Computational Exploration of the BKT Transition in XY-interaction Systems

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Abstract

The Berezinskii-Kosterlitz-Thouless (BKT) Transition is a topological phase transition that appears in systems with spin interactions described by the XY Hamiltonian. Throughout its history, the BKT transition has garnered attention for its unique topological properties, and its application to different superfluid and superconducting systems. In this study, we develop software to simulate various system properties and actions with a computational implementation of the XY model as well as a Markov-Chain Monte Carlo (Metropolis-Hastings) sampling algorithm. Finally, this software is used to observe the BKT transition in a computer-generated spin lattice system, governed by XY spin interactions. The results show that the transition temperature occurs at $T_c \cong 1.17$K, relatively close to experimentally observed values.

The XY Hamiltonian

In correlated spin systems, different models described by Hamiltonians, energy operators, are used to describe the total energy of the system. The BKT transition only occurs exclusively in systems described by the Hamiltonian,

$$H(\mathbf{s}) = -\sum_{i \neq j} J_{ij}\, \mathbf{s}_i \cdot \mathbf{s}_j - \sum_j \mathbf{h}_j \cdot \mathbf{s}_j = -\sum_{i \neq j} J_{ij}\, \cos(\theta_i - \theta_j) - \sum_j h_j \cos\theta_j$$

Where J is the spin-coupling constant, and s_i and s_j are spin moments [1][2][3][4]. This Hamiltonian, true to its name, accounts for spin interactions on a single particle, up and down, and left to right (hence, XY model). This model supports the BKT transition, an second-order topological phase transition. The implementation of this across theoretical systems is often tedious and mathematically repetitive, so computers are often employed for the use of fast and accurate calculation of considerably large (compared to hand-calculated systems, they are still very small) systems.

Transition of Vortex-Antivortex Pairs

Vortices and antivortices are a topological defect that arise theoretically from calculations in perturbation theory, results of evaluating the partition function for a system. Graphically, the description is relatively self explanatory. As shown in Figure 2, the vortex is denoted by a circulation of magnetic moment vectors around a centerpoint. Conversely, the antivortex is shown at the other singularity of moments in the graph, where two adjacent vectors seem to face directly opposite one another. These pairs are initially bounded under a temperature T_c, but eventually evolve into unbounded independent vortices and antivortices.[5]

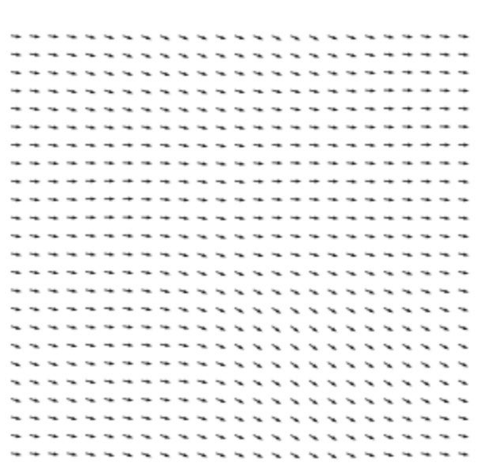

Figure 1 - T=0.0, width=25

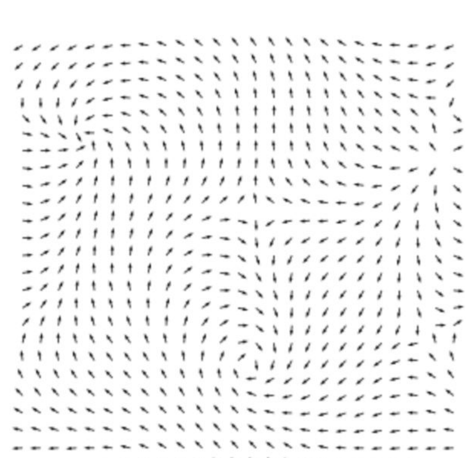

Figure 2 - T=0.9, width=25

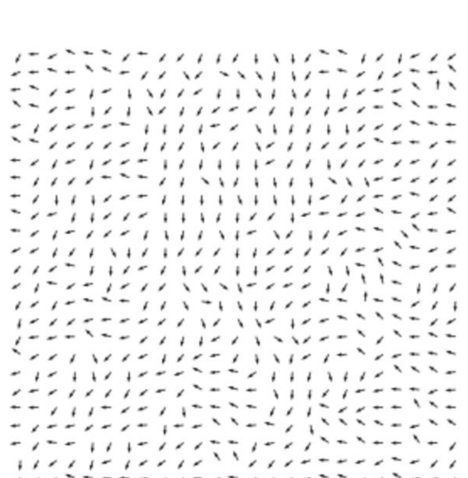

Figure 3 - T=1.1 width=25

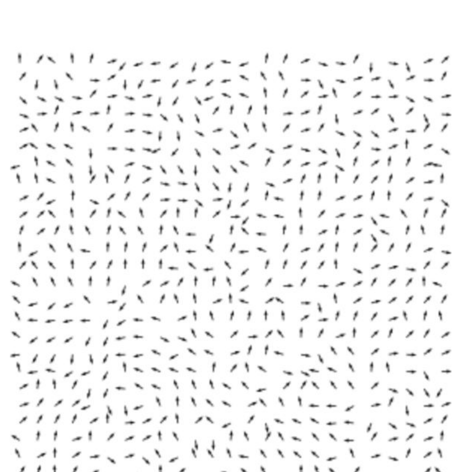

Figure 4 - T=1.5, width=25

A Computational Implementation of the XY Model

The Computational Implementation of the XY Model was grown with the help of open-source code from an implementation of a Metropolis-Hastings sampling algorithm[6] (Markov-Chain Monte Carlo algorithm, aka MCMC) originally developed by Shiling Liang, Ph.D[7]. The final code accounts for various processes relevant to a two-dimensional topological system.

Class 'XYSystem'
Takes in width of lattice and temperature (0 - 50K)
Width parameter limited by our computational power: impacted ability to observe clear formation and unbinding of vortex-antivortex pairs

Construction Function
Generates:
1. Number of spins (based off of width input)
2. Number of interactions (based on number of spins)
3. Energy (based on spin configuration and Hamiltonian)
4. Sideways and up-down interaction constants (based on number of spins and configuration)
5. Spin configurations (random assignment of a variable between zero and 2π on the number of spins)
6. Magnetization (based on average spin configuration)

Apply MCMC Algorithm
Runs through n sweeps to find the final (most thermodynamically favorable) configuration of the lattice at the given temperature
Energy of the configuration calculated

Annealing Function
Does the MCMC method for each step in a given range of temperatures
Shows the system undergoing a process of cooling

Heat Capacity and Free Energy

The specific heat capacity of the lattice can be found using the equation[8]:

$$c/k_B = \frac{\langle E^2 \rangle - \langle E \rangle^2}{N(k_B T)^2}$$

There is a peak at $k_b T/J \approx 1.1671$ in the graph of specific heat capacity against temperature[9]. This peak position and height have been shown to be independent of system size for lattices of linear size greater than 256. Our results show a peak at roughly this value, although the largest lattice we were able to compute was 60 by 60.

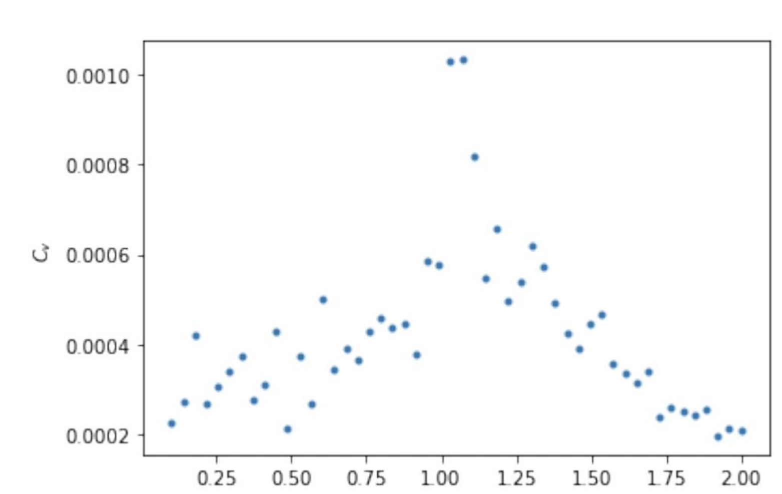

Figure 5 - width=40

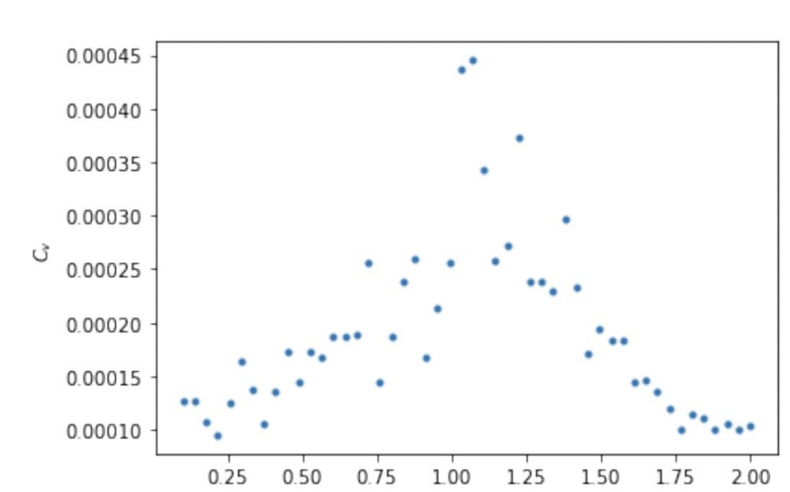

Figure 6 - width=60

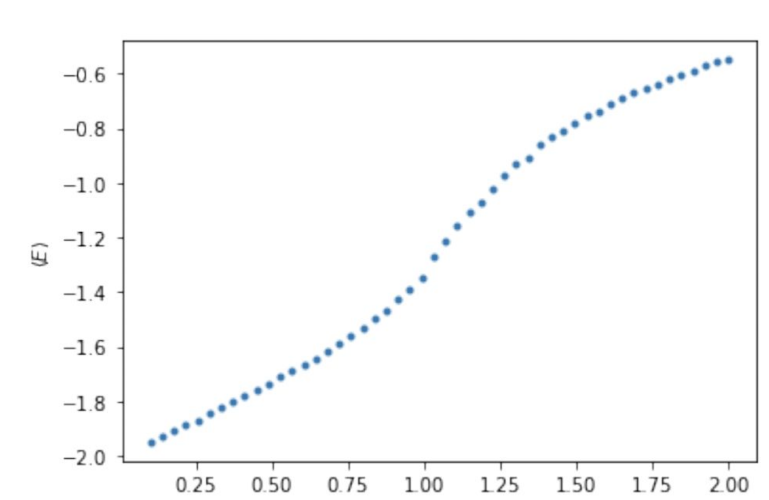

Figure 7 - width=40

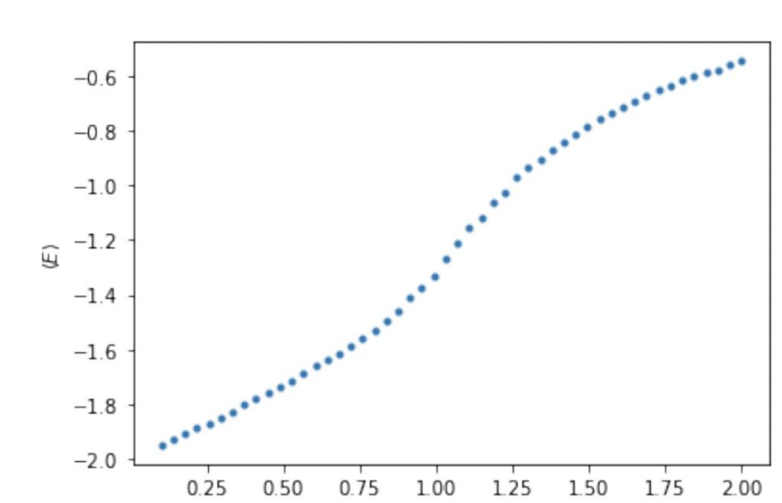

Figure 8 - width=60

The graph of free energy against temperature similarly shows maximum rate of increase at around this value.

Experimental Evidence

BKT phase transitions have been realized experimentally using liquid helium films[10], superconducting Josephson junctions[11], and 2D atomic hydrogen[12]. Taking the last of the three experiments[13] as an example, very cold atomic gas (with temperatures to the order of a few μK) is generated through a Doppler cooling technique[14]. Two high-frequency laser beams are sent through the 3D gas to create 2D layers of matter waves. The observed interference pattern of the waves at different temperatures represent the amount of vortex-antivortex pairs, that is, the interference pattern will be the most distorted when the vortex and antivortex are unbound. As shown in Figure 9, this occurs at a specific mid-temperature, as defined by the theoretical models.

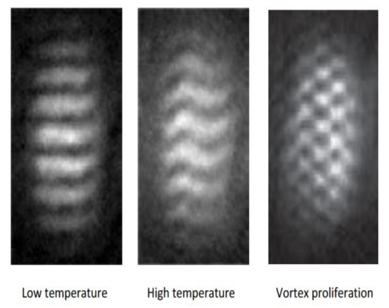

Figure 9 [9]

Conclusion + Future Work

Although the overall goal of the project was met, there were challenges in software development and tuning. Implementation of the Metropolis-Hastings algorithm was particularly challenging, and took a great deal of time to test and confirm proper operation. Additionally, further work could be done from the current state of the project. In condensed matter, this software could be used to characterize correlated magnetic systems, which could also contribute to findings in spintronics, chip design, or various other topics involving computer engineering or related fields. Also, recent breakthroughs in the field of ambient superconductivity have been incredibly promising, and certain programs built on top of this software could possibly model certain candidates for ambient superconductors. Following from these ideas, this piece of software is a tool to work on more accurate material characterization and design, allowing for a smoother workflow between theory and experiment.

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