Monte-Carlo Simulation of the 2D Ising Model

Final project for Computer Fundamentals and Computational Physics
(PHY415)

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Contents

This model was suggested to Ising by his thesis adviser, Lenz. Ising solved the one-dimensional model, an easy task , and on the basis of the fact that the one-dimensional model had no phase transition, he asserted there was no phase transition in any dimension. As we shall see, this is false. It is ironic that on the basis of an elementary calculation and erroneous conclusion, Ising's name has become among the most commonly mentioned in the theoretical physics literature. But history has had its revenge. Ising's name, which is correctly pronounced "E-zing," is almost universally mispronounced as "I-zing"!

Barry Simon[1]

1 Introduction

1.1 Ising model

The Ising Model is a mathematical model which attempts to simulate a domain in a ferromagnetic substance. [2] It consists of an array of N fixed points called lattice points which form an n-dimensional periodic lattice. Associated with each lattice site is a spin variable s_i which can take the values +1 or −1. The energy of the system for the given configuration $\{s_i\}$ is given by

$$E\{s_i\} = -\sum_{<ij>} \epsilon_{ij} s_i s_j - H(t) \sum_{i=1}^{N} s_i \tag{1}$$

$< ij >$ represents the sum over all it's nearest neighbours. For simplicity, we consider isotropic interactions so that all ϵ_{ij} is equal to a given number ϵ. The thermodynamic properties for a $2D$, square lattice in a zero field was worked out by Lars Onsager in 1944.[2]. To perform our simulation we will use the Metropolis algorithm.

1.2 Metropolis algorithm

In this method, configurations are generated from a previous state using a transition probability which depends on the energy difference between initial and final states. [3]. The algorithm proceeds as follows

1. An initial state is picked.

2. An lattice point is chosen at random.

3. The spin is flipped at that random point and the change in energy ΔE is calculated.

4. If ΔE is less than 0 then the change is kept, otherwise, a random number r is chosen such that $0 < r < 1$

5. If, $r < e^{-\frac{\Delta E}{k_B T}}$, the spin change is kept else it is reversed.

6. Another lattice point is picked and the above steps repeated.

After a set number of states are considered, the thermodynamic properties are evaluated and they are added to the statistical average being kept. The standard measure of time is the Monte Carlo Steps per site.

1.3 Expected results

The observables we will be looking at in the absence of external field are the average energy, magnetisation, specific heat and susceptibility.

1.3.1 Onsager's solution for zero field

The exact solutions obtained by Onsager contain very involved mathematical manipulations and due to their inapplicability in other situations they are mainly of historical interest. [4] Here we present only a summary of the results to compare with the results of our numerical simulations. The full solution can be found in [2].

The critical temperature [1] is given by $\frac{k_B T_c}{J} = \frac{2}{1+\sqrt{2}}$, where we set the energy scale using $k_B = 1$ and for $J = 1$ we obtain $T_c \approx 2.269$. The exact solution for the energy is given by

$$E = -2NJtanh(2\beta J) - NJ\frac{sinh2\beta J - 1}{sinh(2\beta J)cosh(2\beta J)}[\frac{2}{\pi}K_1(\kappa) - 1]$$

where $K_1(\kappa)$ is the complete elliptic integral of the first kind. The specific heat can similarly be obtained in terms of the complete elliptic integral of

[1] Rather than going through the full Onsager solution, the critical temperature can be estimated by simpler physical arguments. See [5]

the second kind by differentiating E with respect to temperature. The magnetisation and zero-field susceptibility were calculated by Yang in 1952. The most important features thus is that the energy is a continuous function of temperature, the specific heat diverges logarithmically at $T = T_c$, the magnetisation drops to 0 at $T = T_c$ and the susceptibility diverges as a power law at $T = T_c$.

1.3.2 In the presence of a time dependent magnetic field

The properties of the ising model in the presence of a time varying magnetic field were first worked out in [6]. We summarise here the required results.
Dependence of the hysterisis loop on omega: In the limit $\Omega \to 0$, the hysterisis loop becomes a discontinuity about $H = 0$ and then evolves by stretching out into the familiar loop and in the limit $\Omega \to \infty$ it becomes a straight line, independent of the applied magnetic field.
Dependence of the hysterisis loop on amplitude: An analysis of the monte carlo data shows that the hysterisis loop does not depend on amplitude individually but on a ratio of the frequency of amplitude and frequency.
Dependence of the hysterisis loop on Temperature: The loop shrinks as temperature increases.

2 Numerical results

2.1 Zero field results

The metropolis algorithm described in 1.2 was used to simulate the behaviour of the ising model. The energy average was calculated by keeping the average after every Monte Carlo Step (one Monte-Carlo step (MCS) consists of a single sweep of $N \times N$ points on the lattice. Since the lattice points are chosen randomly in our programme, some lattice points may be swept multiple times and some none at all in one 'sweep.') and the magnetisation is simply the sum of the spins.

The specific heat and susceptibility are calculated using the formulas

$$C = \frac{\langle E^2 \rangle - \langle E \rangle^2}{k_B T^2} \qquad \chi = \frac{\langle M^2 \rangle - \langle M \rangle^2}{k_B T}$$

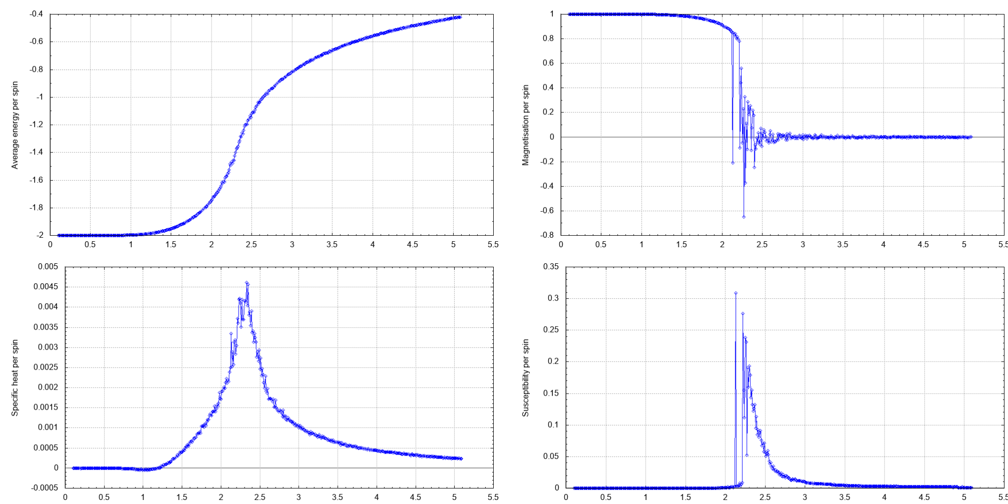

Figure 1: *Simulated results for the thermodynamics properties of the 2D ising model. The various observables are plotted against temperature T in units of* J/K_B*. The values are calculated after 6000 MCS for a* 20×20 *lattice in the absence of a mganetic field.*

The obtained numerical results are plooted in Figure 1 accordance with expected graphs described in section 1.3.1. The specific heat and susceptibility expectedly diverge at around $T \approx 2.3$.

2.2 Time dependent magnetic field

Once equilibrium has been attained, we turned on a time-varying magnetic field H. The magnetic field was constructed by using the sinusoidal function $H(t) = H_0 sin(\Omega t)$. The values for integral t where taken for one-period $\frac{2\pi}{\Omega}$ and then repeated cycles of the hysterisis loop were performed for the system at constant temperature. Since the period is much smaller than the period for the random number generator (for gfortran it is $2^{256} - 1$), the loops will differ through each cycle. Thus, we have plotted an average Hysteresis curve.

2.2.1 Dependence of the hysterisis loop on omega

The hysterisis loop becomes larger as omega increases and ultimately it's axis tilts and it ceases to represent a loop. A way to reach either infinity or

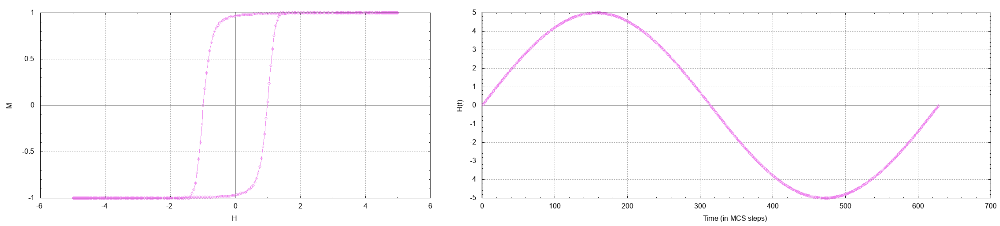

Figure 2: *A typical Hysterisis loop for a* 20×20 *lattice under the action of a sinusoidal magnetic field with* $H_0 = 5$ *and* $\Omega = 0.01$.*The loop is averaged over 955 cyles.*

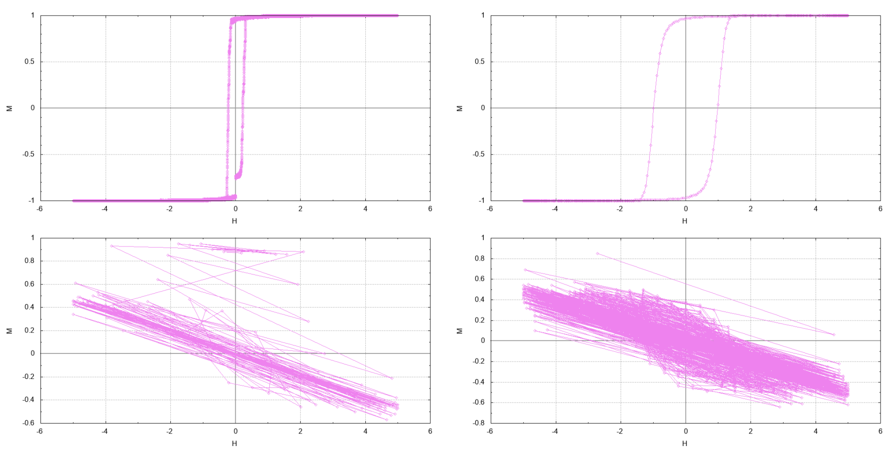

Figure 3: *Hysterisis loops for Omega = 0.0001, 0.01, 10 and 10000000 respectively (clockwise from top left).*

0 could not be found using the sinusoidal magnetic field. It is easier Using a constructed periodic magnetic field as in [6].

2.2.2 Dependence of the hysterisis loop on amplitude

It appears that as H_0 increases, the hysterisis curve goes in the opposite direction to omega i.e. it shrinks for large H_0 and titls for small H_0.

2.2.3 Dependence of the hysterisis loop on Temperature

Quite expectedly the loop shrinks with increase in temperature.

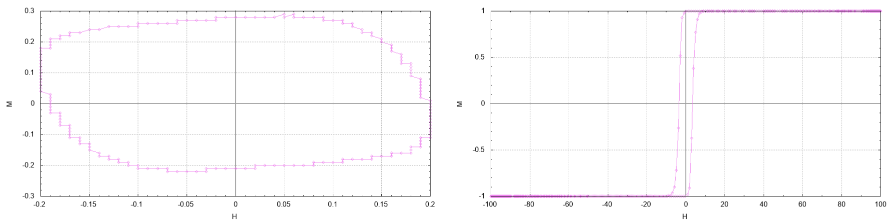

Figure 4: *Hysterisis loops for* $H_0 = 0.2$ *and* $H_0 = 100$.

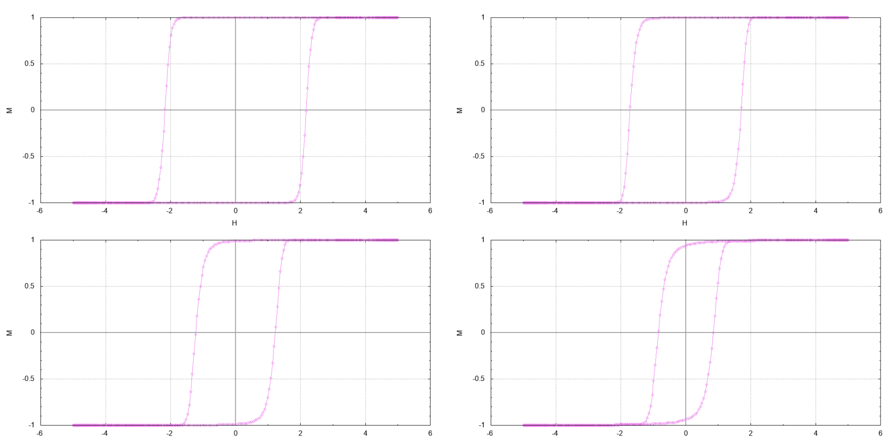

Figure 5: *Hysteresis loops at four different temperatures,* T = *0.6, 1.0, 1.5 and 2.0 respectively (clockwise from top left.)*

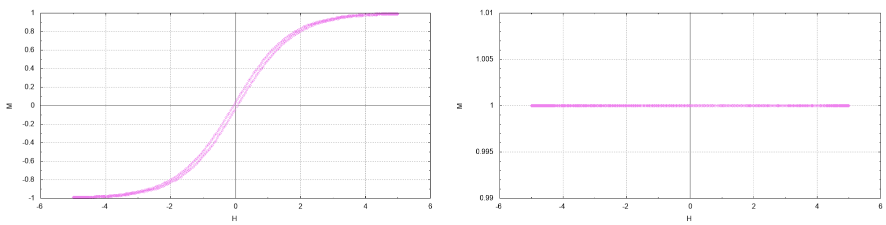

Figure 6: *Hysteresis loops for J = 0.02 and J = 1000 respectively.*

2.2.4 Dependence of the hysterisis loop on interaction energy

For small J_F the loop to the magnetic field almost taking the form of the sinusoidal field. This is because for small J_F the second term n the energy, corresponding to the non-zero magnetic field dominates. For large J_F similarly the loop does not respond to the magnetic field at all as the first term in the energy dominates.

3 Conclusions

Here I have investigated the properties of the hysterisis loop formed by a two dimension ising model under the action of a sinusoidal external field. The same thing has been done before using a constructed periodic magnetic field in [6]. Their analysis is much better because their hand constructed field allows the taking the limit $\Omega \to 0$ and $\Omega \to \infty$. Their analysis is also more complete because they've calculated the error bars for the hysterisis graphs as well taken more data points. Due to machine limitations ,I have been unable to consider lattices larger than 20×20. As pointed out in their paper, a larger lattice gives more accurate results. Nevertheless, their conclusions abut the 2D ising model has mostly been replicated here.

4 Acknowledgements

I'd like to thank my course instructors for this course, Dr. Sanjoy Biswas and Dr. Abhijeet Bhattachary for giving me the opportunity to work in this project. I'd also like to acknowledge the university library collection which allowed me to consult several relevant books.

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