

# Graphical Analysis of Phase Transition in XY Model

Jiachuan Chen, Zhiren He, Chenhao Zhang, Tayyab Nawaz(mentor), Prof. Kay Kirkpatrick(supervisor)



Illinois Geometry Lab

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## Mean Field Theory in XY Model

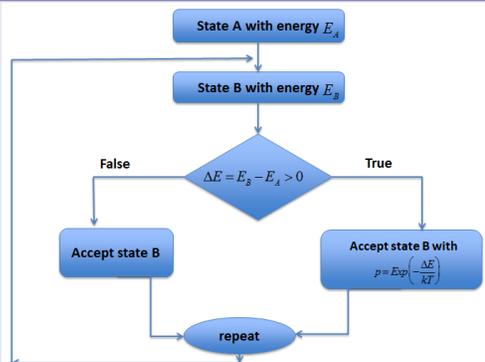
- **XY Model:** Every spin is on the unit circle
- Graphically, it is similar to complete graph, which means that every two distinct particles interact with each other
- **Mean Field Theory:** The study of average effect of all the particles on a particular particle
- The Hamiltonian is given by:  

$$H(\sigma) = -\sum_{ij} J_{ij} \langle \sigma_i, \sigma_j \rangle = -\frac{1}{2N} \sum \cos(\theta_i - \theta_j)$$

## Ordered Parameters' Formulas

- Average Energy:  $\langle E \rangle = \frac{H(\sigma)}{N}$
- Magnetization:  $M = \frac{\sum \sigma_i}{N}$
- Specific Heat:  $C_v = \frac{1}{kT^2} [\langle E^2 \rangle - \langle E \rangle^2]$  scaled variance of Energy, where  $k$  is Boltzmann constant,  $T$  is Temperature
- Susceptibility:  $\chi_M^2 = \frac{1}{T} [\langle M^2 \rangle - \langle M \rangle^2]$

## Metropolis Algorithm



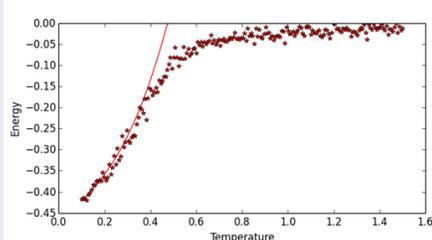
- The algorithm is an 'accept-reject' algorithm where we calculate the difference of the total energy in original configuration and in new configuration;
- If energy of new configuration is larger, we accept new configuration with probability  $\text{Exp}(-\frac{\Delta E}{kT})$ ; if energy of new configuration is smaller, we accept new configuration with probability 1

## Phase Transition

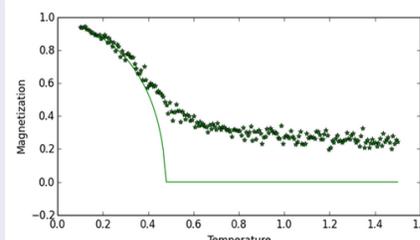
- Physically: Transformation of a thermodynamic system from one phase or state of matter to another one by heat transfer
- Mathematically: The study of non-analyticity of free energy, which is given by

$$U \equiv \langle E \rangle = \sum_r P_r E_r = -\frac{\partial \log Z}{\partial \beta}$$

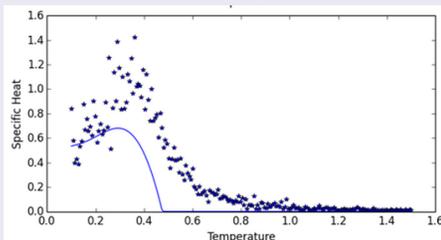
## Ordered Parameters' Graphical Analysis



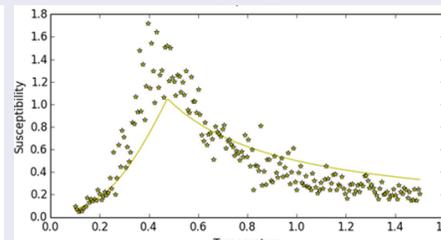
(a) As Temperature rises from 0 to 0.5, Average Energy increases exponentially. After critical temperature 0.5, the Average Energy becomes stable



(b) Before critical temperature 0.5, the increase in temperature leads to decrease in Magnetization; after critical temperature magnetization tends to zero, which indicates at high temperature, particles move in random directions



(c) Specific heat experienced a parabola change before critical temperature; after critical temperature Specific Heat tends to 0 as Temperature increases

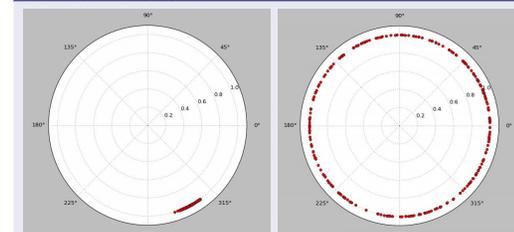


(d) Susceptibility increases as Temperature increases before critical Temperature; after it reaches a peak at critical temperature, Susceptibility decreases as Temperature increases

## Average Spin Behavior in Different Temperature Regimes

- For low temperature, spins are all lined up in same directions, as  $T$  goes down,  $M$  increases,  $|E|$  increases
- For high temperature, spins are pointed randomly in different directions, as  $T$  goes up,  $M$  decreases,  $|E|$  decreases

## Animated Simulation Plot



(e)  $T = 0.01; E = -0.4945; M = 0.9983; \chi_M^2 = 0.01$   
 (f)  $T = 1.50; E = -0.0056; M = 0.0745; \chi_M^2 = 0.37$

## Applications of Superconductors

- Biomagnetism
- Magnetic-levitation
- SQUIDs (Superconducting Quantum Interference Device)

## Future Work

- Study the correlations of spin behaviors under different temperature regions
- Numerical calculation for rate function and Large Deviation Principle for each regime
- Graphical analysis of limit theorems in subcritical/critical/supercritical regimes

## Acknowledgements

- Professor Kay Kirkpatrick
- Mentor Tayyab Nawaz
- Reference:  
<https://github.com/seanshahkarami/demos/blob/master/spindemo.py>  
 Geometry and Topology in Hamiltonian Dynamics and Statistical Mechanics (Marco Pettini)