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

Lennart Voorgang

Bachelorarbeit in Physik
angefertigt am Institute for Advanced Simulation
des
Forschungszentrum Jülich

vorgelegt der
Mathematisch-Naturwissenschaftlichen Fakultät
der
Rheinischen Friedrich-Wilhelms-Universität
Bonn

August 2025

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

Bonn, ..... .....
Date Signature

1. Assessor: Prof. Dr. Stefan Krieg
2. Assessor: TBD

# Contents

# 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 $\mathbb{Z}_2$ symmetry is replaced by a continuous $U(2)$ symmetry.

### 2.2.1. Definition

The XY model describes the spins $\sigma_i$ 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 $\beta J$ 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.

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

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

**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

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

**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* $\Upsilon$ 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

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

(Teitel and Jayaprakash, 1983, eq. 3.2) 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 arbritrary unit vector. One may choose $\vec{e}$ such that it points in a row of the lattice to the right. Thus only neighbours within a row contribute as $\vec{r}_{ij} \cdot \vec{e} = 0$ otherwise.

### 2.2.3. Kosterlitz–Thouless Transition

Unlike the Ising model, the XY model does not feature a 2nd order phase transition of the usual kind "as the ground state is unstable against low-energy spin-wave excitations" (Kosterlitz and Thouless, 1973, p. 1190). It was shown by Kosterlitz and Thouless (1973) that instead there is something we now call the KT phase transition where below a critical temperature $T_C$ metastable states emerge.

#### Vortices

These metastable states "correspond to vortices which are closely bound in pairs" (Kosterlitz and Thouless, 1973, p. 1190). The vortex/antivortex pairs come closer together with decreasing temperature until they pair-annihilate.

## 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. Markov Chain

### 2.3.3. Metropolis Algorithm

The overall procedure for the lattice is as follows:

1. Calculate $E$, $M$ and $\Upsilon$ 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 $\Delta H = \Delta E$, $\Delta M$ and $\Delta\Upsilon$ for the proposed new state.
   c) Accept or reject state with probability $P = \min(1, \exp(-\beta\Delta H))$.
3. Update the observables $E \mathrel{+}= \Delta E$, $M \mathrel{+}= \Delta M$ and $\Upsilon \mathrel{+}= \Delta\Upsilon$ and add them to the result set.
4. Repeat from 2. for a total of $N$ sweeps.

### 2.3.4. Critical Slowing Down

While the Metropolis-Hastings algorithms works well for low and high temperatures it has its problems near the critical temperature.

### 2.3.5. Wolff Cluster Algorithm

As discussed in section 2.3.4 the Metropolis-Hastings algorithm suffers severe critical slowing down effects. In a desire to mititage such effect Swendsen and Wang (1987) introduced a multi-cluster Monte Carlo algorithm for the Potts spin models "giving a highly efficient method of simulation for large systems near criticality" (Swendsen and Wang (1987)).

Adjacent to the multi-cluster Swendson and Wang algorithm, the Wollf algorithm shows similar improvements with regards to the critical exponent while only utilizing a single cluster which makes implementations more straight forward.

The key insight is that the Ising spin-flip operation $\sigma_i \to -\sigma_i$ needs to be generalized to the $U(2)$ symmetry of the XY model. Wolff (1989) Defines the spin-flip as the reflectionalong the hyperplane orthogonal to an arbritarly choosen unit vector $\vec{r}$

$$R(\vec{r})\sigma_i = \sigma_i - 2(\sigma_i \cdot \vec{r})\vec{r} \tag{2.9}$$

which is an idempotent operation $R(\vec{r})^2 = 1$ (Wolff, 1989, eq. 3).

The overall procedure for the Wolff cluster algorithm was taken from (Wolff, 1989, p. 361) with the addition of item 2. This was done, as the probability of a site joining the lattice is lower for unordered states. These states emerge when the temperature is high and this the cluster size tends towards 1. This results in a very uneven distribution of potential updates (*marked* sites in the algorithm procedure). At low temperatures many sites get visited and potentionally updated while at high temperature as few as one site gets updated. To mitigate this, I introduce item 2 as an additional step which should ensure that even at high temperature a sufficient number of potential updates are made.

1. Calculate $E$, $M$ and $\Upsilon$ for the initial lattice configuration. Here the initial configuration is a cold state where $\sigma_i = 0$ for all sites $i$.
2. Perform the following until we marked $L^2$ lattice sites in total:
   a) Choose a random two dimensional unit vector $\vec{r}$ as the reflection vector.
   b) Pick a random lattice site $x$ as the first element of the cluster.
   c) Flip the spin at the initial lattice site $\sigma_x \to R(\vec{r})\sigma_x$ and mark site $x$.
   d) Visit all direct unmarked neighbours $y$ of $x$ and add them to the cluster with propbability

      $$P(\sigma_x, \sigma_y) = 1 - \exp(\min[0, 2\beta(\vec{r} \cdot \vec{\sigma_x})(\vec{r} \cdot \vec{\sigma_y})]) \tag{2.10}$$

      and calculate $\Delta E$, $\Delta M$ and $\Delta\Upsilon$ for the proposed new state.
   e) If site $y$ was accepeted into the cluster its spin is flipped $\sigma_y \to R(\vec{r})\sigma_y$.

f) Site $y$ becomes the new $x$ and continue from item 2d until there are no more sites to add to the cluster.

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

4. Continue from item 2 until the exit condition is fulfilled.

### 2.3.6. 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.

# 3. Implementation

## 3.1. General

## 3.2. Optimizations

## 3.3. Temperature Scanning

## 3.4. Distributed Computing

# 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 6, 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/ .
```

[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`

# List of Figures

# Bibliography

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