Studying the Kosterlitz-Thouless Transition of the two dimensional XY model using Monte Carlo methods

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I hereby declare that this thesis was formulated by myself and that no sources or tools other than those cited were used.

Bonn, ...
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1. Introduction

In physics there are a variaty of problems for which it is either very hard or impossible to find analytical solutions. These problems often involve many particle systems and/or integrals of high dimensionality. With ever increasing compute power available to researchers, it becomes more and more feasible to study such system using Monte Carlo methods. Monte Carlo methods is an umbrella term for numerical methods which employ random numbers.

The perhaps most well-known application of Monte Carlo methods in physics is the Ising model. It describes the magnetizion of lattice structures

It describes the total magnetization of a lattice as the superposition of all spins $\sigma_i = \pm 1$ on the lattice. The Ising model features a phase transition at a critical temperature where the system transitions from an ordered low-temperature to a unordered high-temperature state.

One can now generalize the problem from a discrete $\mathbb{Z}_2$ symmetry to a continuous $U(2)$ symmetry. This is called the XY model and describes the spins as two-dimensional vectors on the unit circle. Unlike the Ising model, the XY model does not have a 2nd order phase transition. It does however have something we call KT phase transition where below a critical temperature T_C metastable states can exist. These metastable states are closely related to vortex/anti-vortex pairs on the lattice. The discovery of the KT phase transition was awared with the Nobel prize in 2016.

In this bachelor thesis I will be employing Monte Carlo methods, namely the Metropolis and Wolff algorithms, to study the two dimensional XY model.

2. Theory

2.1. Phase Transitions in Thermodynamics

Test

2.2. XY Model

The XY model is the generalization of the Ising model where the $\mathbb{Z}$ symmetry is replaced by a continuous $U(2)$ symmetry.

2.2.1. Definition

The XY model describes the spins σ_i as two-dimensional vectors on the unit circle

$$\sigma_i = \begin{pmatrix} \cos\theta_i \\ \sin\theta_i \end{pmatrix} \tag{2.1}$$

parametrized by the angle $\theta_i \in [0, 2\pi)$. The total Energy of the system is given by the Hamiltonian

$$H = -J \sum_{\langle i,j \rangle} s_i \cdot s_j = -J \sum_{\langle i,j \rangle} \cos(\Delta\theta) \tag{2.2}$$

where $\langle i,j \rangle$ are neighbouring spins, $\Delta\theta = \theta_i - \theta_j$ is the angle between two neighbouring spins and $J > 0$ is the interaction strength. The partition function for such a system is given by

$$Z = \sum \exp{-\beta H} = \sum \exp\left(\beta J \sum_{\langle i,j \rangle} \cos(\Delta\theta)\right) \tag{2.3}$$

with $\beta = (k_B T)^{-1}$ so that $[\beta] = \frac{1}{\mathrm{J}}$ and k_B being the Boltzmann constant. The coupling constant J is set to $J = 1\,\mathrm{J}$ so that βJ is dimensionless.

2.2.2. Observables

As the observables of the XY model scale with the number of lattice sites, it is generally more insightful to study the observables per spin. This way, the finite size scaling of the observables can be be better observed.

2. Theory

Energy per Spin   The total energy of the system is given by its Hamiltonien. For the two dimensional lattice with side length L, periodic boundary condition and nearest neighbour approximation the total energy is this

$$E = -\frac{1}{L^2} \sum_{\langle i,j \rangle} \cos(\Delta\theta). \tag{2.4}$$

Specific Heat per Spin   In addition to the energy per spin E one can also record E^2 and derive the specific heat capacity of the system

$$C_V = \frac{\langle E^2 \rangle - \langle E \rangle^2}{T^2}. \tag{2.5}$$

Magnetization per Spin   The total absolute magnetization per spin for a system with side length L is given by

$$|M|^2 = \frac{1}{L^2} \left(\left(\sum \cos\theta_i \right)^2 + \left(\sum \sin\theta_i \right)^2 \right). \tag{2.6}$$

Magnetic Susceptibility   The magnetic susceptibility of the system can be derived as

$$\chi = \frac{\langle M^2 \rangle - \langle M \rangle^2}{T}. \tag{2.7}$$

Helicity Modulus per Spin   According to Teitel and Jayaprakash (1983) one can also derive the *spin stiffness* or *helicity modulus* Υ which "is a measure of the phase correlations of the system" (Teitel and Jayaprakash (1983)). It can be shown that the *helicity modulus* is given by

$$\Upsilon = -\frac{1}{2}\langle E \rangle - \frac{J}{k_B T L^2} \left\langle \left(\sum_{\langle i,j \rangle} \sin(\Delta\theta) \vec{r_{ij}} \cdot \vec{e} \right)^2 \right\rangle \tag{2.8}$$

where, in addition to the existing definitions, $\vec{r}_{i,j}$ is the vector from site i to site j and $\vec{e}$ is an arbitrary unit vector. As only neighbouring spins are included, the set of possibles values of $\vec{r}_{i,j}$ is

$$\vec{r}_{i,j} \in \{s\} \tag{2.9}$$

2.2.3. Kosterlitz–Thouless Transition

2.2.4. Vortices

Test

2.3. Numerical Methods

As stated in the introduction in chapter 1, the goal is to simulate the two dimensional XY model with periodic boundary conditions using the Metropolis-Hastings and the Wolff-Cluster algorithms. In the following section I will present the concepts needed for understanding and implementing the simulation.

2.3.1. Importance Sampling

2.3.2. Metropolis Algorithm

The overall procedure for the lattice is as follows:

1. Calculate E, M and Γ for the initial lattice configuration.

2. Perform a lattice sweep by iterating over all lattice sites. For every site i do:

   a) Propose a new angle $\theta_i \in [0, 2\pi)$ from a uniform distribution.

   b) Calculate $\Delta H = \Delta E$, ΔM and $\Delta\Gamma$ for the proposed new state.

   c) Accept or reject state with probability $P = \min\left(1, \exp\left(-\beta \Delta H\right)\right)$.

3. Update the observables $E \mathrel{+}= \Delta E$ and $M \mathrel{+}= \Delta M$ and add them to the result set.

4. Repeat from 2. for a total of N sweeps.

2.3.3. Wolff Cluster Algorithm

2.3.4. Bootstrapping

Since the Metropolis-Hastings algorithm scales with the number of lattice sites, it is computationally impractical to run the Metropolis-Hastings algorithm for long timescales. Given that we have an observable whose iid samples follow a Gaussian distribution and we already have "enough" iid samples which cover enough of the possible configuration space, we can then use bootstrapping to generate more samples (**?**).

1. Collect B intermediate means by repeating the following:

   a) Take A random samples from the blocked samples obtained in **??** with replacement.

   b) Calculate the mean of those samples and add the result to the set of intermediate means.

2. Calculate the final mean and the sample standard deviation of those B intermediate means.

A. Source Code

The program requires a *gcc*[1] or *Intel® oneAPI DPC++/C++ Compiler*[2] installation with support for *C++26*. The build process was tested with version 15.1.1 and 2025.0.4 respectivly. The source code for the simulation as well as the sources for this report can be obtained from GitHub:

> https://github.com/lennartvrg/physik690-Bachelorarbeit

As the progam makes use of submodules, it is necessary to clone with

> git clone --recurse-submodules [...]

to automatically initialize all submodules.

Dependencies   The program requires several third party libraries to compile. The following packages names are those used in the *Ubuntu launchpad*[3].

```
sudo apt-get install meson libpqxx-dev libsimde-dev
↪   libboost-all-dev libfftw3-dev libtomlplusplus-dev
↪   libflatbuffers-dev libsqlite3-dev libtbb-dev
```

The build process was tested with the versions available in *Ubuntu 25.04* on August 4, 2025. Build errors might occur when using older versions. In particular for `libpqxx-dev` at least version 7.10.x is required.

Building   First create a build directory in the repository root via `mkdir buildDir`. Then, the build files can be generated either for *gcc* via

```
CC=gcc CXX=g++ meson setup --reconfigure
↪   --buildtype=release buildDir/ .
```

or for the *Intel® oneAPI DPC++/C++ Compiler* via

```
CC=icx CXX=icpx meson setup --reconfigure
↪   --buildtype=release buildDir/ .
```

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[1] https://gcc.gnu.org/
[2] https://www.intel.com/content/www/us/en/developer/tools/oneapi/dpc-compiler.html
[3] https://launchpad.net/ubuntu

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