The Analysis of Kosterlitz-Thouless Transition Using Monte Carlo Methods

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1. Introduction

The Nobel Prize in Physics in 2016 is *for theoretical discoveries of topological phase transitions and topological phases of matter* [1].

David J. Thouless
Prize share: 1/2

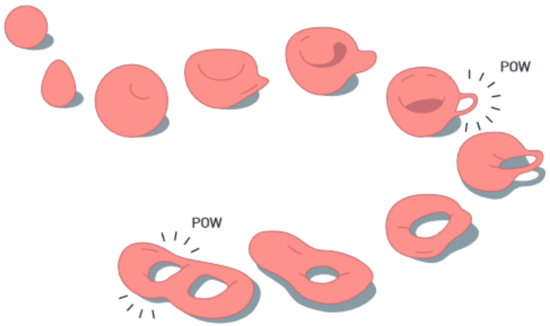
F. Duncan M. Haldane
Prize share: 1/4

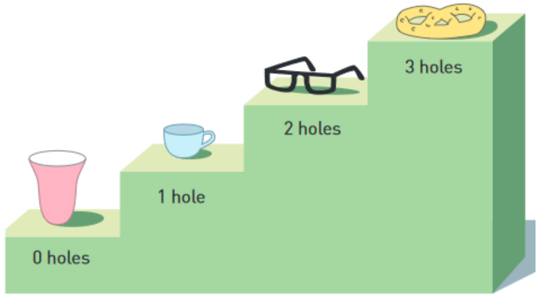
J. Michael Kosterlitz
Prize share: 1/4

The Nobel Prize in Physics in 2016 consists Three parts.

- TKNN formula
- Haldane conjecture
- Kosterlitz-Thouless transition $\leftarrow$ I will introduce

Key Word : **Topology**





2. Mermin-Wagner's Theorem

Mermin-Wagner's Theorem

When spacetime dimension d is 2, **continuous symmetry** is not spontaneously broken at finite temperature. When $d = 1$, continuous symmetry is not spontaneously broken including absolute zore temperature[1][2].

[1] Ising model has $\mathbb{Z}_2$ symmetry for spin flip, which is discrete symmetry so, $d = 2$ Ising model has spontaneous symmetry breaking phase in finite temperature.

3. A definition of Classical $\mathbf{2}d$ XY Model

The Hamiltonian is

$$\begin{aligned}\mathcal{H} &= -J \sum_{\langle i,j \rangle} \boldsymbol{S}_i \cdot \boldsymbol{S}_j \\ &= -J \sum_{\langle i,j \rangle} \left(S_i^x S_j^x + S_i^y S_j^y \right) \\ &= -J \sum_{\langle i,j \rangle} \cos\left(\theta_i - \theta_j\right)\end{aligned} \tag{1}$$

We defined $S_i^x = \cos\theta_i$, $S_i^y = \sin\theta_i$ [3], [4].

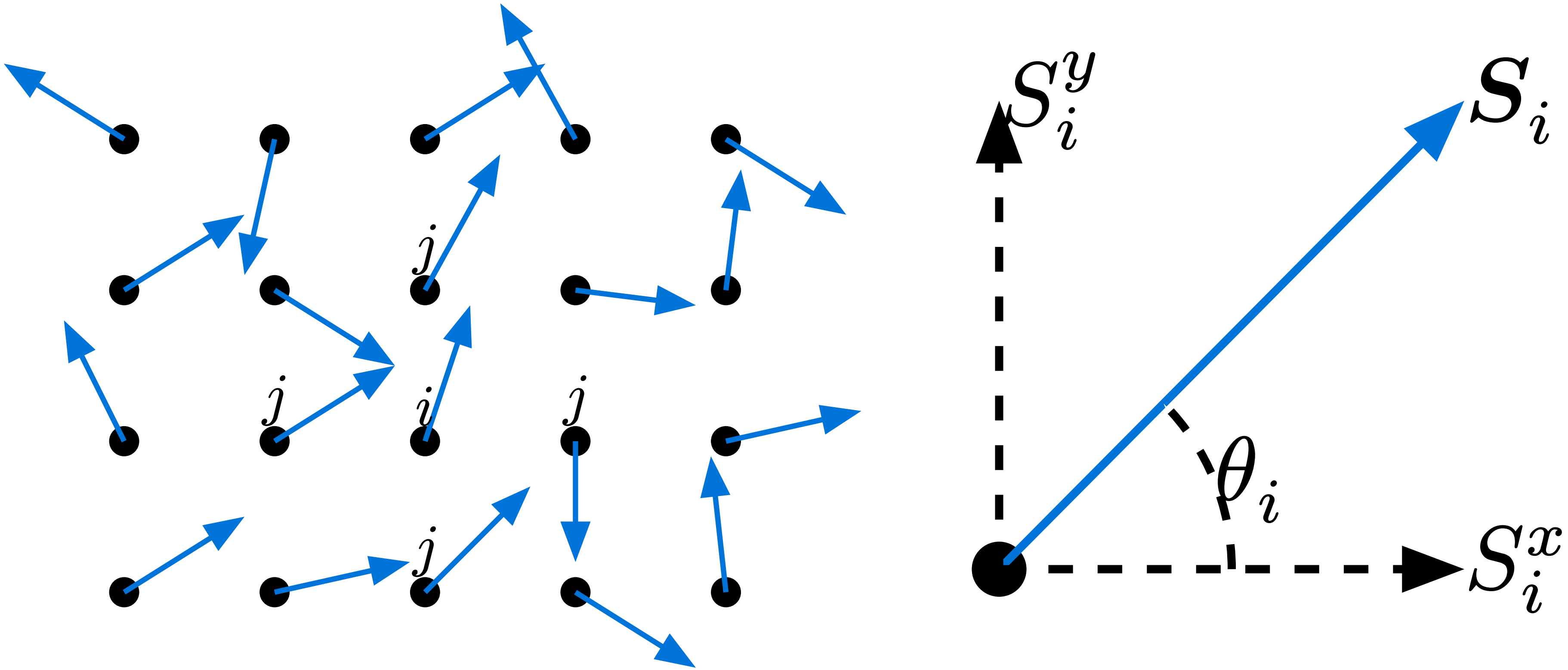


Figure 3: definitions of $\langle i, j\rangle$, $\boldsymbol{S}_i$, S_i^x, S_i^y, θ_i

4. Correlation Function

In low temperature, we use **spin wave approximation**.

In high temperature, we use **high temperature expansion**.

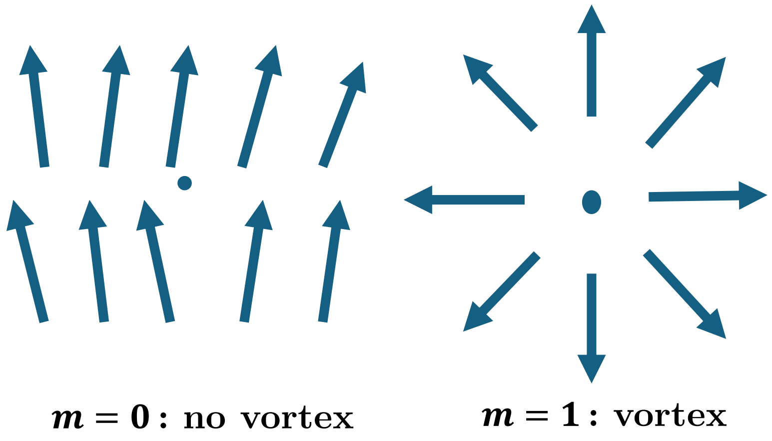
$$\begin{aligned} &\text{Low } T : \langle \boldsymbol{S}_i \cdot \boldsymbol{S}_j \rangle = \left(\frac{1}{\left| \boldsymbol{r}_i - \boldsymbol{r}_j \right|} \right)^{-\frac{1}{2\pi J\beta}} \\ &\text{High } T : \langle \boldsymbol{S}_i \cdot \boldsymbol{S}_j \rangle = \exp\left(-\frac{\left| \boldsymbol{r}_i - \boldsymbol{r}_j \right|}{\xi} \right), \quad \xi = \left(\log \frac{2}{\beta J} \right)^{-1} \end{aligned} \tag{2}$$

5. “Topological Excitation

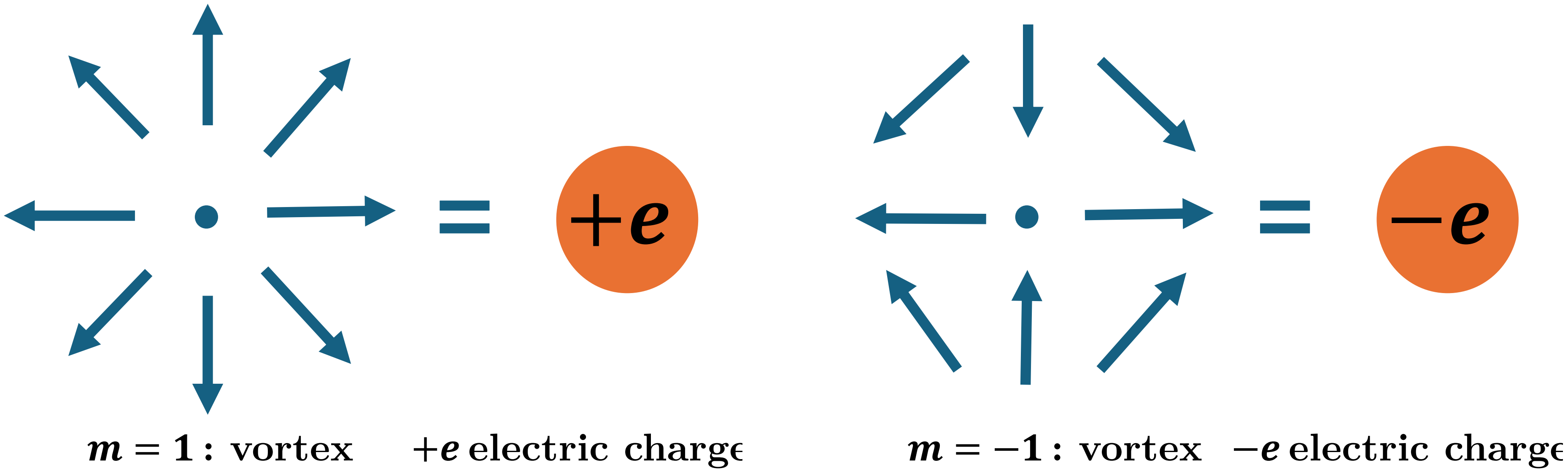
What are vortices? $\Rightarrow$ singular spin configuration.

Topological charge m defines

$$m = \frac{1}{2\pi} \oint d\boldsymbol{r} \cdot \boldsymbol{\nabla}\theta = 0, \pm 1, \pm 2, \ldots \tag{3}$$



We can regard the topological charge m as the electrical charge q in $2d$.



In $T > T_c$, vortex excitations can occur.

6. Monte Carlo Simulation

We want to calculate this expectation value

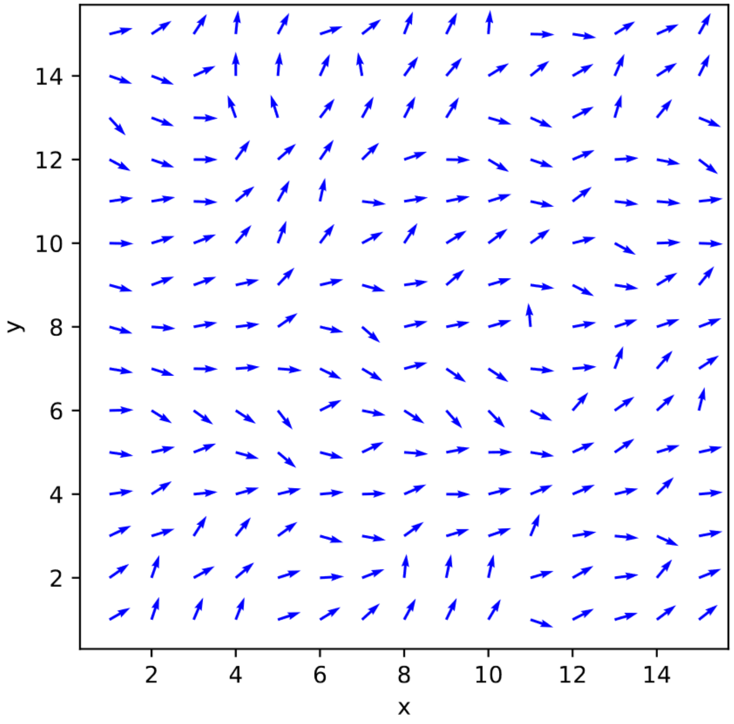
$$\langle \boldsymbol{S}_j \cdot \boldsymbol{S}_k \rangle = \sum_i \boldsymbol{S}_j \cdot \boldsymbol{S}_k \frac{1}{Z} \exp\left(-\frac{E(C_i)}{k_B T} \right) \tag{4}$$

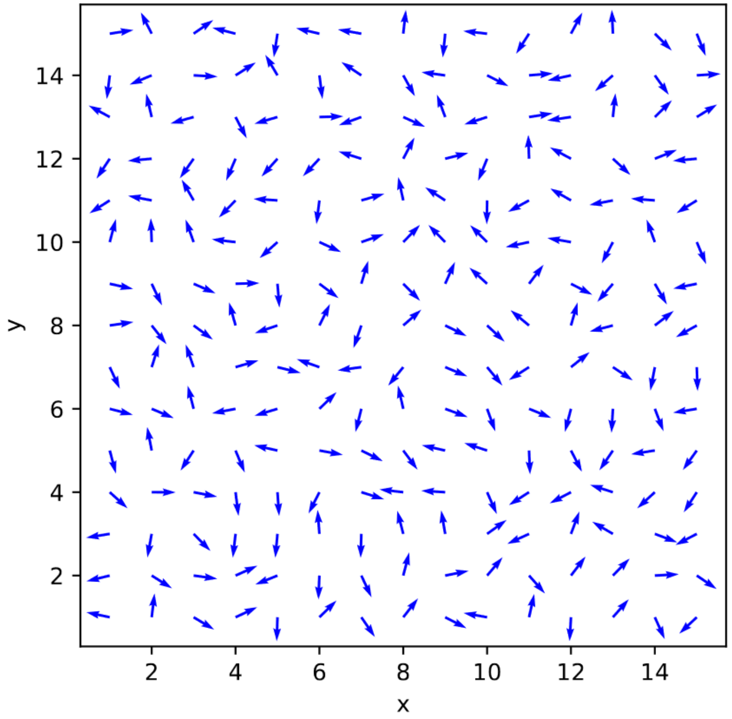
C_i is a ith certain spin configuration, $E(C_i)$ is a total energy of spin configuration C_i.

$\Longrightarrow$ I used Metropolis Monte Carlo Method [5] to generate C_i

1. consider we change the spin configuration C_i to C_{i+1}.
2. Calculate the energy differences $\Delta E = E(C_{i+1}) - E(C_i)$.
3. If $\Delta E < 0$, the spin configuration changes C_{i+1} .

4. If $\Delta E > 0$, the spin configuration changes to C_{i+1} with probability $\exp\left(-\frac{\Delta E}{k_B T}\right)$.





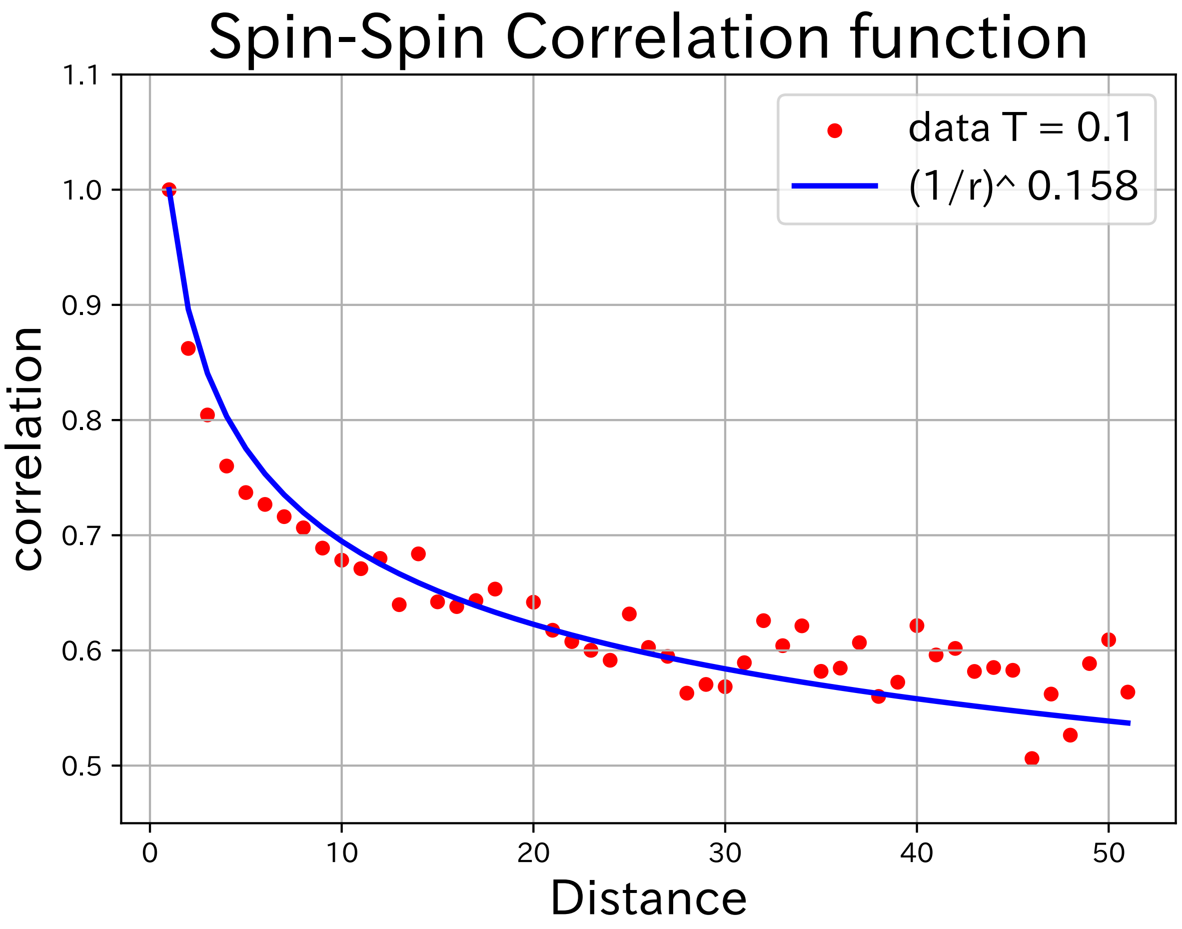


Figure 6: spin configuration at $T < T_c$. system size $= 100 \times 100$.

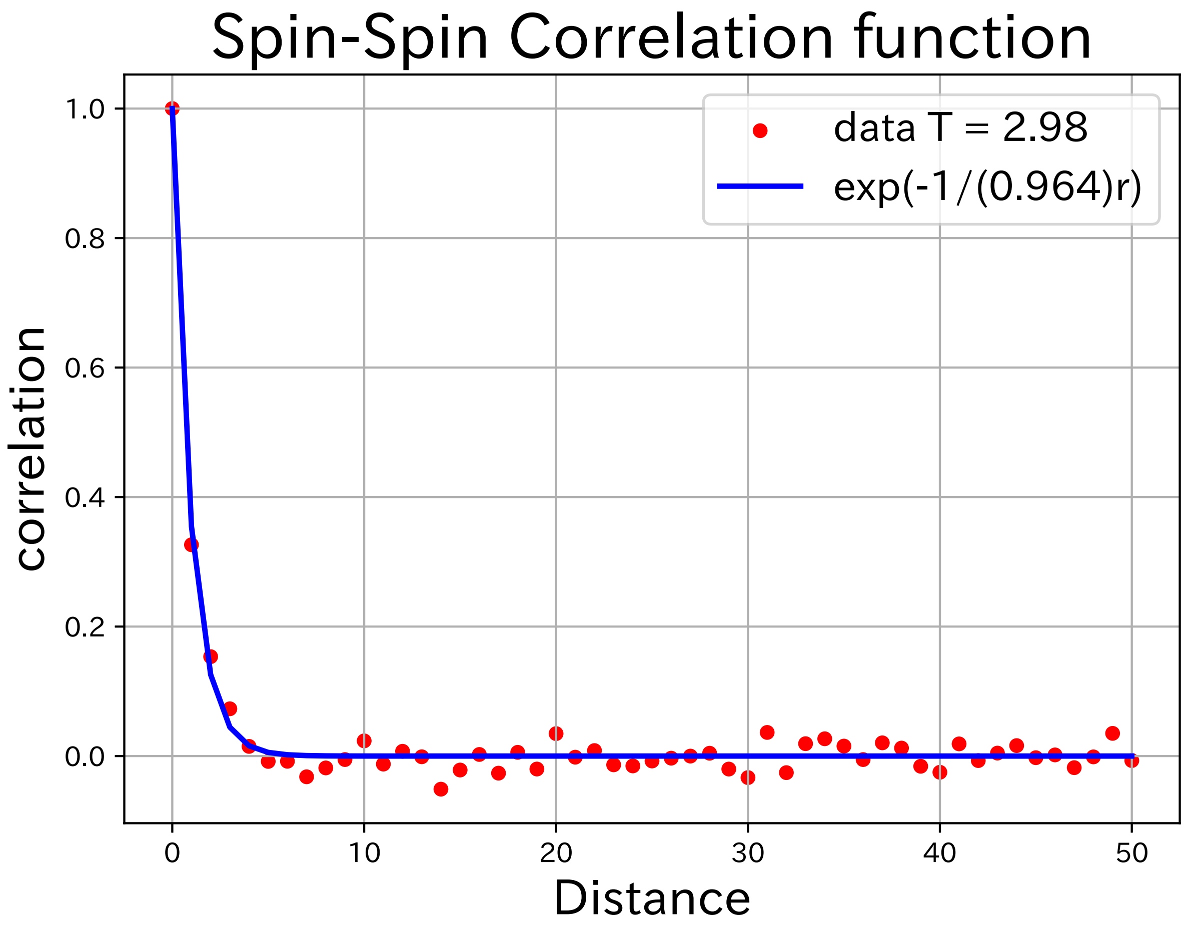


Figure 7: spin configuration at $T > T_c$. system size = 100×100.

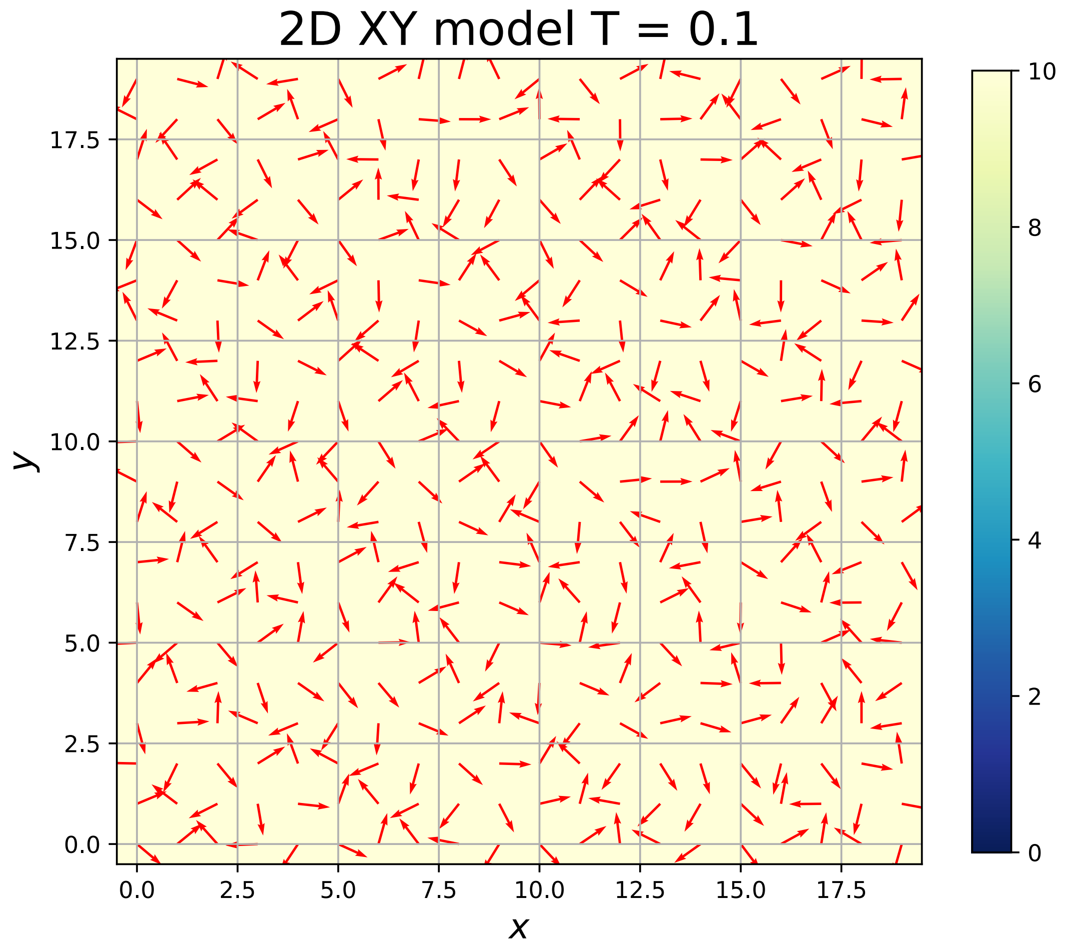


Figure 8: spin configuration at $T < T_c$. system size = 20×20

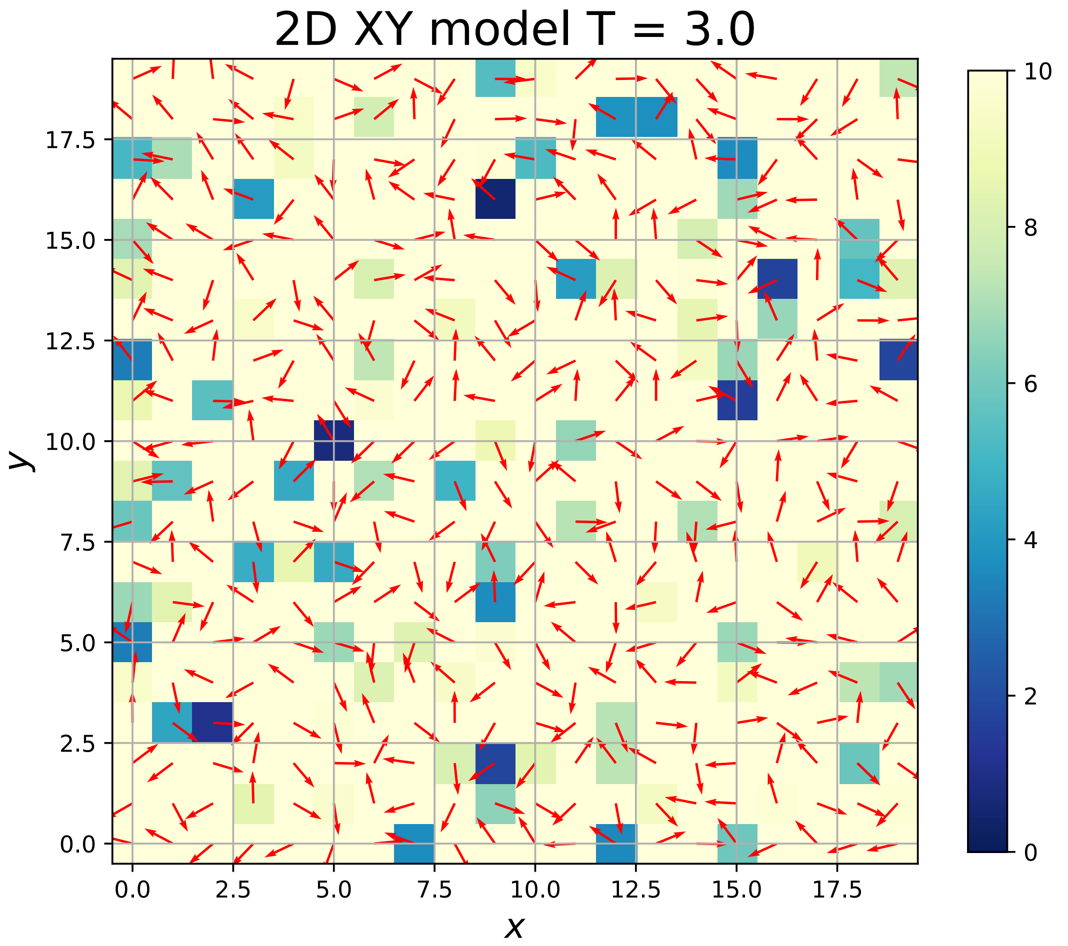


Figure 9: spin configuration at $T > T_c$. system size = 20×20

7. Conclusion

- In two dimensions, continuous symmetry breaking does not occur at finite temperature.
- Topological excitations, namely vortices, cause changes in the correlation function.
- We confirmed that correlation function changes between low and high temperature and viewd vortices excitations as demonstrated by the Monte Carlo method.

Other topics related to today's talk

- Renormalization Group Analysis in the Kosterlitz-Thouless Transition [6].
- Experimental Realizations of the Kosterlitz-Thouless Transition.
- Nambu-Goldstone's Theorem and its Generalization.
- What is the phase of matter?
- What is Topological Condensed Matter Physics?

Bibliography

[1] “Topological phase transitions and topological phases of matter”, *Royal Swedish Academy of Sciences*, 2016.

[2] 永長直人, “物性論における場の量子論”, 岩波オンデマンドブックス, Jun. 2014.

[3] J. M. Kosterlitz and D. J. Thouless, “Ordering, metastability and phase transitions in two-dimensional systems”, *Journal of Physics C: Solid State Physics*, vol. 6, no. 7, p. 1181, Apr. 1973, doi: 10.1088/0022-3719/6/7/010.

[4] 高橋和孝, “相転移・臨界現象とくりこみ群”, 丸善出版, Apr. 2017.

[5] 永井佑紀, “1 週間で学べる！Julia 数値計算プログラミング”, 講談社, Jun. 2022.

[6] J. B. Kogut, “An introduction to lattice gauge theory and spin systems”, *Rev. Mod. Phys.*, vol. 51, Oct. 1979, doi: 10.1103/RevModPhys.51.659.