CONTINUOUS SPINS

Jay Nash & Wilson Hernandez

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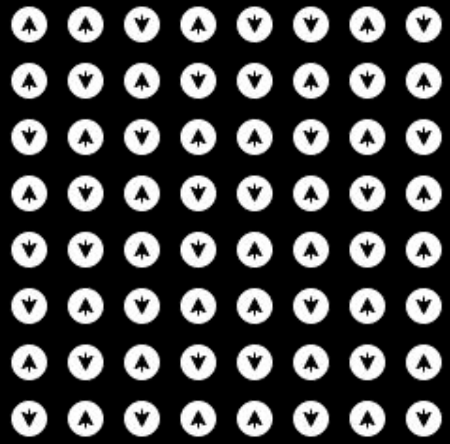
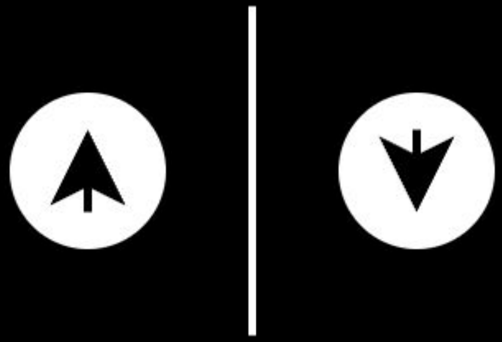
Ising Model





Select Random Spin, Then:

1. Flip spin if flip results in negative energy change
2. Flip spin with probability if flip results in positive energy

Lattice of Spins

- Lattie size is some length
- Spins subject to periodic boundary conditions

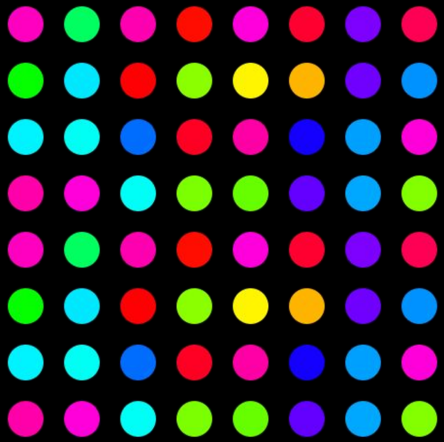
Binary Spins

- Spins can either be spin up or spin down
- Spins all have the same magnitude

Spins Flip With Prob.

- A change is accepted if the energy decreases or with probability $e^{-\beta\Delta E}$

Continuous XY Model



Select Random Spin, Then:

1. Flip spin if random rotation results in negative energy change
2. Flip spin with probability if random rotation results in positive energy

Lattice of Spins

- Lattie size is some length
- Spins subject to periodic boundary conditions

Cont. Spin Value

- Spins may have any angle $\theta \in [0,2\pi)$
- Spins all have the same magnitude

Spins Flip With Prob.

- A change is accepted if the energy decreases or with probability $e^{-\beta\Delta E}$

Energy Calculation

Ising Model

Spin Energy

- $E_s = \sum \sigma_i \sigma_j$
- Where σ_i is the value of a spin and σ_j are the surrounding spin values

Change In Energy

- $\Delta E = E_i - E_{new}$

Avg. Energy Per Spin

- $E_{tot} = \sum E_s$
- $E_{avg} = (E_{tot} / 2) / N$
- Where N is the number of spins

XY Model

Spin Energy

- $E_s = \sum \cos(\theta_i - \theta_j)$
- Where θ_i is the angle of a spin and θ_j are the surrounding spin angles

Change In Energy

- $\Delta E = E_i - E_{new}$

Avg. Energy Per Spin

- $E_{tot} = \sum E_s$
- $E_{avg} = (E_{tot} / 2) / N$
- Where N is the number of spins

Other Measurements

Magnetization

Ising Model:

- $M = N^{-1}\sum \boldsymbol{\sigma}_i$
- Where $\boldsymbol{\sigma}_i$ is the value of a spin

XY Model:

- $M_{x/y} = \sum \cos\theta_i \,;\, \sum \sin\theta_i$
- $M = N^{-1}(M_x^{\,2} + M_y^{\,2})$
- Where θ_i is the angle of a spin

Specific Heat & Susceptibility*

When in equilibrium at temperature T:

- $M_{var} = \langle M^2 \rangle - \langle M \rangle^2$
- $\mathscr{X} = N\,(M_{var} / T)$
- $E_{var} = \langle E^2 \rangle - \langle E \rangle^2$
- $C_V = E_{var} / T^2$

Vortex Count*

For every 2x2 square of spins:

- $\Delta\theta$ = Total Angular Change
- $N_v = \sum 1(|\Delta\theta| \geq 2\pi)$

Specific Heat & Susceptibility

Boltzmann Statistics Says:

- The partition function is:
  - $Z = \sum e^{-\beta E\_i}$
- The probability of a state *i* is:
  - $p_i = Z^{-1}\, e^{-\beta E\_i}$
- For any quantity the expectation value is given by:
  - $\langle X \rangle = \sum X_i p_i$
  - Therefore:
    - $\langle M \rangle = \sum M_i Z^{-1}\, e^{-\beta E}$

If an external field $\dot{M}$ is applied then the energy is given by:

- $E = E_i - \dot{M} M$

This changes both the partition function and p_i :

- $Z_{\dot{M}} = \sum e^{-\beta E\_i}\, e^{\beta \dot{M} M}$
- $p_i = Z_{\dot{M}}^{-1}\, e^{-\beta E} e^{\beta \dot{M} M}$

If $\dot{M}$ is small, we can approximate $e^{\beta \dot{M} M}$ as a taylor series:

- $e^{\beta \dot{M} M} \cong 1 + \beta \dot{M} M + (\beta \dot{M}^2 M^2 / 2!) + \ldots$
- Thus:
  - $Z_{\dot{M}} \cong Z\,(1 + \beta \dot{M} \langle M \rangle_0 + (\beta \dot{M}^2 \langle M^2 \rangle_0 / 2!) + \ldots)$
  - $\langle M \rangle_{\dot{M}} = \sum M_i Z_{\dot{M}}^{-1}\, e^{-\beta E} e^{\beta \dot{M} M}$

After expansion/approximation we get:

- $\langle M \rangle_{\dot{M}} \cong (\, Z\, (M + \beta \dot{M} \langle M^2 \rangle_0 + \ldots\,)\,) / Z_{\dot{M}}$

This reduces to:

- $\langle M \rangle_{\dot{M}} \cong \langle M \rangle_0 + \beta \dot{M} (\langle M^2 \rangle_0 - \langle M \rangle_0^{\,2}) + \ldots$

Susceptibility is defined as:

- $\mathscr{X} = \partial \langle M \rangle_{\dot{M}} / \partial \dot{M}$
- If we take the derivative of the first 2 terms of $\langle M \rangle_{\dot{M}}$:
  - $\mathscr{X} = \beta (\langle M^2 \rangle_0 - \langle M \rangle_0^{\,2})$

If we expand β and set $k_B = 1$:

- $\mathscr{X} = (\langle M^2 \rangle_0 - \langle M \rangle_0^{\,2}) / T\,)$

Since M is normalized to N:

- $\mathscr{X} = N\,(\, M_{var} / T\,)$
- Where $M_{var} = (\langle M^2 \rangle_0 - \langle M \rangle_0^{\,2})$

If we follow the same process for E and consider a change in T instead of applying an external magnetic field:

- $E \cong E_i - \partial E / \partial T\, \Delta T$

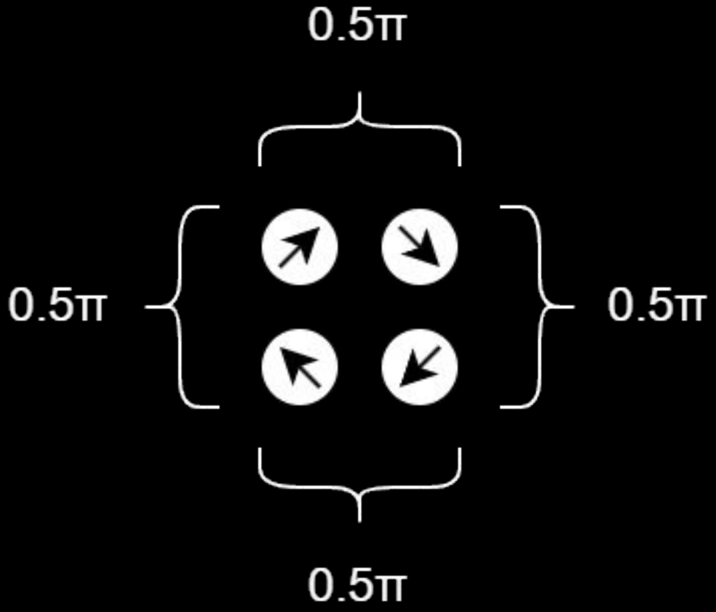
We can expand similarly as we did with M and get:

- $C_V = \partial E / \partial T = (\langle E^2 \rangle_0 - \langle E \rangle_0^{\,2}) / T^2\,)$

Vortex Count

To find vortexes:

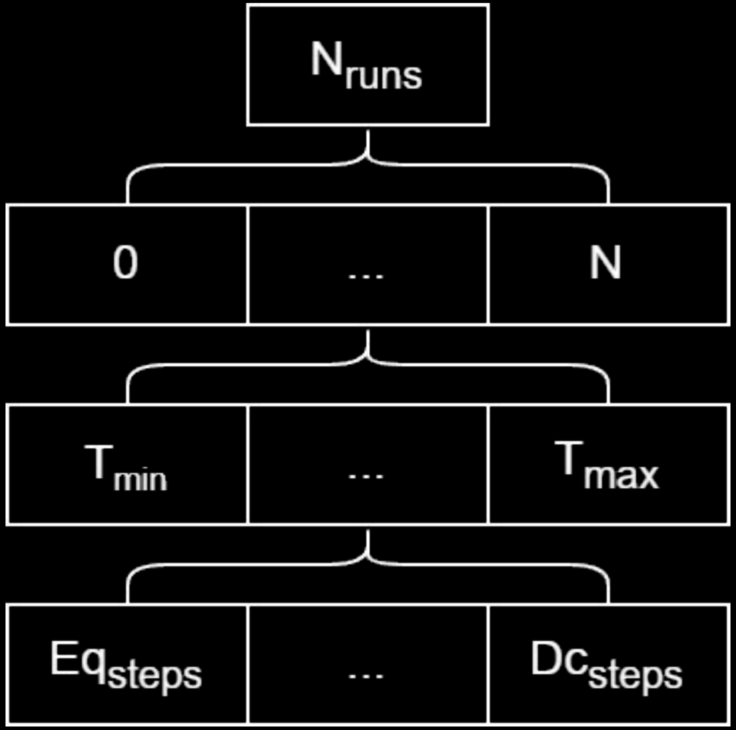
- A vortex occurs when spins fully rotate around a point
- Use a sliding 2x2 window with a step of 1
    - For each 2x2 block:
        - Find $\Delta\theta$ between spins
        - Adjust $\Delta\theta$ to $[-\pi,\pi]$
        - If $|\Delta\theta| \geq 2\pi$ then there is a vortex
    - Sum number of vortexes found
- After finding total number of vortexes:
    - Scale to lattice size by dividing by total number of spins in the lattice
    - This gives us the vortex density



Data Collection

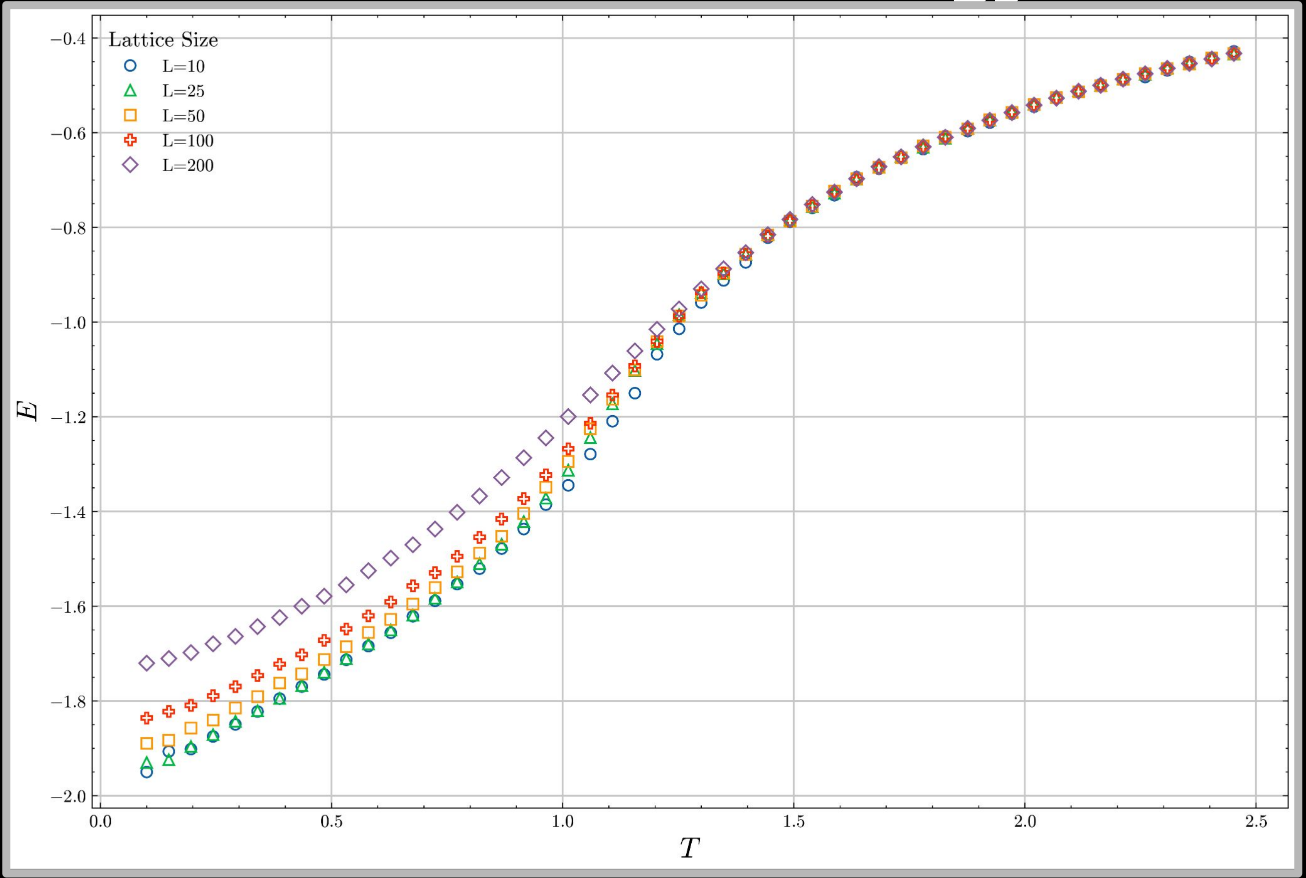
Data Collection Methodology:

- A set of lattice sizes are defined:
  - 10, 25, 50, 100, 200
- For each lattice size:
  - Run simulation for T values
    - With 50 evenly spaced values of T between 0.1 and 2.5
  - Equilibrate system for 1M steps of the metropolis algorithm before data collection
  - Collect data for 1M steps after equilibration
    - Data point collected every 10k steps
- Repeat 10 times to get average results

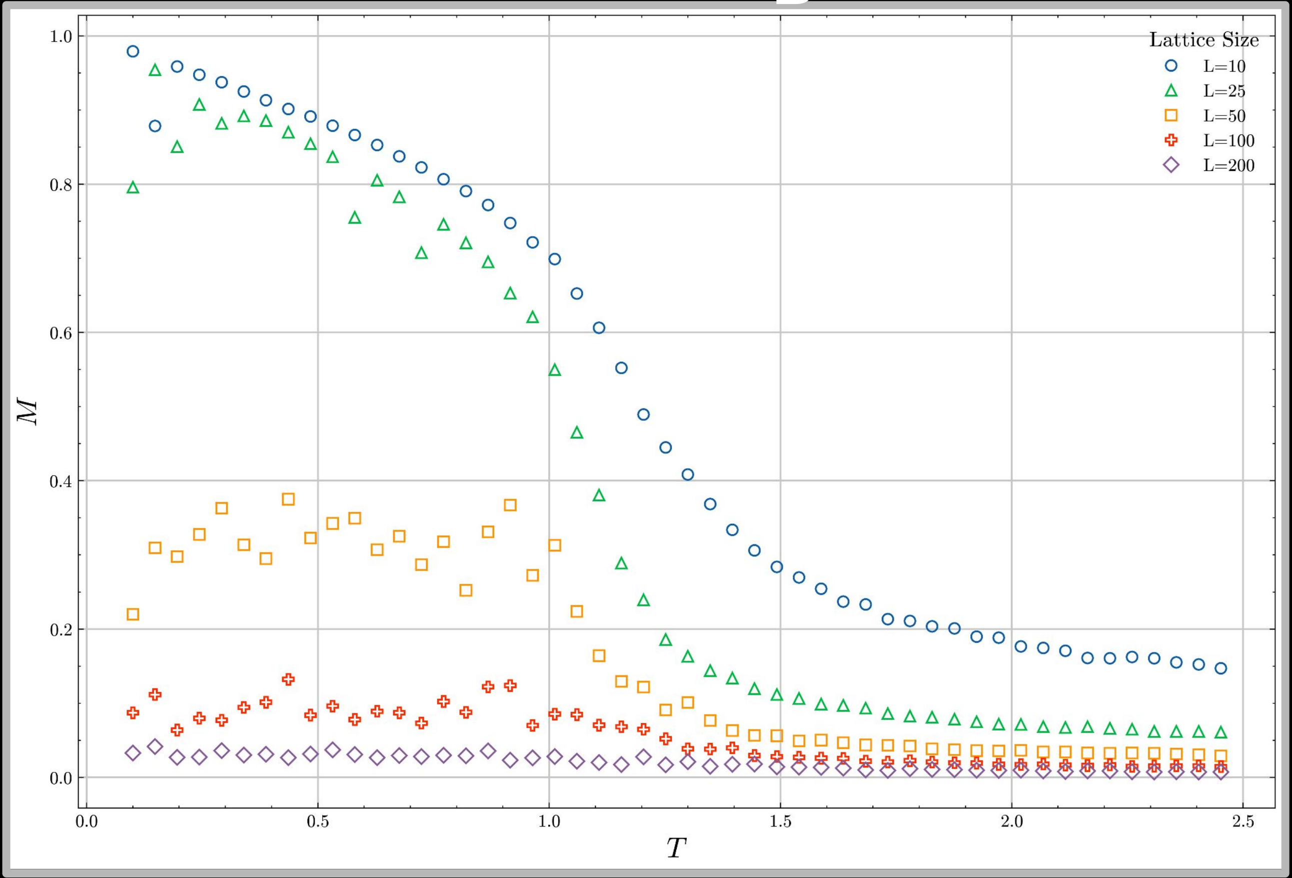


Code/Demo

Results - Energy

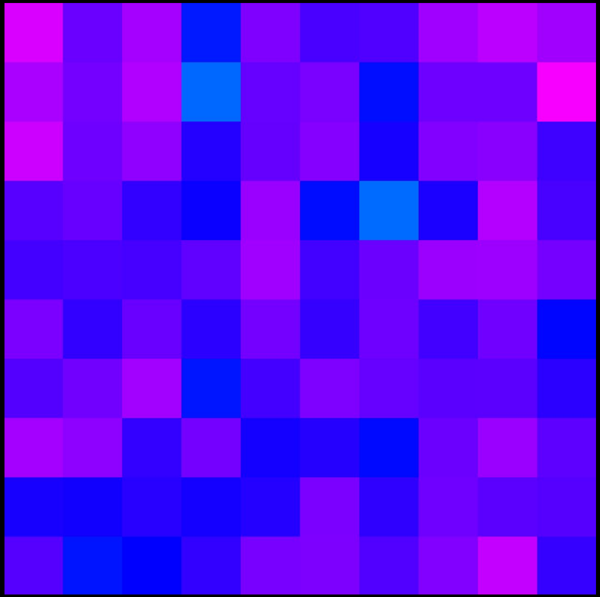


Results - Magnetism

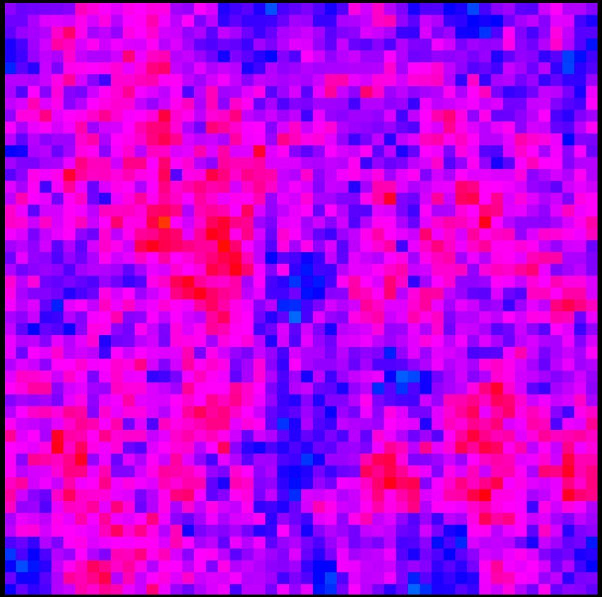


Results - Magnetism

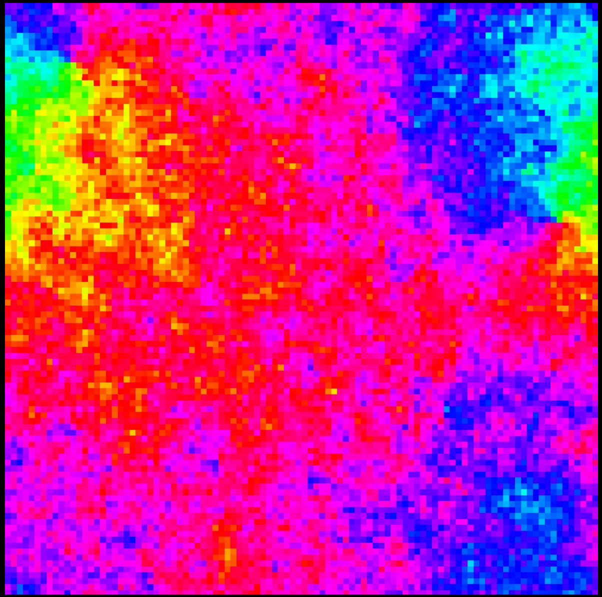
T = 0.25



L = 10

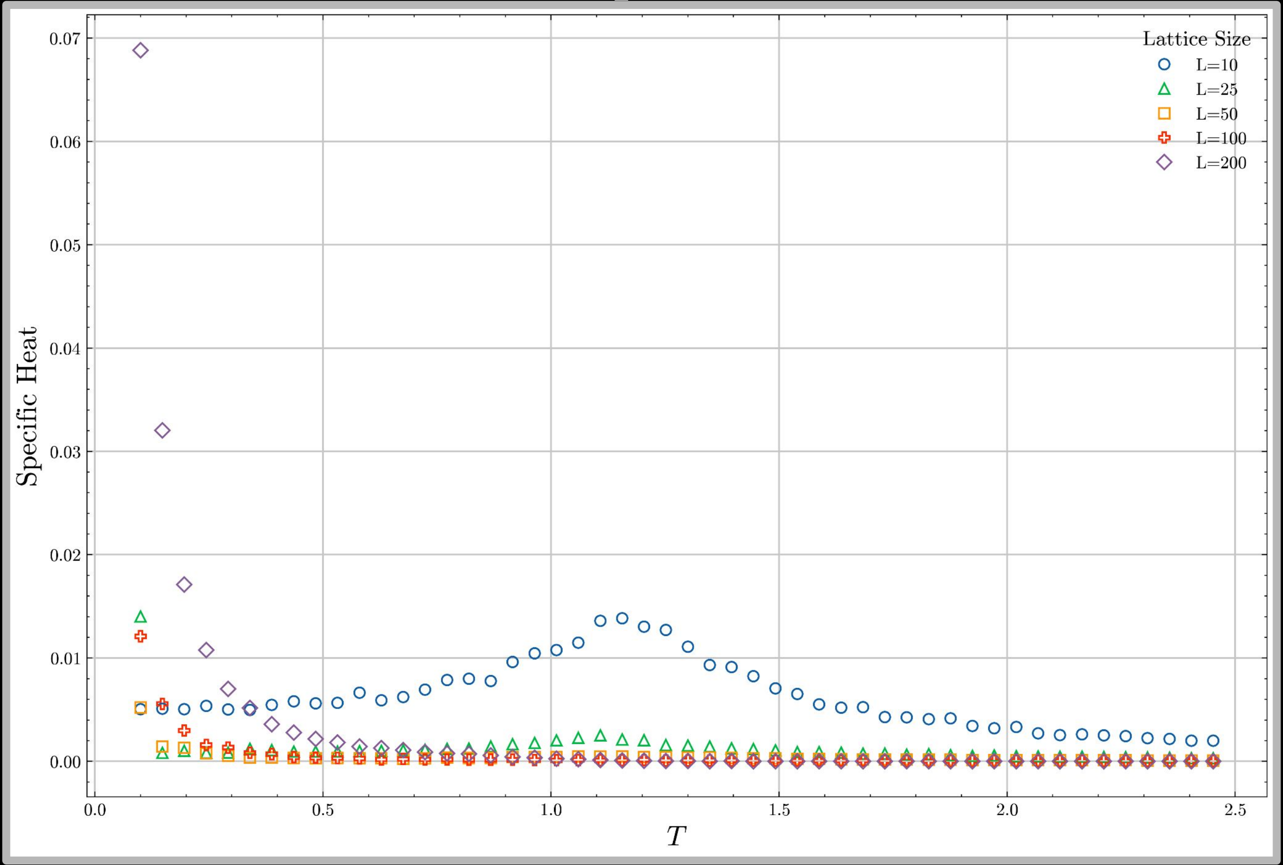


L = 50

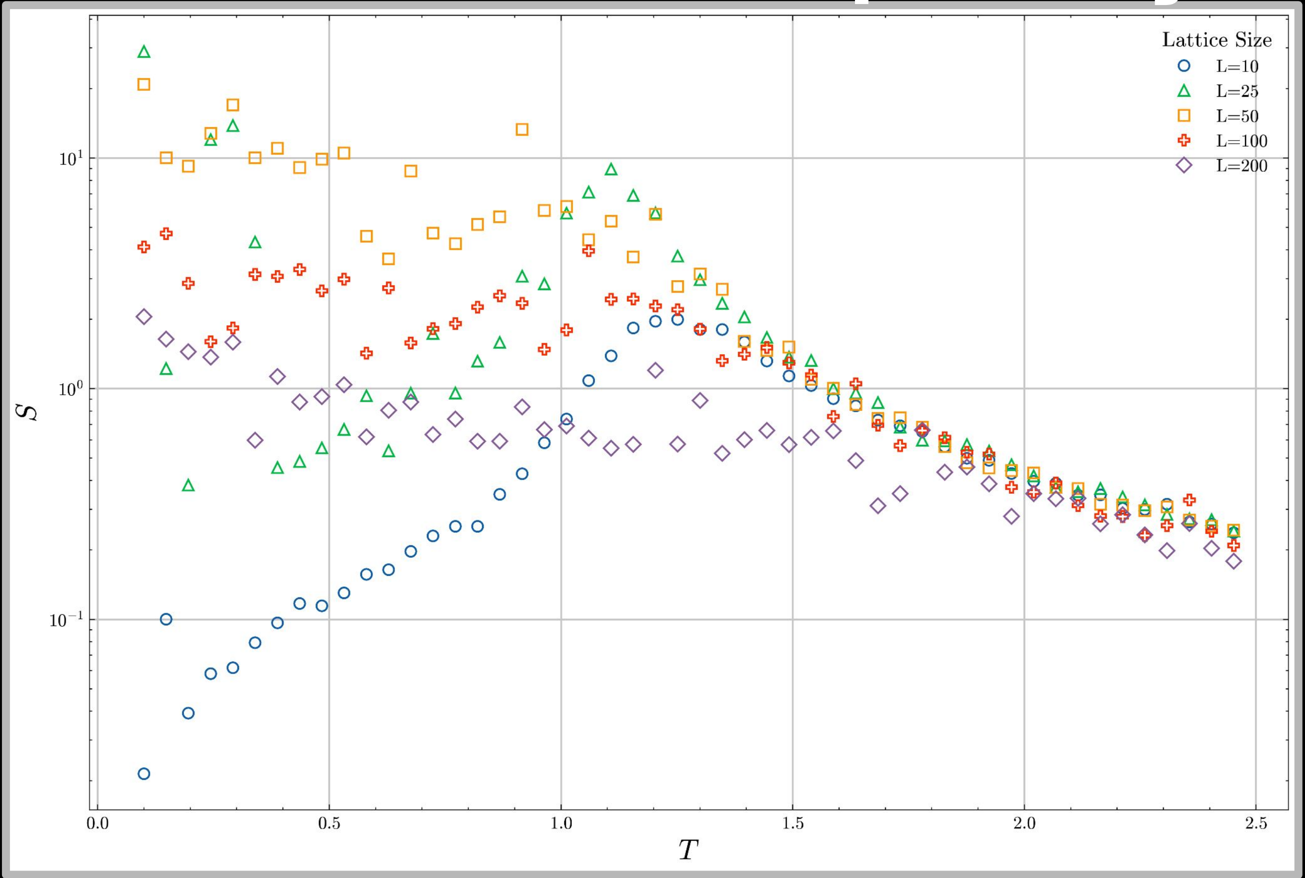


L = 100

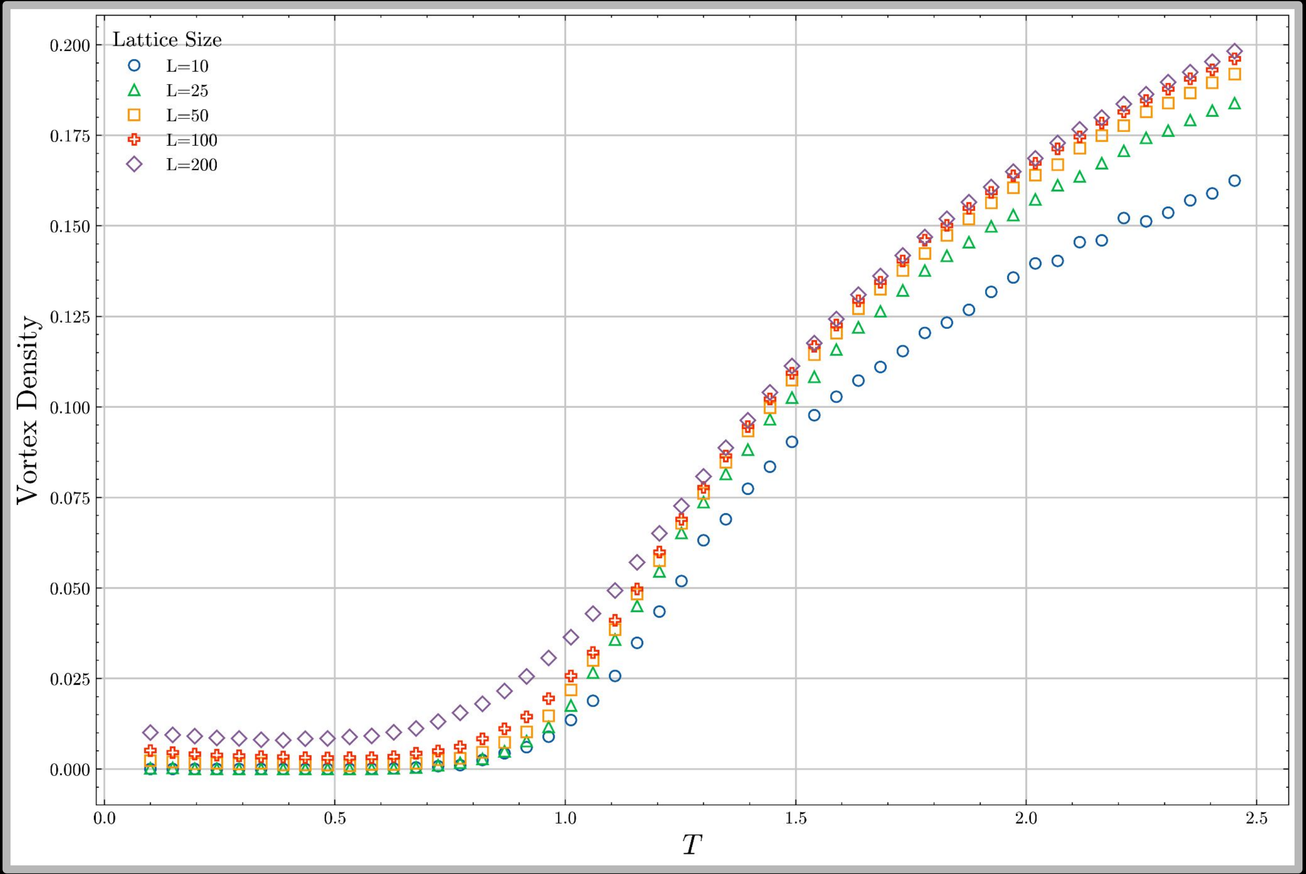
Results - Specific Heat



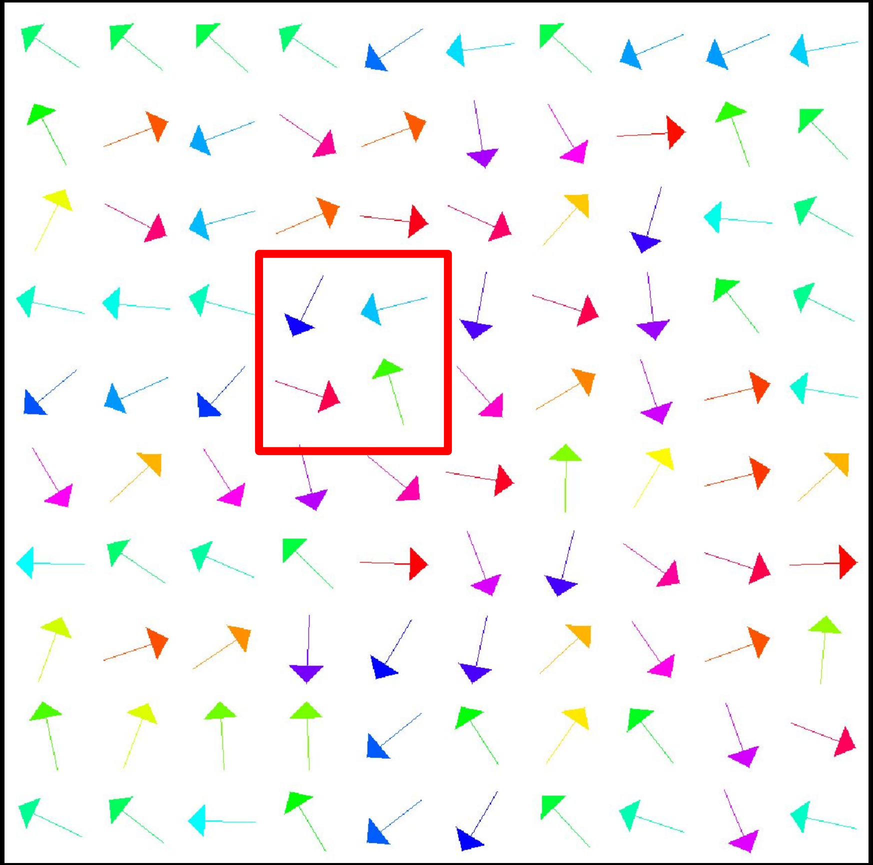
Results - Susceptibility



Results - Vortex Count

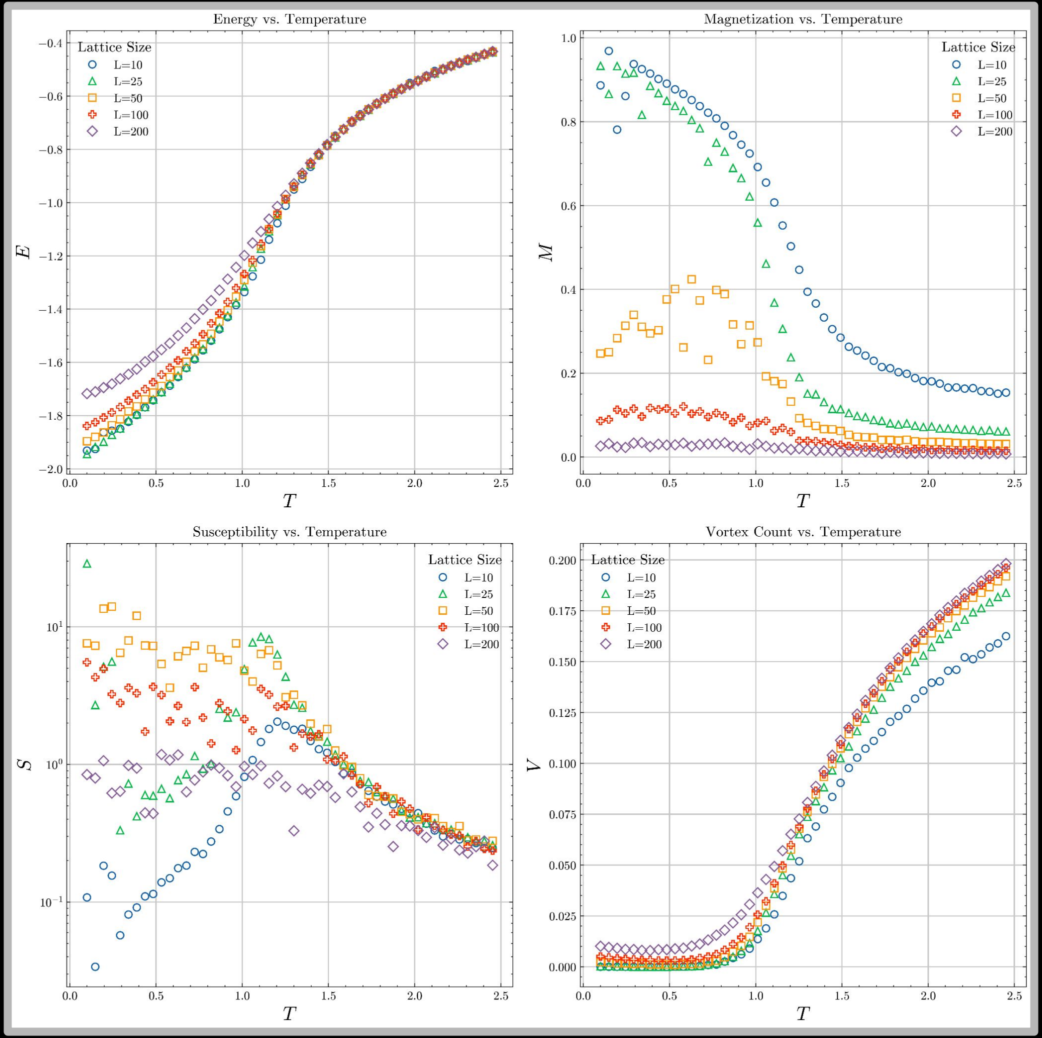


Results - Vortex Count



Result Analysis

- All graphs* have an inflection point at T ≅ 1.10
- In the XY Model this inflection point is the Berezinskii-Kosterlitz-Thouless (BKT) transition temperature
    - Above this temperature vortices are unbound and disorder the system
    - BKT temperature has been estimated to be ≅ 1.120, which agrees with the reported results
- Approaching the BKT transition:
    - The energy landscape changes
    - Long-range correlations between spins decay exponentially, reducing net magnetism
    - Fluctuations, then decay, of magnetism cause susceptibility to spike, then decay
    - The number of free vortices increase sharply as bound vortices unbind
    - Specific heat plateaus as the system is more affected by small changes in T



Questions