The XY-Model

David-Alexander Robinson Sch.[*]
08332461

17th January 2012

Contents

Abstract

The *XY-Model* was used to model the spin interactions of a system of 32×32 spin states as implemented with C++ coding. A *Markov Chain* of configuration states was used to find the equilibrium state as updated using the *Metropolis-Hastings Algorithm*.

Furthermore a `double` function was written to calculate both the real and imaginary parts of the *Magnetisation* of the field. *Monte Carlo* simulation was used to calculate the dependence of the expectation value of the square of the magnetisation, $< |M^2| >$, versus the Lagrange multiplier of the Canonical Ensemble, β, and a graph was plotted. It was seen that the system undergoes a Kosterlitz-Thouless transition at a *beta* value of 0.40 ± 0.05.

Finally the *Two-Point Correlation Functions* were calculated for seperations along the x-axis. The dependence of the correlation function C versus the seperation length d was found and again a graph was plotted, here using a logarithmic scale.

1 Introduction & Theory

1.1 The XY-Model

The *Classical XY-Model* is a statistical mechanical model of spin interactions which may be used to predict magnetic behaviour. For a two dimensional lattice $\mathscr{G}$ of side length N, the spin $\vec{\theta}$ may be given as a complex number of unit length where

$$\begin{aligned} \sigma_{\vec{x}} &= \exp(i\theta_{\vec{x}}) \\ &= \cos(\theta_{\vec{x}}) + i\sin(\theta_{\vec{x}}) \end{aligned} \tag{1}$$

The expectation value of an observable O is then

$$< O >= \frac{1}{Z} \int_{-\pi}^{\pi} \prod_{\vec{x} \in \mathscr{G}} d\theta_{\vec{x}}\, O(\theta) \exp(-\beta S(\theta)) \tag{2}$$

where Z is the *Zustandssumme*, or the *Partition Function*, given by

$$Z = \int_{-\pi}^{\pi} \prod_{\vec{x} \in \mathscr{G}} d\theta_{\vec{x}} \exp(-\beta S(\theta))$$

with

$$\beta = \frac{1}{k_B T}$$

Moreover, the action S is given by

$$\begin{aligned} S(\vec{\theta}) &= \sum_{\vec{x}} \sum_{\vec{y} \in n(\vec{x})} 1 - \Re\{\sigma_{\vec{x}} \cdot \sigma_{\vec{y}}\} \\ &= \sum_{\vec{x}} \sum_{\vec{y} \in n(\vec{x})} 1 - \cos(\theta_{\vec{x}} - \theta_{\vec{y}}) \end{aligned} \tag{3}$$

where here $\vec{y} \in n(\vec{x})$ is all $\vec{y}$ in the neighbourhood of $\vec{x}$.

1.2 Markov Chains

A *Markov Chain* is a system which undergoes transitions from one state to another in a random memoryless process. In this sense, the next state in the sequence depends only on the current state, and not on the sequence of states that came before it. A Markov chain may be used to create statistical mechanical models of processes, such as the alignment of spins in a magnetic system.

1.3 The Monte Carlo Method

The *Monte Carlo Method* is a algorithm to compute definite integrals based on random sampling. Here a state is generated randomly from the set of possible states, and the integral approximated. This process is then repeated for a large number of steps N, and the results summed. On completion of the sampling the result is renormalised with respect to the number of steps.

By taking a large number of steps the error in the expectation value of the integral is reduced by a factor of

$$\frac{1}{N}$$

1.4 The Metropolis-Hastings Algorithm

The *Metropolis-Hastings Algorithm* is a Markov chain Monte Carol method for choosing a sequence of random samples of states from a sequence of such states. The algorithm uses two steps, a proposal state, and an accept or reject step respectively.

On storing the current state of the system, $\psi = \psi_k$ a new state ψ' is generated for proposal. The probability of acceptance r is then calculated by

$$r = \min\left(1\,,\,\frac{P(\psi')}{P(\psi)}\right) \tag{4}$$

The proposed state is then accepted with probability r, or rejected in favour of keeping the current state with probability $1 - r$.

For the XY-Model the probability density is given by

$$P(\vec{\theta}) = \frac{1}{Z}\exp(-\beta S(\theta_{\vec{x}}))$$

and so the probability r becomes

$$r = \min(1\,,\,\exp[-\beta(S' - S)]\,) \tag{5}$$

where S' is the action of the proposed state ψ'.

1.5 Magnetisation

The magnetic properties of a material are determined by the spin configuration of the microscopic particles of which the material is made. For a simple model

$$M = \sum_{\vec{x}} \sigma_{\vec{x}} \tag{6}$$

or in terms of the real and imaginary components of the magnetisation

$$M = \sum_{\vec{x}} \cos(\theta_{\vec{x}}) + i \sum_{\vec{x}} \sin(\theta_{\vec{x}}) \tag{7}$$

Below a certain critical temperature, known as the *Curie Temperature*, or equivalently above a certain value of thermodynamic beta, a system of spins may align to exhibit *Ferromagnetism*. This transition from the highly disordered high temperature phase to the ordered low temperature phase is known as a *Kosterlitz-Thouless Transition*.

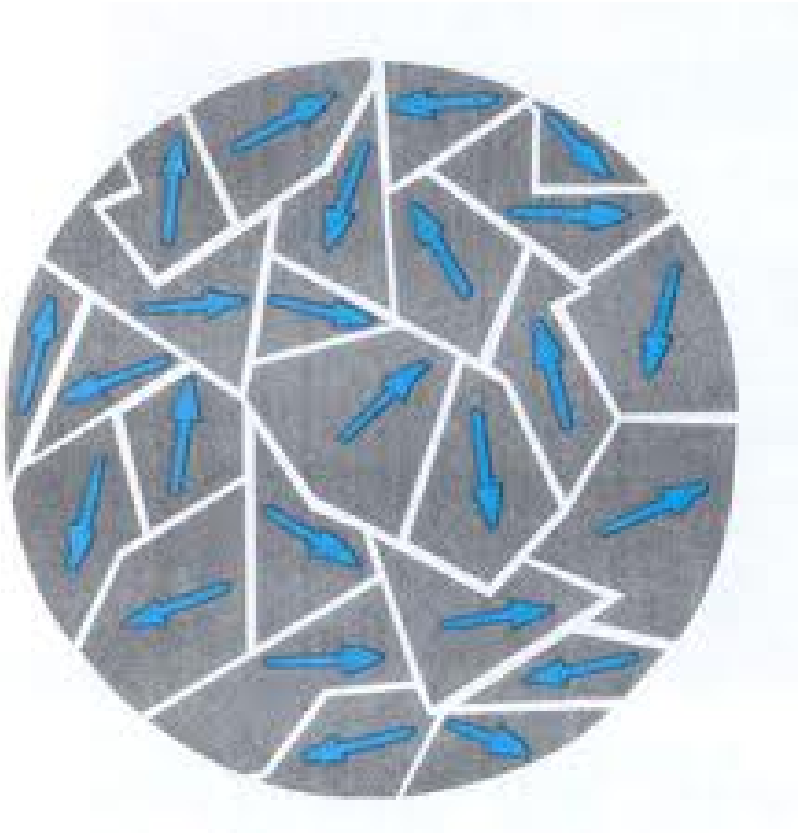

Figure 1: Ferromagnetic Domains

1.6 Correlation Functions

A *Correlation Function* is a measure of the order in a statistical mechanical system. In a system of spins the correlation function between two points describes how aligned or lack thereof these spins are. Here

$$C(d) = \sum_{\vec{x}} \cos(\theta_{\vec{x}} - \theta_{\vec{x}+d\,\vec{e_x}}) \tag{8}$$

where d is the separation and

$$\vec{e_x} = (1, 0)$$

is the unit vector in the x-direction. For a system of nearest neighbour interactions the correlation function is expected to drop off for large seperations.

2 Experimental Method

2.1 The XY-Model

A `class` was written called `one_one_tensor` to represent an n×n-matrix as an n×n-array such that objects declared in this class could be arguments of any new functions to be written, to hold the value of the complex spin $\sigma_{\vec{x}}$.

A `void` function `initial_data` was then written to assign a random value between $-\pi$ and π to the spin of each point by `for`-looping over all points `(i,j)` in in the lattice.

A function was also written to simulate a Markov chain of spin states, using the Metropolis-Hastings algorithm. To do this a `double` function `action` was written to calculate the action due to the interaction of a spin `(i,j)` with its nearest neighbours.

A new spin value was then proposed for the state `(i,j)`, and the action of the proposed spin configuration calculated. The Metropolis-Hastings algorithm was then used to accept or reject the proposed state.

The was repeated for all $(\mathtt{i}, \mathtt{j}) \in \mathscr{G}$, and iterated over the entire lattice for a large number of steps N, as per the Monte Carlo Method.

2.2 Magnetisation Calculations

The C++ code was edited to read the command `magnetisation` from the command line, so as to specify it to preform a calculation of the expectation value of the square of the magnetisation, $< |M^2| >$. To this end, a `double` function `magnetisation` was written to sum over all lattice sites $(\mathtt{i}, \mathtt{j}) \in \mathscr{G}$ where

$$< |M^2| >= \left[\sum_{\vec{x}} cos(\theta_{\vec{x}})\right]^2 + \left[\sum_{\vec{x}} \sin(\theta_{\vec{x}})\right]^2 \tag{9}$$

A `for` loop was then added to the `main` function to run the Markov chain of spin configuration states and calculate the magnetisation for a range of values of thermodynamic β. A graph of the expectation value of the square of the magnetisation versus thermodynamic β was then plotted.

2.3 Correlation Functions

A `double` function `correlation` was written to calculate the correlation function for the spin configuration state by `for`-looping over all lattice sites $(\mathtt{i}, \mathtt{j}) \in \mathscr{G}$.

A `for` loop was then added to the `main` function to calculate the correlation function for a range of values of lattice site separation d.

In addition, a `for` loop was added to sample the correlation function sereval times, and an average value was taken to reduce the errors in C, as per the Monte Carol method.

Finally a logscale graph of the resulting correlation functions C versus the lattice site spearation d was made.

3 Results & Analysis

3.1 The XY-Model

The code was found to converge on a final spin state corresponding to a minimum of the action function on running the Markov chain for a large number of iterations.

3.2 Magnetisation Calculations

The expectation value of the square of the magnetisation $< |M^2| >$ was calculated for a range of values of thermodynamic β and the following graph was plotted

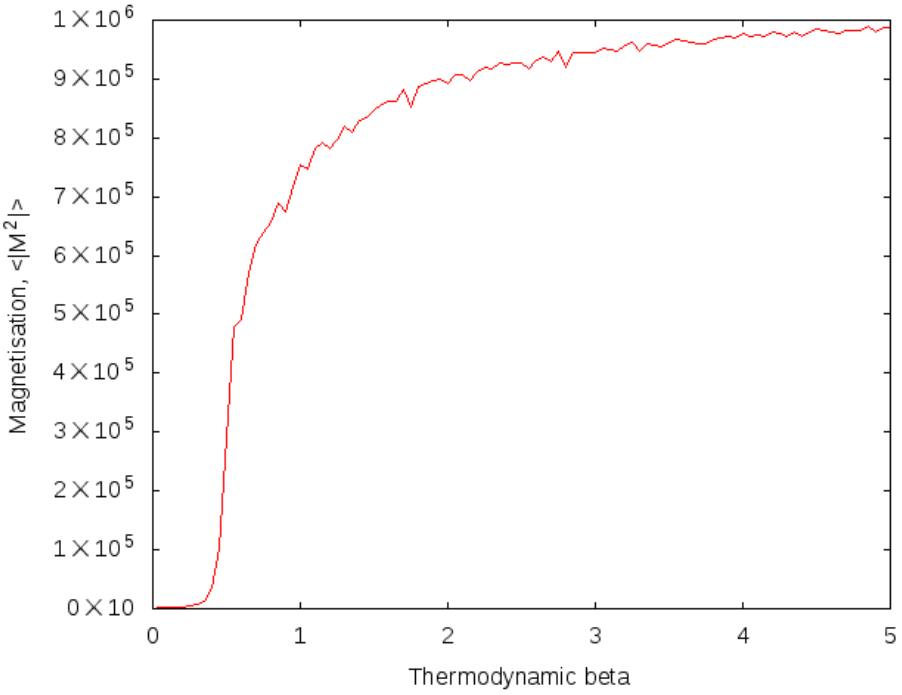

Figure 2: The Expectation Value of The Square of The Magnetisation Versus Thermodynamic β

3.3 Correlation Functions

The correlation function C was calculated for a range of values of lattice site separation d and the following logscale graph of the results was made

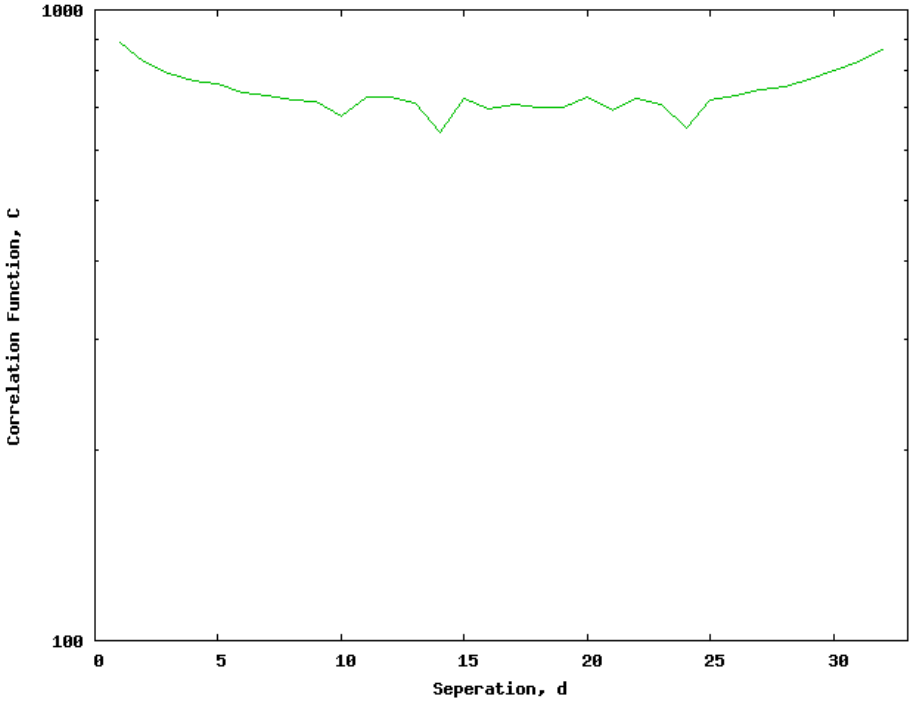

Figure 3: The Correlation Function versus the Seperation

4 Conclusions

It was found that the Metropolis-Hastings algorithm was able to be effectively used to generate a Markov chain of spin configuration states as implimented with the C++ programing code.

In addition, code could be written to calculate the expectation value of the square of the magnetisation for a range of values of thermodynamic β. It was found that the spin system underwent a Kosterlitz-Thouless transition at a *beta* value of 0.40 ± 0.05.

Finally, it was possible to calculate the correlation functions for a range of values of lattice site separation d. It was seen that the correlation function dropped off for increased separation, as was expected. Furthermore, it was found the the graph of the correlation function versus the lattice site separation was symmetric.