Two Dimensional Ising Model

Using Metropolis Algorithm

Abdallah Sayyed-Ahmad
Birzeit University, Department of Physics
e-mail address: asayyeda@birzeit.edu

Large classical systems have so many degrees of freedom. An exact description of positions and velocities of every molecule is completely intractable. For example, it is totally impractical and not useful to know the exact micro-state (positions and momenta of all molecules) of a large volume of gas. A statistical approach works very well, since the number of degrees of freedom is extremely large. In this project we will study the Ising model of a lattice as a simple model of real physical systems. It is also relevant to a variety of other systems linked by the theory of critical phenomena and phase transitions, e.g. thermodynamics. The existence of Analytic solutions for some simple cases is very useful for checking the accuracy of numerical techniques used. We will use Monte Carlo methods to calculate some of the thermodynamic properties of this system.

I. INTRODUCTION

The Ising Model[1-3] is a simple and crude description of a magnetic material consists of spin degrees of freedom interacting with each other and with an external magnetic field. As a special case, we will deal with two-dimensional lattice of spin variables ($Nx \times Ny$). The spin can be labeled as S_{ij}, where i,j are the indices of the two spatial directions, or in general as Sα, where α is a generic site label. Each of these spin variables can be either "up" ($S_\alpha = +1$) or down ($S_\alpha = -1$). If we take spins as classical degrees of freedom, the Hamiltonian of the system is

$$H = -J \sum_{\langle \alpha\beta \rangle} S_\alpha S_\beta - B \sum_\alpha S_\alpha$$

The notation $\langle \alpha\beta \rangle$ means that the sum is over the nearest neighbor pairs of spins. The coefficient J determines the strength of spin-spin interaction. Periodic boundary conditions are assumed on the lattice. For example, the lower neighbors of the spins with $i = N_x$ are those with $i = 1$. This means the lattice wraps around on itself to form a torus which has been shown to give the smallest finite size effects.

The partition function of the canonical ensemble of the spins is

$$Z(J,B) = \sum_S e^{-H(S)}$$

And the probability of each spin configuration is

$$w(S) = \frac{e^{-H(S)}}{\sum_S e^{-H(S)}}$$

In this project, we will consider the following thermodynamic properties:

1) The Magnetization: Unpaired electron spins couple and align. The sum of their magnetic fields gives rise to macroscopic magnetism.

$$M = \frac{\partial \ln Z}{\partial B} = \sum_S \left(w(S) \sum_\alpha S_\alpha \right)$$

2) The Magnetic Susceptibility :

$$\chi = \frac{\partial M}{\partial B} = \sum_S w(S) \left(\sum_\alpha S_\alpha \right)^2 - M^2$$

3) The Energy:

$$E = \sum_S w(S) H(S)$$

4) The specific heat:

$$C_B = \sum_S w(S) H^2(S) - E^2$$

II. COMPUTATIONAL METHODS

To calculate sums (or integrals, if the spins are continuous-valued) over such a large number of degrees of freedom, we resort to Monte Carlo techniques. With the Monte Carlo integration, we could just generate configurations at random, and approximate the real thermal averages by Monte Carlo averages. The problem here is that because of the rapidly varying exponential function in the Boltzmann distribution, most randomly chosen configurations will

make a negligible contribution to the sums due to their relatively large Hamiltonian values.

In order to get sensible, accurate results when simulating statistical systems with a rapidly varying distribution, it is vital to use the idea of importance sampling in Monte Carlo integration[4]. Clearly the ideal situation would be to sample configurations with a probability given by their weight $w(S)$. To do so we will use Metropolis algorithm. The Metropolis algorithm does not specify how the changes to the configuration should be made. It just says that any proposed change to the system should be accepted with a certain probability that depends on the change in energy.

For the Ising Model, the change in the configuration is to try to update or flip a spin. However, if too many spins changed at time, the energy difference between the two consecutive configurations will be relatively large. This means the probability of accepting the change will be small. To avoid this, we need to update one spin at a time. In this case the update is local and the energy difference between the two configurations will depend only on the updated spin and its neighbors. The acceptance probability is given by

$$r = e^{-2S_\alpha(Jf+B)}$$

Where

$$f = S_{i+1j} + S_{i-1j} + S_{ij} + S_{ij-1}$$

III. RESULTS AND DISCUSSION

Test Case:

Useful theoretical results exist for the Ising model with spins interaction coupling constant $J = 0$[5]. The system can be considered as a $N = (Nx \times Ny)$ independent distinguishable spins. It is easy to show that

$$Z = (e^B + e^{-B})^N$$
$$E = -BN \tanh B$$
$$M = N \tanh B$$
$$\chi = N(1 - \tanh B)$$
$$C_B = B^2(\chi + M^2) - E^2$$

For this case, we carried out a simulation using our code using the following parameters

N_x=16
N_y=16
J=0
B=0,…,1 in steps of 0.01
Ngroup=10
Size=5
Freq=5
Therm=10

The thermodynamic variables values from the simulation are comparable to the exact solution, However the fluctuation were very large in calculation the susceptibility, and the specific heat.

Test Case 2:

When studying any macroscopic system with a very large number of degrees of freedom, invariably make an approximation and simulate a smaller and/or discretized model system. This introduces systematic errors called finite size effects. For spin models, we have a finite d-dimensional lattice of sites. But only get a true phase transition (i.e., divergence) when the size of the lattice goes to infinity. However, for a finite system, we get rounded peaks rather than divergences. The peaks narrow and increase in height as the dimensions are increased, and the location of the peak shifts slightly. Many problems require an empirical extrapolation to an infinite system. For infinite lattice, and when the external magnetic field is zero. An exact expression for the thermodynamic variables exists.

We run the code using

N_x=64
N_y=64
J=0,..,0.6 in steps of 0.01
B=0
Ngroup=10
Size=5
Freq=5
Therm=10

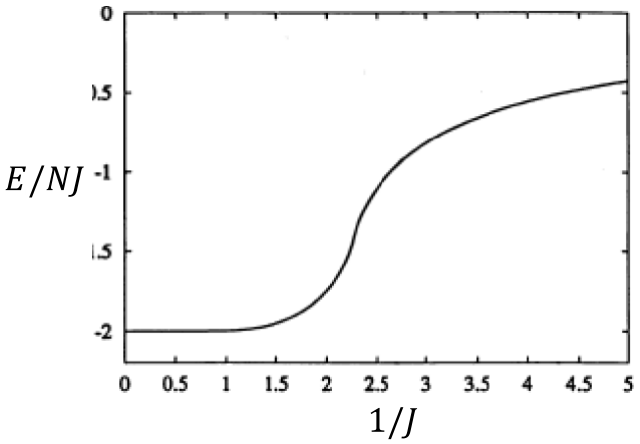

Figure. 1: Internal Energy per lattice point for the 2D ising model as a function of 1/J.

The energy values agreed with the infinite lattice solution as seen in Figure 1. For the magnetization, and specific heat it is clear that we have a phase transition around $J = 0.4406$ (see Figure 2) . However, to understand these, and be able to extrapolate to an infinite system, we need to do a number of simulations at different system sizes.

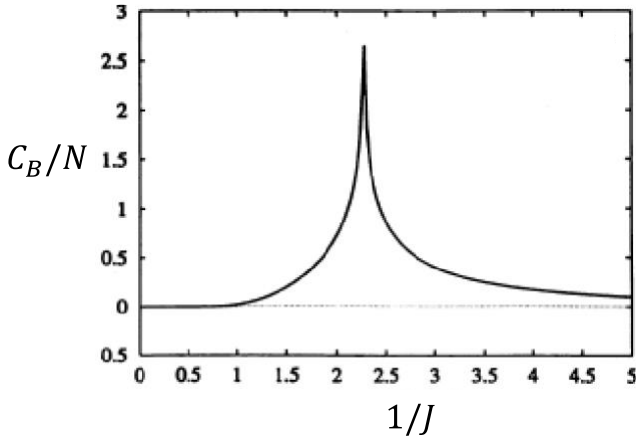

Figure. 2: Specific heat of the system as function of 1/J.

IV. REFERENCES

1) Chamberlin, R.V. Mean-field model for the critical behaviour of ferromagnets. Nature 408, 337-339 (2000).
2) Peryard, M. Melting the double helix, Nature Phys 2, 13-14 (2006). 3.
3) Onsager, L. Crystal Statistics. I. A Two-Dimensional Model with an OrderDisorder Transition. Phys.Rev 65,117-149 (1944).
4) Newman, M.E.J & Barkema, G.T., Monte Carlo Methods in Statistical Physics (Oxford University Press, 1998).
5) Pathria, R.K., Statistical mechanics. (Pergamon, 1972).

V. APPENDICES

Individual Contributions
ASA designed the project and implemented the computational code; A.S.A. performed simulations and analysis; A.S.A. wrote and critically reviewed the report.

Machine Details
Desktop computer with intel i7 9700k CPU and 16GB of DDR4 3200GHz RAM and Samsung 870 QVO SATA III 2.5" SSD 1TB

Files

- montecarlo.m: perform montecarlo simulation on 2D grid and report the results for a range of coupling constants.
- obserrvables.m: compute the various thermodynamics properties
- infinite_lattice.m: compute the asymptotic results for an infinite lattice.
- Independent_spins.m : solve the problem in the limiting case where the coupling constant is zero

Log Book

* 10/12/2020
-> design project
Team met for 3 hours.
Total hrs = 3 * 3 = 9 hrs.

* 10/15/2020
-> montecarlo.m, independent_spins.m
Team met for 3 hours. 1.5 hrs design, 1.5 hr coding and testing.
Total hrs = 3 * 3 = 9 hrs.

* 10/19/2020
-> infinite_lattic.m, independent_spins
Team met for 2 hours. 2 hr testing.
Total hrs = 2 * 3 = 6 hrs.

* 10/26/2020
-> Comparing results, writing report and finalizing results
Team met for 2 hours.
Total hrs = 2 * 3 = 6 hrs.

Total Hrs = 30 hrs.