Studies of Phase Transitions in Magnetic Fields

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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.

II. Theory

In its simplest form the energy of the Ising model is expressed as, without an externally applied magnetic field,

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

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. We will assume that we have a ferromagnetic ordering, viz $J > 0$. We will use periodic boundary conditions and the Metropolis algorithm only. The material on the Ising model can be found in chapter 13 of the lecture notes. The Metropolis algorithm is discussed in chapter 12.

i. 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

$$\chi(T) \sim |T_C - T|^{\gamma}, \tag{1}$$

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

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

$$\xi(T) \sim |T_C - T|^{-\nu}. \tag{2}$$

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

$$T_C(L) - T_C(L = \infty) = aL^{-1/\nu}, \tag{3}$$

with a a constant and ν defined in Eq. (2). We set $T = T_C$ and obtain a mean magnetisation

$$\langle \mathcal{M}(T) \rangle \sim (T - T_C)^{\beta} \to L^{-\beta/\nu}, \tag{4}$$

a heat capacity

$$C_V(T) \sim |T_C - T|^{-\gamma} \to L^{\alpha/\nu}, \tag{5}$$

and susceptibility

$$\chi(T) \sim |T_C - T|^{-\alpha} \to L^{\gamma/\nu}. \tag{6}$$

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