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

Lennart Voorgang

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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, ...
Date Signature

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

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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 emply random numbers to simulate a particular system.

The perhaps most well-known application of Monte Carlo methods is the Ising model. It describes the total magnetization of a lattice as the superposition of all spins $\sigma = \pm 1$ 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

2.2.1. Definition

The XY model describes spins 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 $\theta_i \in [0, 2\pi)$.

2.2.2. Observables

2.2.3. Kosterlitz–Thouless Transition

2.2.4. Vortices

Test

2.3. Numerical Methods

2.3.1. Metropolis Algorithm

The overall procedure for the lattice is as follows:

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

2.3.2. Wolff Cluster Algorithm

2.3.3. 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 *clang*[2] installation with support for *C++26*. The build process was tested on the development machine with *gcc 15.1.1* and *clang 20.1.8*. 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 nescarry to clone with

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

Dependencies The program makes use of several third party libraries which are also required to compile the program. The following packages names are those used in the *Ubuntu launchpad*[3]. Please note that some package versions are only available on the newest release *Ubuntu 25.04*.

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

[1] https://gcc.gnu.org/
[2] https://clang.llvm.org/
[3] https://launchpad.net/ubuntu

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