

## §2 Symmetry breaking and phase transitions

### \* Kosterlitz - Thouless transition (cont'd)

- Link variable and tensor network representation

$$\begin{aligned} Z_{XY} &= \int \prod_{i=1}^N d\theta_i e^{\beta J \sum_{\langle i,j \rangle} \cos(\theta_i - \theta_j)} \\ &= \int \prod_{i=1}^N d\theta_i \prod_{\langle i,j \rangle} e^{\beta J \cos(\theta_i - \theta_j)} \\ &\quad \downarrow \\ &\sum_{l=-\infty}^{\infty} A_l e^{il(\theta_i - \theta_j)} \end{aligned}$$

$$A_l = A_{-l} \geq 0, \quad A_l \geq 0 = \sum_{n=0}^{\infty} \left( \frac{\beta J}{2} \right)^{n+l} \frac{1}{(n+l)! n!}$$

$A_l$  : modified Bessel function of the first kind.

Define link variable  $l_{ij} \in \mathbb{Z}$  and

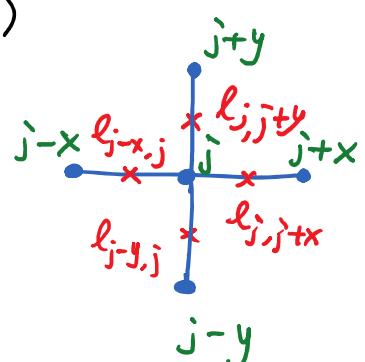
perform integrations over  $\theta_j$  :

$$\int_0^{2\pi} d\theta_j e^{i\theta_j(l_{j,j+x} + l_{j,j+y} - l_{j-x,j} - l_{j-y,j})}$$

$$= 2\pi \delta_{l_{j,j+x} + l_{j,j+y} - l_{j-x,j} - l_{j-y,j}, 0} = 0$$

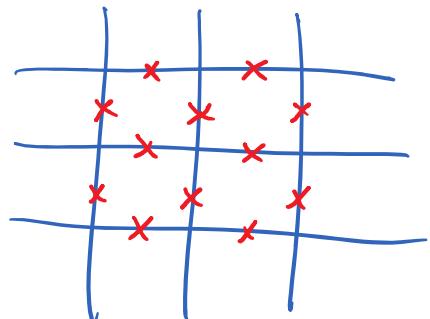
$$= 2\pi \delta_{\sum_j l_{j,j}, 0}$$

→ "Gauss law":  $l_{j,j+x} + l_{j,j+y} = l_{j-x,j} + l_{j-y,j}$



All angle integrations can be performed:

$$Z_{XY} = \sum_{\{l_{ij}\}=-\infty}^{\infty} \left( \prod_{ij} A_{l_{ij}} \right) \left( \prod_j \delta_{\sum l_j=0} \right)$$

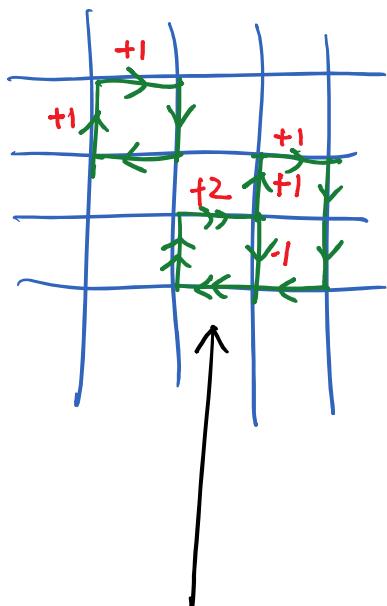


Graphical representation:

$$i \rightarrow j \quad l_{ij} = 0$$

$$i \rightarrow j \quad \begin{array}{c} \uparrow \\ \downarrow \end{array} \quad l_{ij} = +1$$

$$i \leftarrow j \quad \begin{array}{c} \uparrow \\ \downarrow \end{array} \quad l_{ij} = -2$$



Gauss Law:

For each vertex, incoming and outgoing arrows must "conserve".

(This is due to the U(1) symmetry of the XY model.)

Each link variable is assigned with weight  $A_{l_{ij}} \geq 0$

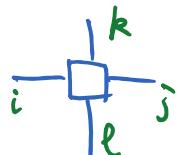
This form is suitable for Monte Carlo simulations.

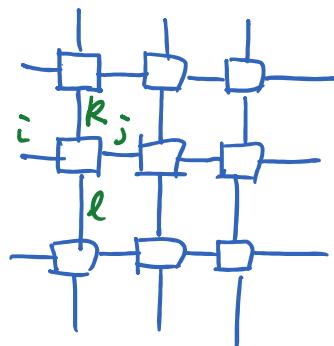
Modern terminology:  $Z_{XY}$  is a tensor network.

$$Z_{XY} = \sum_{\{ijkl\}} (\dots T_{ijkl} \dots)$$

$$T_{ijkl} = \sqrt{A_i A_j A_k A_l} \quad \delta_{j+k-i-l=0}$$

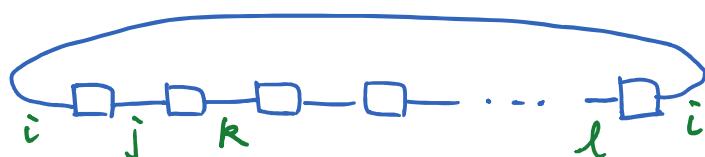
Gauss law





connected indices  
imply summation

Calculation easy for  $d=1$ :



(periodic boundary)

$$Z_{d=1}^{XY} = \sum_{\{ijkl\}} T_{ij} T_{jk} \dots T_{li}$$

$$= \sum_i (T^L)_{ii}$$

$$= \text{tr } T^L$$

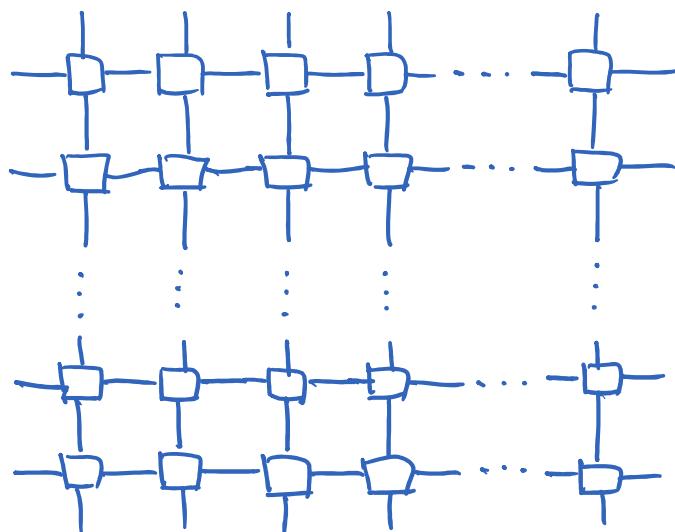
diagonalize  $T$  and find  
the largest eigenvalue  $\lambda_{\max}$ .

$$\xrightarrow{L \rightarrow \infty} \lambda_{\max}^L$$

The case with degenerate largest eigenvalues is similar.

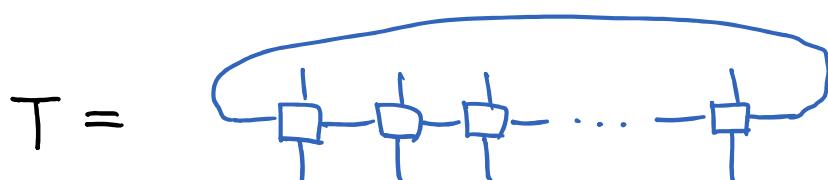
This is a general way for solving  $d=1$  classical statistical models.

Calculation difficult for  $d \geq 2$ :



$$\sum_{d=2}^{XY} = \text{tr}(T^{L_y}) \quad \xrightarrow{\text{row-to-row transfer matrix}}$$

matrix-product operator (MPO) in tensor network language



diagonalization difficult when  $L_x$  is large!

(computation cost  $\sim e^{L_x}$ )

Analytical side: integrability (e.g. Bethe ansatz) is applicable for diagonalizing row-to-row transfer matrices, but this only works for a limited number of models ...

Ising, Potts, ... all (?) exactly solvable  $d=2$  statistical models.

Unfortunately, XY model does not belong to this family.

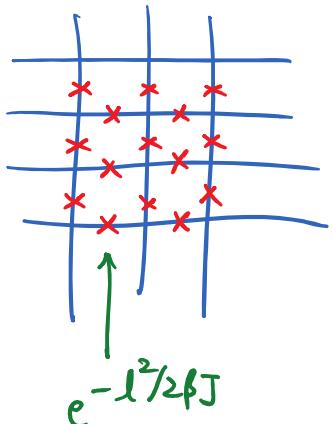
— Villain model

Modify the Boltzmann weight assigned to the link variables:

$$Z_{XY} = \sum_{\{l_{ij}\}=-\infty}^{\infty} \left( \prod_{ij} A_{l_{ij}} \right) \left( \prod_j \delta_{\sum l_j=0} \right)$$

↓

$$Z_V = \sum_{\{l_{ij}\}=-\infty}^{\infty} \left( \prod_{ij} e^{-\frac{1}{2\beta J} l_{ij}^2} \right) \left( \prod_j \delta_{\sum l_j=0} \right)$$



$$A_{l_{ij}} \approx e^{-\frac{1}{2\beta J} l_{ij}^2} \quad \text{for } \beta \rightarrow \infty \quad (T \rightarrow 0)$$

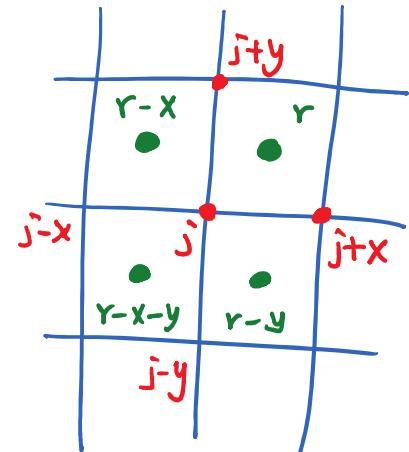
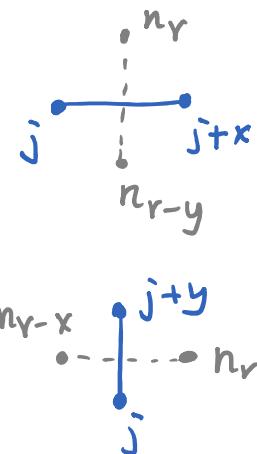
so Villain's model can reproduce the low T behavior of the XY model.

Still not exactly solvable, but easier to develop a field theory description, and the key feature is still there (KT transition between low T and high T phases).

Vortex (dual) description:

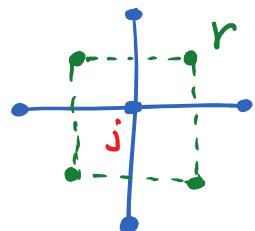
$$l_{j,j+x} = n_r - n_{r-y}$$

$$l_{j,j+y} = n_{r-x} - n_r$$



Constraint automatically resolved:

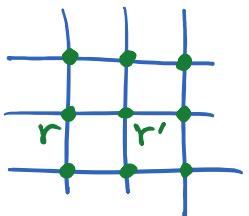
$$\begin{aligned} & l_{j,j+x} + l_{j,j+y} - l_{j-x,j} - l_{j-y,j} \\ &= (\cancel{n_r} - \cancel{n_{r-y}}) + (\cancel{n_{r-x}} - \cancel{n_r}) \\ &\quad - (\cancel{n_{r-x}} - \cancel{n_{r-x-y}}) - (\cancel{n_{r-x-y}} - \cancel{n_{r-y}}) \\ &= 0 \end{aligned}$$



Rewrite  $Z_v$  by using  $n$ -variables on the dual lattice:

$$Z_v = \sum_{\{l_j\}=-\infty}^{\infty} \left( \prod_{\langle i,j \rangle} e^{-\frac{1}{2kT} l_{ij}^2} \right) \left( \prod_j \delta_{\sum_j l_j = 0} \right)$$

$$= \sum_{\{n_r\}=-\infty}^{\infty} \prod_{\langle r,r' \rangle} e^{-\frac{1}{2kT} (n_r - n_{r'})^2}$$



dual lattice

⑦

$$\begin{aligned}
 Z_V &= \sum_{\{n_r\}=-\infty}^{\infty} e^{-\frac{1}{2\beta J} \sum_{r,r'} (n_r - n_{r'})^2} \\
 &= \underbrace{\int_{-\infty}^{\infty} \frac{\pi}{r} d\phi_r}_{\text{}} \sum_{\{m_r\}=-\infty}^{\infty} \underbrace{\frac{\pi}{r} \delta(\phi_r - n_r)}_{\text{}} e^{-\frac{1}{2\beta J} \sum_{r,r'} (\phi_r - \phi_{r'})^2} \\
 &\quad \text{||} \\
 &\quad \sum_{\{m_r\}=-\infty}^{\infty} \underbrace{\frac{\pi}{r} e^{2\pi i m_r \phi_r}}_{\text{}} \text{ (poisson summation)} \\
 &= \underbrace{\int_{-\infty}^{\infty} \frac{\pi}{r} d\phi_r}_{\text{}} \sum_{\{m_r\}=-\infty}^{\infty} e^{-\frac{1}{2\beta J} \sum_{r,r'} (\phi_r - \phi_{r'})^2 + 2\pi i \sum_r m_r \phi_r} \\
 &\quad \xrightarrow{\text{now becomes Gaussian integration}} \\
 &= \int_{-\infty}^{\infty} \frac{\pi}{r} d\phi_r \sum_{\{m_r\}=-\infty}^{\infty} e^{-\frac{1}{2\beta J} \sum_{r,r'} \phi_r (G^{-1})_{r,r'} \phi_{r'} + 2\pi i \sum_r m_r \phi_r} \\
 &\quad \downarrow \\
 &\quad \text{determine the propagator } G^{-1}: \\
 \sum_{r,r'} (\phi_r - \phi_{r'})^2 &= \sum_r \sum_{s=\hat{ax}, \hat{ay}} (2\phi_r^2 - 2\phi_r \phi_{r+s}) \\
 &= \sum_r 4\phi_r^2 - 2 \sum_r \sum_{s=\hat{ax}, \hat{ay}} \phi_r \phi_{r+s} \\
 &= \sum_{r,r'} \phi_r (G^{-1})_{r,r'} \phi_{r'}
 \end{aligned}$$

$$(G^{-1})_{\vec{r}, \vec{r}'} = 4 \delta_{\vec{r}, \vec{r}'} - \sum_{s=\pm \hat{ax}, \pm \hat{ay}} \delta_{\vec{r}', \vec{r} + \vec{s}}$$

$$\begin{aligned}
 Z_V &= \sum_{\{m_r\}} \left[ \prod_r d\phi_r \exp \left[ -\frac{1}{2\beta J} \sum_{r,r'} (\phi_r - 2\beta J \pi i m_{r_1} G_{r,r}) (G^{-1})_{rr'} \right. \right. \\
 &\quad \left. \left. \times (\phi_{r'} - 2\beta J \pi i G_{r',r_2} m_{r_2}) \right] \right] \quad \text{Summation over } r_1, r_2 \text{ assumed} \\
 &\quad \times e^{-2\pi^2 \beta J \sum_{r_1, r_2} m_{r_1} \underbrace{G_{r_1, r_2}}_{\text{to be determined...}} m_{r_2}} \\
 &= \sqrt{\frac{(2\pi\beta J)^N}{\det G^{-1}}} \sum_{\{m_r\}=-\infty}^{\infty} e^{-2\pi^2 \beta J \sum_{r,r'} m_{r_1} \underbrace{G_{r,r_2}}_{\text{to be determined...}} m_{r_2}}
 \end{aligned}$$

$Z_{\text{spin-wave (sw)}}$        $Z_{\text{vortex}}$

No approximation has been made. The partition function  $Z$  factorizes into two parts, meaning that they separately contribute to the free energy:

$$\begin{aligned}
 F &= -\frac{1}{\beta} \ln Z = -\frac{1}{\beta} \ln Z_{\text{sw}} - \frac{1}{\beta} \ln Z_{\text{vortex}} \\
 &= F_{\text{sw}} + F_{\text{vortex}}
 \end{aligned}$$

The reason why they are associated with "spin-wave" and "vortex" will be clear in a minute.

The variables  $m_r$  live in each site of the dual lattice, or equivalently, center of the plaquette in the original lattice. They correspond to vortices ( $m$  is the winding number).

The interactions between vortices are mediated by

$G_{\vec{r}, \vec{r}'}$  (see  $Z_{\text{vortex}}$ ), which needs to be calculated:

$$(G^{-1})_{\vec{r}, \vec{r}'} = 4\delta_{\vec{r}, \vec{r}'} - \sum_{\vec{s}=\pm a\hat{x}, \pm a\hat{y}} \delta_{\vec{r}', \vec{r} + \vec{s}}$$

Fourier transformation:

$$\begin{aligned} (G^{-1})_{\vec{k}, \vec{k}'} &= \frac{1}{N} \sum_{\vec{r}, \vec{r}'} e^{i\vec{k} \cdot \vec{r}} (G^{-1})_{\vec{r}, \vec{r}'} e^{-i\vec{k}' \cdot \vec{r}'} \\ &= (4 - 2\cos k_x a - 2\cos k_y a) \underbrace{\delta_{\vec{k}, \vec{k}'}}_{\text{diagonal in } \vec{k}\text{-space, because of translation invariance}} \end{aligned}$$

$$\Rightarrow G_{\vec{k}, \vec{k}'} = \frac{1}{4 - 2\cos k_x a - 2\cos k_y a} \delta_{\vec{k}, \vec{k}'}$$

Inverse Fourier transformation:

$$\begin{aligned} G_{\vec{r}, \vec{r}'} &= \frac{1}{N} \sum_{\vec{k}, \vec{k}'} e^{-i\vec{k} \cdot \vec{r}} G_{\vec{k}, \vec{k}'} e^{i\vec{k}' \cdot \vec{r}'} \\ &= \frac{1}{N} \sum_{\vec{k}} \frac{e^{i\vec{k} \cdot (\vec{r}' - \vec{r})}}{4 - 2\cos k_x a - 2\cos k_y a} \end{aligned}$$

$$Z_{SW} = \sqrt{\frac{(2\pi\beta J)^N}{\det G^{-1}}}$$

use  $(G^{-1})_{\vec{k}, \vec{k}'}$ , which is diagonal

$$= \sqrt{\frac{(2\pi\beta J)^N}{\frac{\pi}{k}(4 - 2\cos k_x a - 2\cos k_y a)}}$$

This is exactly the spin-wave contribution.

To see this one could go back to "spin-representation" of Villain's model (or use spin-wave expansion of the XY model  $\Rightarrow$  At low T, equivalent to Villain's model).

Below we derive the "spin-representation" of  $Z_V$ :

$$Z_V = \sum_{\{l_{ij}\}} e^{-\sum_{ij} \frac{1}{2\beta J} l_{ij}^2}$$

$\underbrace{\prod_j \delta_{\sum l_j = 0}}$

$$\propto \int_0^{2\pi} \prod_{j=1}^N d\theta_j \sum_{\{l_{ij}\}} e^{\sum_{ij} \left[ -\frac{1}{2\beta J} l_{ij}^2 + i l_{ij} (\theta_i - \theta_j) \right]}$$

↑  
integration over  $\theta$   
generates Gauss-law Constraint

$$Z_V \propto \int_0^{2\pi} \prod_{j=1}^N d\theta_j \sum_{\{l_{ij}\}} e^{\sum_{ij} \left[ -\frac{1}{2\beta J} l_{ij}^2 + i l_{ij} (\theta_i - \theta_j) \right]}$$

$$= \int_0^{2\pi} \frac{\pi}{j} d\phi_j \int_{-\infty}^{\infty} D\phi_{ij} \underbrace{\sum_{\{l_{ij}\}} \frac{\pi}{j} \delta(\phi_{ij} - l_{ij})}_{\sum_{\{P_{ij}\}} e^{2\pi i P_{ij} \phi_{ij}}} \\$$

$$X e^{\sum_{i,j} \left[ -\frac{1}{2k_j} \phi_{ij}^2 + i \phi_{ij} (\theta_i - \theta_j) \right]}$$

↑ integrate out  $\phi_{ij}$

$$= \int_0^{2\pi} \frac{\pi}{j} d\theta_j \sum_{\{P_{ij}\}} \int d\phi_{ij} e^{-\frac{1}{2\beta J} \sum_{\langle ij \rangle} [\phi_{ij} - i\beta J(\theta_i - \theta_j + 2\pi P_{ij})]^2} \\ \times e^{-\frac{\beta J}{2} \sum_{\langle ij \rangle} (\theta_i - \theta_j + 2\pi P_{ij})^2}$$

$$\alpha \int_0^{2\pi} \prod_j \frac{d\theta_j}{j} \sum_{\{P_{ij}\}} e^{-\frac{\beta_j}{2} \sum_{\langle ij \rangle} (\theta_i - \theta_j + 2\pi P_{ij})^2}$$

low T,  $P_{ij} = 0$  favored, sp

low T,  $P_{ij} = 0$  favored, spin-wave expansion:

$$\int D\theta e^{-\frac{F_J}{2} \sum_{\langle i,j \rangle} (\theta_i - \theta_j)^2} = \int D\theta e^{-\frac{F_J}{k} \sum_{\substack{i \\ \text{half } F}} (4 - 2\cos kx_i - 2\cos ky_i) \theta_i^* \theta_i}$$

$$\propto \left[ \frac{\pi}{k} (4 - 2 \cos k_x a - 2 \cos k_y a) \right]^{-1/2}$$

Precisely  $Z_{SW}$  in page 10 up to trivial factors !

This gives an indication that  $Z_{\text{vortex}}$  indeed describes vortices, which spin-wave expansion misses.

Let us analyze  $Z_{\text{vortex}}$  (c.f. Page ⑧)

$$G_{\vec{r}, \vec{r}'} \simeq -\frac{1}{2\pi} \ln \frac{|\vec{r} - \vec{r}'|}{a} - \frac{1}{4} + G(0) \sim \ln \frac{R_c}{a}$$

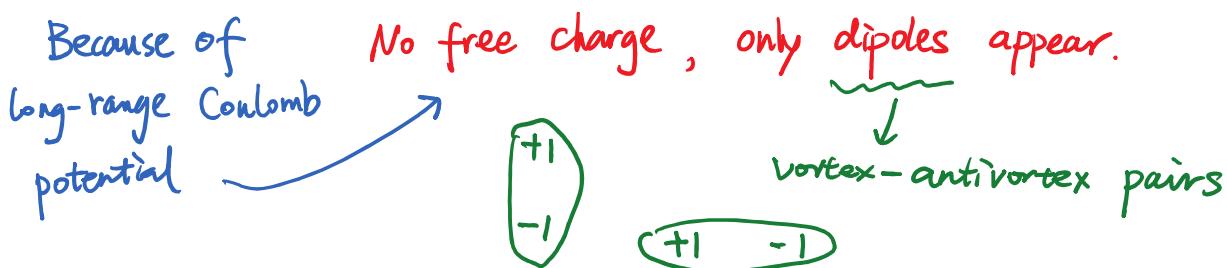
$$\Rightarrow Z_{\text{vortex}} \propto \sum_{\{m_r\}} e^{-2\pi^2 \beta J G(0) \left(\sum_r m_r\right)^2} \times e^{\frac{\pi^2}{\sum_r} \beta J \sum_{r \neq r'} m_r m_{r'} + \pi \beta J \sum_{\vec{r} \neq \vec{r}'} m_{\vec{r}} \ln \frac{|\vec{r} - \vec{r}'|}{a} m_{\vec{r}'}}$$

Coulomb potential in  $d=2$

$m_r \in \mathbb{Z}$  : vortices are interpreted as charges

Low T: charge neutral condition  $\sum_r m_r = 0$

(because  $\beta$  large,  $G(0)$  large)



high T: free single charges (vortices).

Coulomb potential screened and becomes a short-range potential.