Studies of Phase Transitions in Magnetic Fields

Andreas Fagerheim*

Department of Physics, University of Oslo, Norway

November 19, 2019

Abstract

This article set forth to integrate a six-dimensional integral which is used to determine the ground state correlation energy between two electrons in a helium atom. The integral appears in many quantum mechanical applications. We will first solve the integral through a brute force manner using Gauss Quadrature (Gauss-Legendre) and Monte Carlo method. By changing coordinate frame and choosing a better suited probability distribution function (PDF) we implemented improved methods respectively Gauss-Laguerre and Monte Carlo with Importance Sampling. This article will show that by doing these implementations of improvement we can get better precision off our numerical methods for integration. All programs developed and used are available in the github link in the footnote.

I. Introduction

The aim of this project is to study a widely popular model to simulate phase transitions, the so-called Ising model in two dimensions. At a given critical temperature, this model exhbits a phase transition from a magnetic phase (a system with a finite magnetic moment) to a phase with zero magnetization. This is a so-called binary system where the objects at each lattice site can only take two values. These could be 0 and 1 or other values. Here we will use spins pointing up or down as the model for our system. But we could replace the spins with blue and green balls for example. The Ising model has been extremely popular, with applications spanning from studies of phase transitions to simulations in statistics. In one and two dimensions its has analytical solutions to several expectation values and it gives a qualitatively good underatanding of several types of phase transitions.

We will assume that we have a ferromagnetic ordering, viz $J > 0$. We will use periodic boundary conditions and the Metropolis algorithm only.

*https://github.com/AndreasFagerheim/Project-4

II. Theory

i. Ising Model

The total energy of the Ising Model can in the simplest form be expressed as

$$E = -J \sum_{<kl>}^{N} s_k s_l - B \sum_{k}^{N} s_k$$

with $s_k = \pm 1$. The quantity N represents the total number of spins and J is a coupling constant expressing the strength of the interaction between neighboring spins. The symbol $< kl >$ indicates that we sum over nearest neighbors only. B is an external magnetic field interacting with the magnetic moment set up by the spins [Hjorth-Jensen, 2015]. This article will look closer at the case of witch there is no interacting external magnetic field and the energy can the be expressed as:

$$E = -J \sum_{<kl>}^{N} s_k s_l \tag{1}$$

The expectation value, the mean energy, can be calculated given a probability distribution P_i as

$$\langle E \rangle = \sum_{i=1}^{M} E_i P_i(\beta) \tag{2}$$

hvor the probability distribution is given by the Boltzmann distribution

$$P_i(\beta) = \frac{e^{-\beta E_i}}{Z}$$

where $\beta = 1/k_b T$ is the inverse temperature, k_b is the Boltzmann constant, E_i is is the energy of a microstate i. The partition function is Z and is given for the canonical ensemble as a sum over all microstates, M;

$$Z = \sum_{i=1}^{M} e^{-\beta E_i}.$$

Further the the expectation values for magnetic moment $|M|$

$$\langle |M| \rangle = \sum_{i=1}^{M} M_i P_i(\beta). \tag{3}$$

The variance of E and $|M|$ is given receptively as

$$\sigma_E^2 = \langle E^2 \rangle - \langle E \rangle^2$$

$$\sigma_M^2 = \langle M^2 \rangle - \langle M \rangle^2$$

This lets us express the specific heat capacity constant volume as

$$C_v = \frac{1}{k_b T^2}(\langle E^2 \rangle - \langle E \rangle^2) \tag{4}$$

$$\chi = \frac{1}{k_b T}(\langle M^2 \rangle - \langle M \rangle^2) \tag{5}$$

ii. Analytic solutions for the Ising Model of 2x2 lattice

Looking closer at a 2x2 lattice to find analytical solutions which will serve as a bechmark for the method implemented later with T = 1. **Table 1** shows the different energies and magnetization states. Using the known states we can find analytical solutions:

$$Z = \sum_{i=1}^{M} e^{-\beta E_i} = 2e^{\beta 8J} + 2e^{-8\beta J} + 12e^0.$$

with $\beta = 1/kT$ and $T = 1$ with unit kT/J we get:

$$Z = 2e^8 + 2e^{-8} + 12e^0.$$

This gives us the energy

$$\langle E \rangle = \sum_{i=1}^{M} E_i P_i(\beta) = \frac{1}{Z}\sum_{i=1}^{M} E_i e^{-\beta E_i} \tag{6}$$

Table 1: *The different energy states of the 2x2 Ising Model*

No. of spins	Degeneracy	Energy	Magnetization
4	1	-8J	4
3	4	0	2
2	4	0	0
2	2	8J	0
1	4	0	-2
0	1	-8J	-4

Showing the different energy and magnetization for the two-dimensional Ising model with periodic boundary conditions.

$$\langle E \rangle = \frac{1}{Z}(-8e^8 + 8e^{-8} + 8e^{-8} - 8e^8) = -7.9839$$

$$\frac{\langle E \rangle}{N} = -1.99598$$

hvor $N = 4$. In the same way the magnetization turns out to be

$$\langle |M| \rangle = \frac{1}{Z}\sum_{i=1}^{M} M_i e^{E_i} = 3.9946 \tag{7}$$

$$\frac{\langle |M| \rangle}{N} = 0.9986$$

The heat capacity then becomes:

$$\langle E^2 \rangle = \frac{1}{Z}\sum_{i=1}^{M} E_i^2 e^{E_i} = \frac{128e^8 + 128e^{-8}}{5973.917} \tag{8}$$

$$\frac{C_V}{N} = \frac{\langle E^2 \rangle - \langle E \rangle^2}{4} = 0.12832 = 0.03208$$

The magnetic susceptibility can in the same way be calculated to $\frac{\chi}{N} = 0.00401$.

iii. Studies of phase transitions.

Near T_C we can characterize the behavior of many physical quantities by a power law behavior. As an example, for the Ising class of models, the mean magnetization is given by

$$\langle M(T) \rangle \sim (T - T_C)^{\beta},$$

where $\beta = 1/8$ is a so-called critical exponent. A similar relation applies to the heat capacity

$$C_V(T) \sim |T_C - T|^{\alpha},$$

and the susceptibility

$$\chi(T) \sim |T_C - T|^{\gamma}\,, \tag{9}$$

with $\alpha = 0$ and $\gamma = 7/4$. Another important quantity is the correlation length, which is expected to be of the order of the lattice spacing for $T >> T_C$. Because the spins become more and more correlated as T approaches T_C, the correlation length increases as we get closer to the critical temperature. The divergent behavior of ξ near T_C is

$$\xi(T) \sim |T_C - T|^{-\nu}\,. \tag{10}$$

A second-order phase transition is characterized by a correlation length which spans the whole system. Since we are always limited to a finite lattice, ξ will be proportional with the size of the lattice. Through so-called finite size scaling relations it is possible to relate the behavior at finite lattices with the results for an infinitely large lattice. The critical temperature scales then as

$$T_C(L) - T_C(L=\infty) = aL^{-1/\nu}, \tag{11}$$

with a a constant and ν defined in Eq. (10). We set $T = T_C$ and obtain a mean magnetisation

$$\langle \mathcal{M}(T) \rangle \sim (T - T_C)^{\beta} \rightarrow L^{-\beta/\nu}, \tag{12}$$

a heat capacity

$$C_V(T) \sim |T_C - T|^{-\gamma} \rightarrow L^{\alpha/\nu}, \tag{13}$$

and susceptibility

$$\chi(T) \sim |T_C - T|^{-\alpha} \rightarrow L^{\gamma/\nu}. \tag{14}$$

MC cycles	E/N	C_V/N	$\|M\|/N$	χ/N
Analytisk	-1.9959	0.03208	0.9986	0.00401
20000	-1.9951	0.03910	0.9983	0.005288
40000	-1.9966	0.02755	0.9988	0.003669
60000	-1.9966	0.02715	0.9988	0.003345
80000	-1.9964	0.02875	0.9987	0.003707
100000	-1.9966	0.02699	0.9989	0.003455

Table 2: *Comparison of the analytical values and the numerical values with increasing number of Monte Carlo cycles*

III. Methods

IV. Results

V. Conclusion

References

[Hjorth-Jensen, 2015] Hjort-Jensen, M. (2015). Computational Physics.

[Hjorth-Jensen] Hjort-Jensen, M. https://github.com/CompPhysics/ComputationalPhysics