Kosterlitz-Thouless Phase Transition in the 2D XY Model

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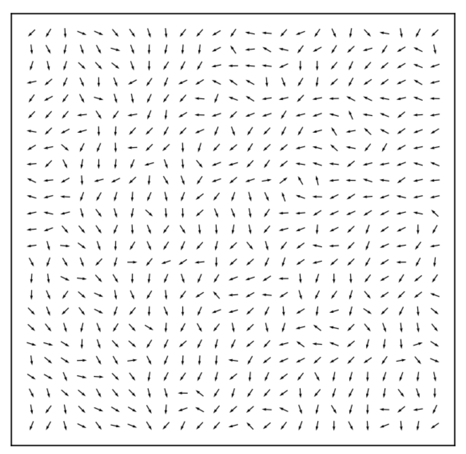
Introduction to 2D XY model

The 2D XY model is a system of interacting spins arranged on a lattice, resembling a ferromagnetic system. Each spin can make an arbitrary angle $0 \leq \theta \leq 2\pi$ with the x-axis.



We can write each spin s_i as a 2-D vector $\boldsymbol{s_i}$ given by $(\cos\theta_i, \sin\theta_i)$. The most general form of the Hamiltonian for such a system is given by,

$$\mathcal{H} = -\sum_{i,j=nn(i)} J_{ij} s_i \cdot s_j - \sum_j h_j s_j, \tag{1}$$

where J_{ij} gives the strength of the interactions between spins i, j and h_j is the external field at the lattice site j. In our project, we have no external field, and set the interaction term $J_{ij} = 1 \; \forall \; i, j$. Thus, the Hamiltonian takes the form,

$$\mathcal{H} = -\sum_{i,j=nn(i)} \cos(\theta_i - \theta_j). \tag{2}$$

The energy of the system is minimised when neighbouring spins point in the same direction. This simple model provides an example of a phase transition.

Phase Transition Characteristics

This system was studied by Michael Kosterlitz and David Thouless who found that it undergoes a topological phase transition between ordered and disordered states of the system, which occurs due to topological defects known as 'vortexes' in the lattice. This phase transition occurs at a specific temperature known as the critical temperature, and marks specific changes in:

- Energy
- Specific heat
- Magnetization
- Susceptibility
- Correlation length
- Vorticity

Looking at the changes in form and the discontinuities in these quantities around the critical temperature, we can get the critical exponents of the system. The critical temperature of the 2D XY model was estimated theoretically by Mattis (1984) to be $\mathbf{\frac{k_B}{J} T_{KT} = 0.8816}$

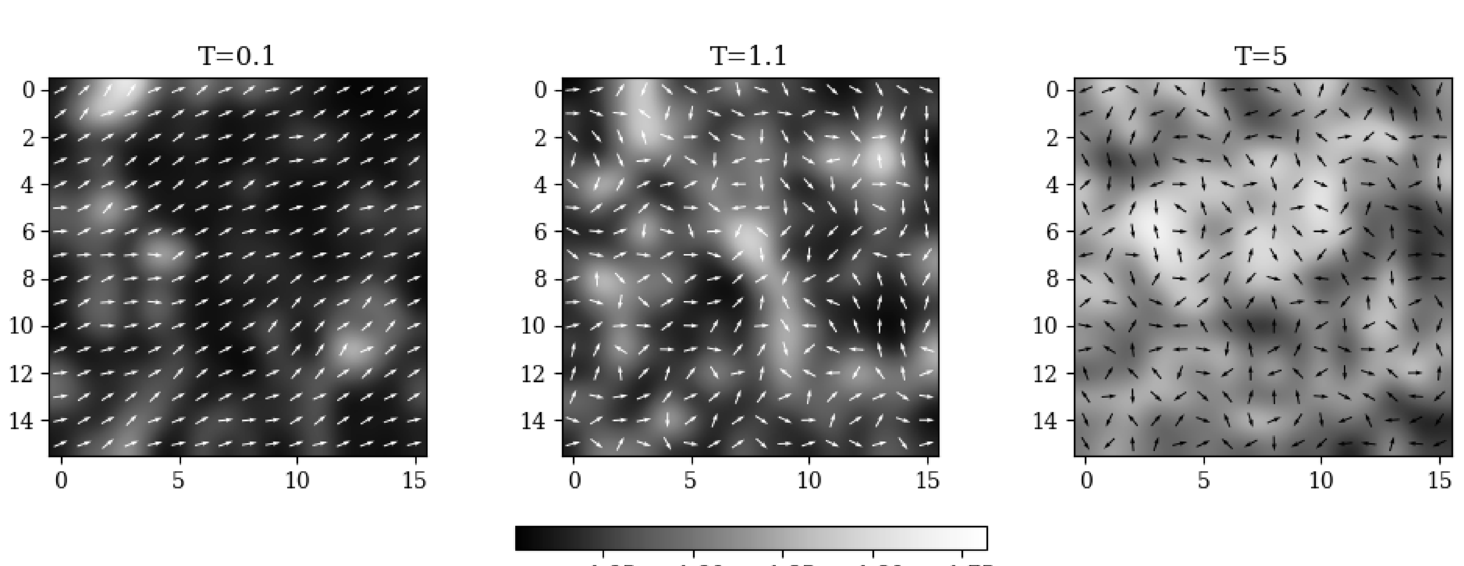
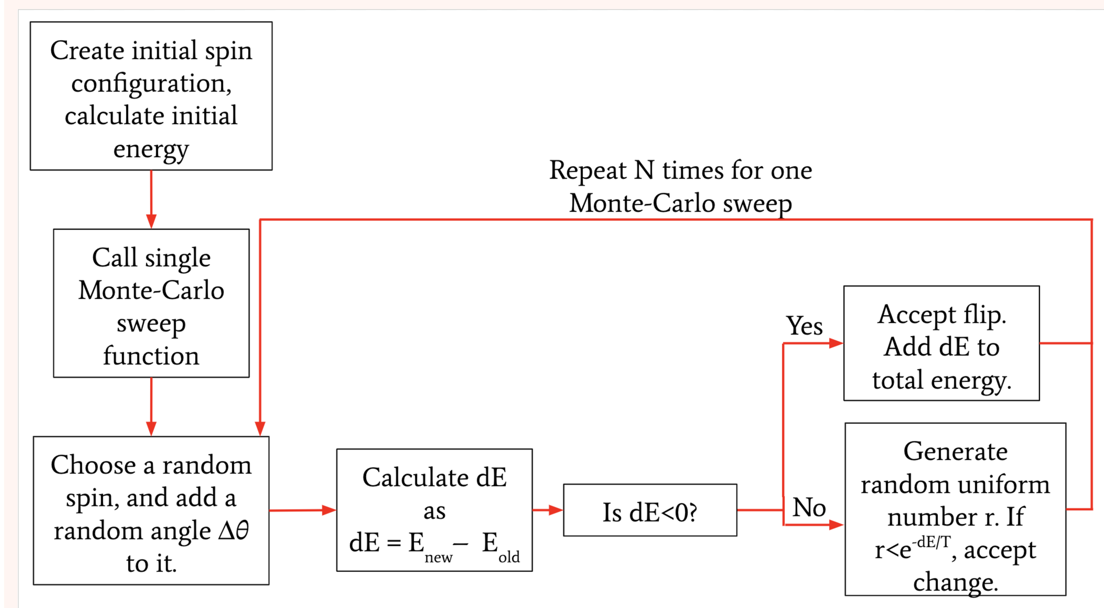


Figure 1. 2D XY model at different temperature, showing lower energies for ordered config. and higher energy for disordered config.

Monte-Carlo steps and the Metropolis algorithm



The algorithm used for Monte-Carlo evolution of the system, using the Metropolis-Hastings algorithm. This uses a Boltzmann weighted distribution. We execute around 10,000 such sweeps to allow the system to reach equilibrium.

Vortexes and Antivortexes

A vortex is topological defect in the spin system, that is formed by spins that rotate by a multiple of 2π in a counterclockwise circle. They annihilate when they collide with an antivortex.

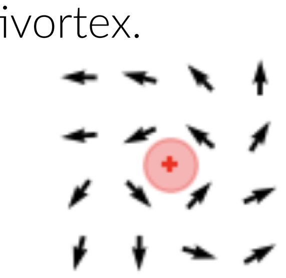


Figure 2. Vortex: spins rotate by $+2\pi$ in a counterclockwise direction.

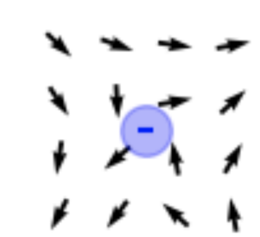


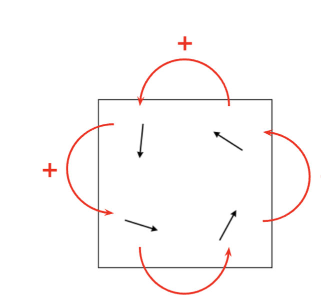
Figure 3. Antivortex: spins rotate by -2π in a counterclockwise direction.

Vortexes are generally not formed at low temperatures as they add a large amount of energy to the system. However, the energy of a *bound vortex-antivortex pair* is much lower than the individual defects, so bound pair can exist at low temperatures. This leads to a phase transition: at low T, a few vortexes and antivortexes exist in bound pairs that do not move too far from each other. Above some critical temperature T_{KT}, The vortexes suddenly unbind and move about freely, and a huge number of new vortexes are formed.

Vortex detection:

1. The absolute sum of differences between one spin and the next (going counterclockwise) is 2π.
2. The product of these differences is negative.

For a vortex, there will be 3 positive differences and 1 negative; for an antivortex, there will be 3 negative and 1 positive.



Correlation function and length

Divergence of the correlation length ξ is a characteristic of the phase transition. The correlation function $C(r)$ is a measure of how much spins separated by a distance influence each other. The correlation length is the characteristic length over which the correlation function decays. We evaluate the spin-spin correlation function as,

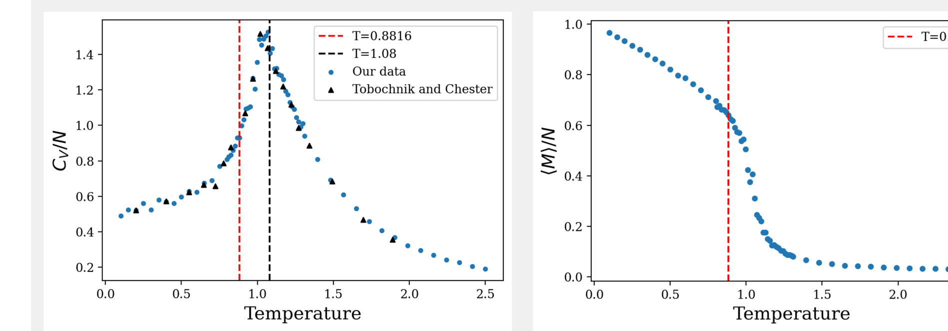
$$C(r) = \langle s_i s_j \rangle - m^2 = \cos(\theta_i - \theta_j) - m^2, \tag{3}$$

where m is the average magnetization per spin in the system. We expect:

- $C(r)$ will follow a power-law decay for temperatures below T_{KT}
- $C(r)$ will show exponential decay above the T_{KT}.
- The system will be infinitely responsive at $T_{KT}k$- for an infinite lattice, the correlation length would go to infinity.

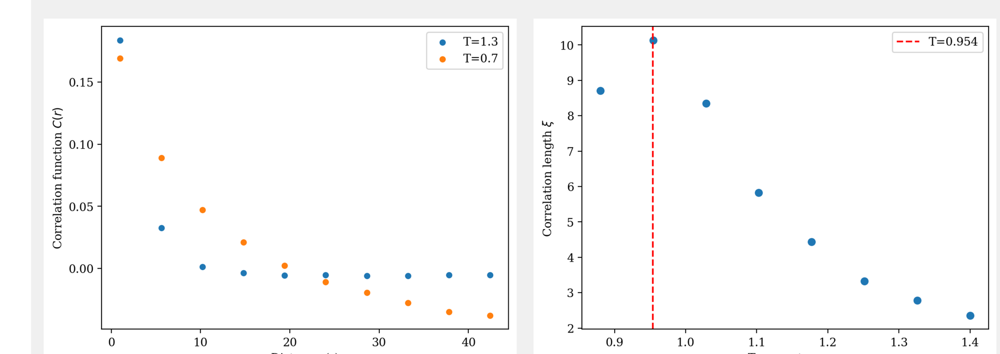
Results

Specific Heat and Magnetization



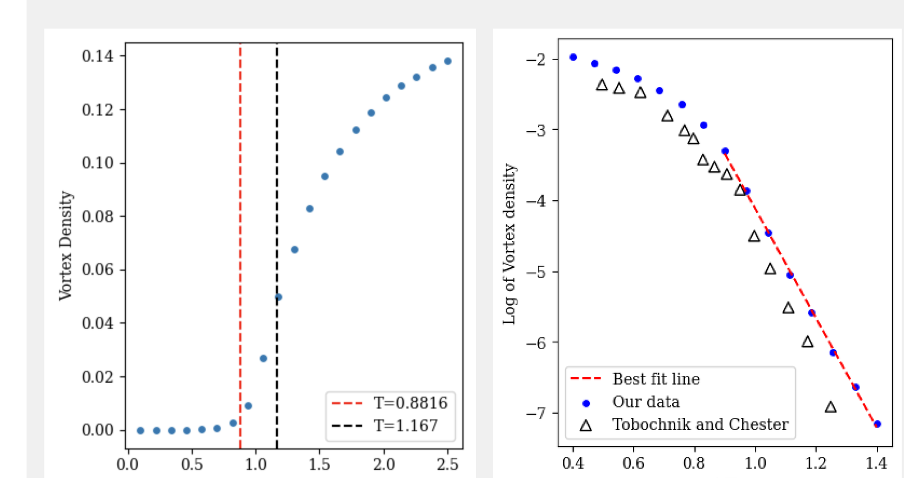
Left: Specific heat per spin plotted against temperature. Data obtained by Tobochnik and Chester is included. The peak is observed near $T \sim 1.08$, which is slightly above the critical temperature, as expected.
Right: Average magnetization per spin plotted against temperature. The critical temperature T_{KT} marks a change in behaviour from linear to exponential form.

Correlation Length



Left: Correlation function against distance. The curve falls exponentially of the form ($e^{-\frac{r}{\xi}}$ where ξ is the correlation length) for $T = 1.3$ and as a power law for $T = 0.7$.
Right: Correlation length as a function of temperature- diverges near the critical temperature and then falls exponentially as a function of temperature.

Vorticity



Left: Graph of vorticity at different temperatures from 1024 spin system.
Right: Graph of $\ln v$ versus $1/T$, with data from Tobochnik and Chester (1979), and best fit line of the linear portion below T_{KT}.
Just below the critical temperature before the phase transition, the vorticity v is expected to change as $v \sim e^{2\mu/T}$. 2μ is the energy required to create one vortex-antivortex pair. We obtain the energy of a vortex pair to be $2\mu \approx 7.740$.

Numerical Results

Parameter->	Critical Temp. (T_{KT})	Critical Exponent (ν)	Vortex-pair energy (2μ)
Simulation data:	0.88	0.756	7.74
Theoretical estimate:	0.8816	0.5	10.2

Future Work

- Calculate error bars for all plots.
- Obtaining critical temperature using correlation length curve.
- Exploring the effects of lattice size on vorticity and correlation length.
- Detecting vortices at larger scales (4x4 sections).

References

1. *Statistical and Thermal Physics: With Computer Applications, Second Edition* by Tobochnik & Gould
2. *Monte Carlo study of the planar model*, Tobochnik & Chester, Physical Review B, 1979.
3. *First-order transition in a 2D classical XY-model using microcanonical Monte Carlo simulations*, Ota et. al, Pramana Journal of Physics, 1993.

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