{i}{\sqrt{N}} \frac{e^{-i\vec{k} \cdot \vec{R}_j} - e^{-i\vec{k} \cdot \vec{R}_l}}{c(\omega_n^2 + \omega_{\vec{k}}^2)} \right]}$$

$$\times e^{-\frac{1}{2\beta N} \sum_{\vec{k}, i\omega_n} \frac{1}{c(\omega_n^2 + \omega_{\vec{k}}^2)} (e^{i\vec{k} \cdot \vec{R}_j} - e^{i\vec{k} \cdot \vec{R}_l}) (e^{-i\vec{k} \cdot \vec{R}_j} - e^{-i\vec{k} \cdot \vec{R}_l})}$$

$$= e^{-\frac{1}{2\beta N} \sum_{\vec{k}, i\omega_n} \frac{1}{c(\omega_n^2 + \omega_{\vec{k}}^2)} \{2 - 2 \cos[\vec{k} \cdot (\vec{R}_j - \vec{R}_l)]\}}$$

$$= e^{-\frac{1}{N} \sum_{\vec{k}} [n_B(\omega_{\vec{k}}) + \frac{1}{2}] \frac{1}{c\omega_{\vec{k}}^2} \{1 - \cos[\vec{k} \cdot (\vec{R}_j - \vec{R}_l)]\}}$$

$$\xrightarrow{N \rightarrow \infty} e^{-\frac{a^d}{c} \int_{-\pi/a}^{\pi/a} \frac{d^d \vec{k}}{(2\pi)^d} [n_B(\omega_{\vec{k}}) + \frac{1}{2}] \frac{1}{\omega_{\vec{k}}^2} \{1 - \cos[\vec{k} \cdot (\vec{R}_j - \vec{R}_l)]\}}$$

we are interested in the behavior of $C(\vec{R}_j - \vec{R}_l)$
when $|\vec{R}_j - \vec{R}_l| \gg a$ (asymptotic behavior)

Case 1: $T > 0$ (Low T)

Integral:

$$\int_{-\pi/a}^{\pi/a} d^d \vec{k} \left[n_B(\omega_{\vec{k}}) + \frac{1}{Z} \right] \frac{1}{\omega_{\vec{k}}} \left\{ 1 - \cos[\vec{k} \cdot (\vec{R}_j - \vec{R}_\ell)] \right\}$$

\downarrow
 $\frac{1}{\beta \omega_{\vec{k}}}$

\downarrow
 $|\vec{R}_j - \vec{R}_\ell| \gg a$

i) No divergence: $1 - \cos[\vec{k} \cdot (\vec{R}_j - \vec{R}_\ell)] \simeq \frac{1}{2} [\vec{k} \cdot (\vec{R}_j - \vec{R}_\ell)]^2$ for $|\vec{k}| \rightarrow 0$
 integral behaves as $\int_0^{k_c} d|\vec{k}| |\vec{k}|^{d-1} \frac{1}{|\vec{k}|^2} |\vec{k}|^2 \sim \int_0^{k_c} d|\vec{k}| |\vec{k}|^{d-1}$
 No divergence for any d

ii) asymptotic behavior for $|\vec{R}_j - \vec{R}_\ell| \gg a$:

Integral small for $|\vec{k}| \in [0, \frac{1}{|\vec{R}_j - \vec{R}_\ell|} \ll a^{-1}]$

$$\text{Integral} \sim \int_{|\vec{R}_j - \vec{R}_\ell|^{-1} \rightarrow 0}^{k_c \sim \frac{\pi}{a}} d|\vec{k}| |\vec{k}|^{d-1} \frac{T}{v_s |\vec{k}|^2}$$

$$\sim \int_{|\vec{R}_j - \vec{R}_\ell|^{-1}}^{k_c} d|\vec{k}| |\vec{k}|^{d-3} T$$

$$= \begin{cases} \text{const} + \text{const} \cdot T |\vec{R}_j - \vec{R}_\ell| & d=1 \\ \text{const} + \text{const} \cdot T \ln |\vec{R}_j - \vec{R}_\ell| & d=2 \end{cases}$$

Case 2: $T = 0$

Integral:

$$\int_{-\pi/a}^{\pi/a} d^d \vec{k} \left[\underbrace{n_B(\omega_{\vec{k}}) + \frac{1}{2}}_{\downarrow 0 \text{ except for } \vec{k}=0} \right] \frac{1}{\omega_{\vec{k}}} \left\{ 1 - \cos[\vec{k} \cdot (\underbrace{\vec{R}_j - \vec{R}_\ell}_{\gg a})] \right\}$$

$$\sim \int_{|\vec{R}_j - \vec{R}_\ell|^{-1} \ll a^{-1}}^{k_c (\sim \frac{\pi}{a})} d|\vec{k}| \cdot |\vec{k}|^{d-1} \frac{1}{v_s |\vec{k}|}$$

$$\sim \int_{|\vec{R}_j - \vec{R}_\ell|^{-1}}^{k_c} d|\vec{k}| \cdot |\vec{k}|^{d-2}$$

$$\sim \text{const} + \text{const} \cdot \ln |\vec{R}_j - \vec{R}_\ell| \quad d=1$$

Correlation function:

$$C(\vec{R}_j - \vec{R}_\ell) \sim \begin{cases} e^{-T|\vec{R}_j - \vec{R}_\ell|/\xi} & , \quad d=1 \ \& \ T > 0 \\ |\vec{R}_j - \vec{R}_\ell|^{-\eta T} & , \quad d=2 \ \& \ T > 0 \\ |\vec{R}_j - \vec{R}_\ell|^{-8} & , \quad d=1 \ \& \ T = 0 \end{cases}$$

Powerlaw decaying correlation \Rightarrow quasi-LRO

$d=2 \ \& \ T > 0$:  powerlaw \rightarrow exponential (high-T expansion)

At least one phase transition! (NO local order parameter)

Kosterlitz-Thouless transition (Nobel Prize in 2016)

*) Kosterlitz - Thouless transition

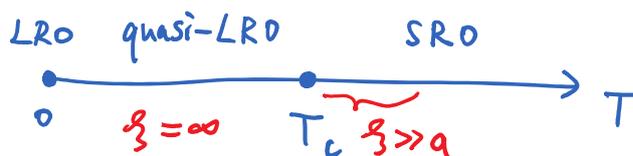
$d=2$ classical XY model

$$Z = \int \prod_{j=1}^N d\theta_j e^{-\beta H}$$

$$H = -J \sum_{\langle ij \rangle} \cos(\theta_i - \theta_j)$$

$$\langle e^{i\theta_j} e^{-i\theta_l} \rangle \sim \begin{cases} |\vec{R}_j - \vec{R}_l|^{-\eta T} & \text{low } T \\ e^{-|\vec{R}_j - \vec{R}_l|/\xi} & \text{high } T \end{cases}$$

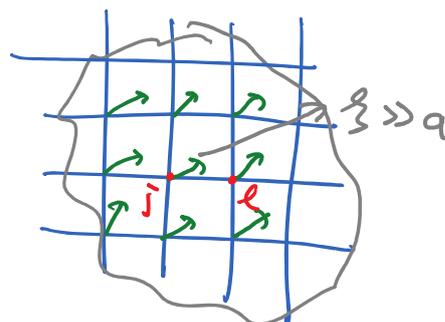
Q: What happens in between?



$\xi \gg a \Rightarrow$ field theory in the continuum limit

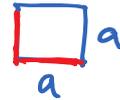
$\theta_j - \theta_l \ll \pi$ within a radius of ξ

$$\begin{aligned} \cos(\theta_j - \theta_l) &\approx 1 - \frac{1}{2}(\theta_j - \theta_l)^2 \\ &\rightarrow 1 - \frac{1}{2} \left[\vec{\nabla} \theta \left(\frac{\vec{R}_j + \vec{R}_l}{2} \right) \cdot (\vec{R}_j - \vec{R}_l) \right]^2 \\ &\rightarrow 1 - \frac{a^2}{2} \left[(\partial_x \theta(\vec{R}))^2 + (\partial_y \theta(\vec{R}))^2 \right] \\ &\rightarrow 1 - \frac{a^2}{2} \left[\vec{\nabla} \theta(\vec{R}) \right]^2 \end{aligned}$$

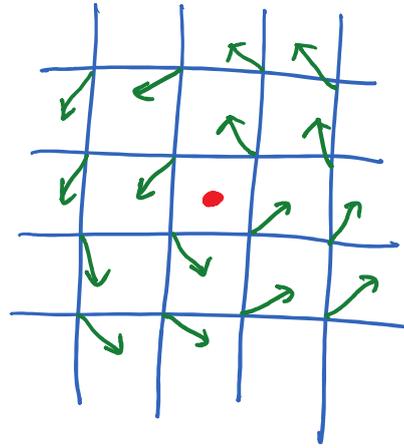
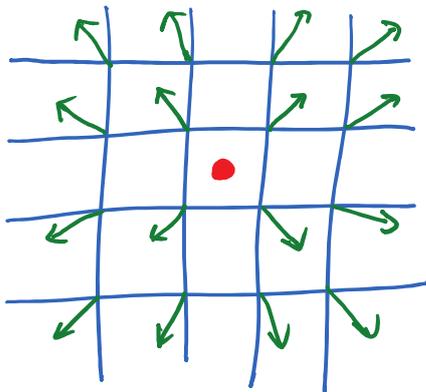


$$\Rightarrow H = -J \sum_{\langle j,l \rangle} \cos(\theta_j - \theta_l)$$

$$\rightarrow \frac{J}{2} \int d^2\vec{R} (\vec{\nabla} \theta(\vec{R}))^2 + \text{const.}$$



- Topological defect in $d=2$: vortex



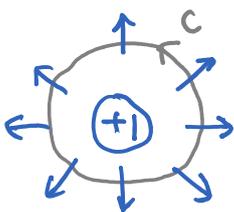
The above two vortex configurations are related to each other by a global $O(2)$ rotation $\theta_j \rightarrow \theta_j + \frac{\pi}{2}$.

Formal definition in the continuum limit:

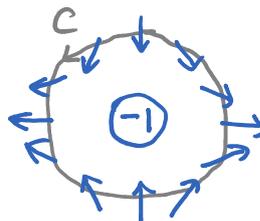
$$\oint_c \vec{\nabla} \theta \cdot d\vec{l} = 2\pi n, \quad n \in \mathbb{Z}$$

↑ closed path ↑ winding number of $\theta(\vec{R})$

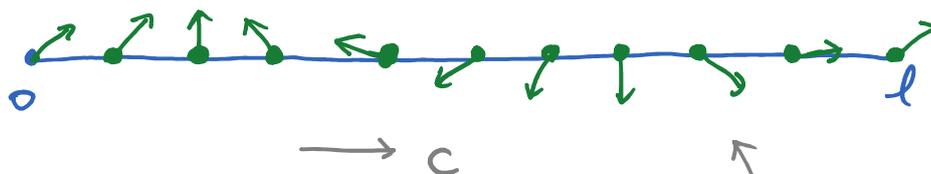
, $(n=0$: no vortex)



vortex ($n=1$)



anti-vortex ($n=-1$)



$$2\pi n = \int_0^l \frac{d\theta(l)}{dl} dl = \int_{\theta(0)}^{\theta(l)} d\theta(l) = 2\pi$$

$$\Rightarrow n=1$$

Winding numbers are topological invariants,

which do not change under smooth deformation of $\theta(\vec{R})$.

One needs to estimate their contributions to the thermodynamics, which was missing in the previous spin-wave analysis (Gaussian approximation).

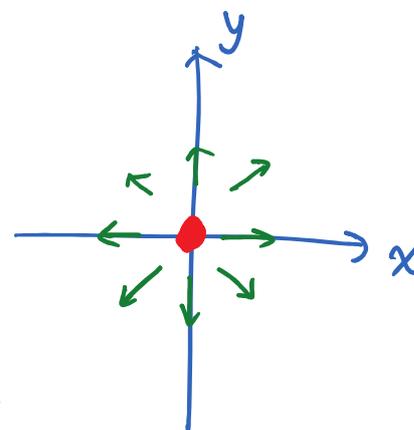
Warm-up: single vortex with $n=1$

Vortex core at $(x, y) = (0, 0)$,

size $\sim a$

$$\theta_{\text{vortex}}(\vec{R}) = \text{Im} \ln z$$

$$z = \sqrt{x^2 + y^2} e^{i \arctan \frac{y}{x}}$$



$$\Rightarrow \theta_{\text{vortex}}(x, y) = \arctan \frac{y}{x}$$

27.11.18

⑦

$$\begin{aligned}
 \vec{\nabla} \theta_{\text{vortex}} &= \left(\frac{\partial}{\partial x} \arctan \frac{y}{x}, \frac{\partial}{\partial y} \arctan \frac{y}{x} \right) \\
 &= \left(\frac{1}{1 + \left(\frac{y}{x}\right)^2} \cdot \left(-\frac{y}{x^2}\right), \frac{1}{1 + \left(\frac{y}{x}\right)^2} \cdot \frac{1}{x} \right) \\
 &= \left(\frac{-y}{x^2 + y^2}, \frac{x}{x^2 + y^2} \right)
 \end{aligned}$$

winding number: $2\pi n = \oint_c \vec{\nabla} \theta \cdot d\vec{\ell}$

choose a circle with radius $r \gg a$,

parametrization: $\vec{r}(t) = r(\cos(2\pi t), \sin(2\pi t)), \quad t \in [0, 1]$

$$\vec{\nabla} \theta_{\text{vortex}}(t) = \frac{1}{r} (-\sin(2\pi t), \cos(2\pi t))$$

$$\begin{aligned}
 \Rightarrow 2\pi n &= \oint_c \vec{\nabla} \theta_{\text{vortex}} \cdot d\vec{\ell} \\
 &= \int_0^1 dt \vec{\nabla} \theta_{\text{vortex}}(t) \cdot \vec{r}'(t) \\
 &= \int_0^1 dt 2\pi \\
 &= 2\pi \quad \Rightarrow \quad n = +1 \quad \checkmark
 \end{aligned}$$

Generalization: vortex with winding number $\pm n$,
at position z_0

$$\theta_{\text{vortex}} = \pm n \operatorname{Im} \ln(z - z_0)$$

27.11.18

⑧

Energy of the single vortex with $n=1$ at $z=0$:

$$E_{\text{vortex}} = \frac{J}{2} \int d^2\vec{R} \left(\underbrace{\vec{\nabla} \theta_{\text{vortex}}(\vec{R})}_{\frac{1}{x^2+y^2}(-y, x)} \right)^2$$

$$= \frac{J}{2} \int dx dy \frac{1}{x^2+y^2}$$

$$= \frac{J}{2} \int_a^{R_c} dR \cdot 2\pi R \frac{1}{R^2}$$

R_c : size of the whole system

← ultraviolet cutoff:

$$= \pi J \ln \frac{R_c}{a}$$

we had a lattice and the smallest length scale for the continuum theory should be the lattice spacing.

(Within the vortex core, the continuum Hamiltonian is "blind".)

The single vortex has a divergent energy when $R_c \rightarrow \infty$!

But for thermodynamics we need to consider free energy instead of energy!

of single-vortex configurations $\sim \left(\frac{R_c}{a}\right)^2$

Entropy: $S_{\text{vortex}} \sim \ln \left(\frac{R_c}{a}\right)^2 = 2 \ln \frac{R_c}{a}$

Free energy of single-vortex configurations:

$$\begin{aligned}
 F_{\text{vortex}} &= E_{\text{vortex}} - T S_{\text{vortex}} \\
 &= \pi J \ln \frac{R_c}{a} - T \cdot 2 \ln \frac{R_c}{a} \\
 &= (\pi J - 2T) \ln \frac{R_c}{a}
 \end{aligned}$$

$$\begin{array}{c}
 \text{~~~~~} \\
 \downarrow \\
 T_c = \frac{\pi}{2} J
 \end{array}$$

State-of-the-art
numerics:

$$T_c \approx 0.893 J$$

$T < T_c$: single vortex NOT favored

$T > T_c$: single vortex favored

However, this is a very rough estimate.

For example, many-vortex configurations not included,
vortex-vortex interactions not considered ...