Monte Carlo study of a 2D Ising lattice

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Abstract

A ferromagnetic Ising lattice has been studied on a computer using a Monte Carlo simulation. The critical temperature, specific heat, magnetic susceptibility and pair correlation have been investigated. The results are analyzed and plotted. The results agree with the theoretical expectations.

I. Introduction

We know that the expactation value of a thermodynamic quantity can be calculated as follows:

$$\langle A \rangle = \frac{\sum_r A_i exp^{-\beta E_r}}{\sum_r exp^{-\beta E_r}} \quad (1)$$

This might be possible for a small system but becomes very impractical for larger systems. A 20x20 spin lattice for instace, has already 2**400 of states.

Instead of sampling all states and weighing them by their Boltzman factor it makes sense to sample states based on their Boltzman factor, weighing them equally. This is what is done in the Metropolis algorithm, an *importance sampling* method also known as a Monte Carlo method.

II. Theory

Mention some theory, what can we expect? Theory surrounding measured quantities. What is expected of the critical temperature and why?

What is expected of the magnetic susceptibility and why? An external magnetic field has to work against the preferred spin of the lattice and against temperature. Much below the critical temperature the preferred spin direction makes the lattice insusceptible to an external magnetic field. Much above the critical temperature the temperature prevents a build up of magnetization. Thus the maximum magnetic susceptibility is expected around the critical temperature.

Detailed Balance. Fluctuation Dissipation Theorem.

III. Method of computation

What is a Monte Carlo method, Markov chain, metropolis, critical slowdown around the cirtical point. Need for Wolff

I. Wolff algorithm

To avoid critical slowdown, we made use of the Wolff algorithm. The Wolff algorithm differs mainly from the Metropolis algorithm in the method of growing clusters. Instead of randomly picking a new position each step, the Wolff algorithm tries to grow a cluster with its neighbours. This is done as follows, first a random position is selected and flipped, we call this position the base position. Secondly, a neighbour with the same spin as the original value of the base position is flipped with probability $P = 1 - exp^{-2\beta J}$. As ususal, $\beta = \frac{1}{K_b T}$ and J is the coupling constant in the Ising hamiltonian. Neighbours with opposite spin are never flipped. Thirdly, if the neighbour is flipped, the neighbour position now becomes the new

*Para enviar comentario y sugerencias sobre ésta investigación

base position, and one follows the procedure as described in the second step again. If the neighbour was not flipped, the base position remains the original value and one proceeds with step two again but now with another neighbour. This is programmed recursively, a simple example of this is given in [**?**]. After a number of steps, the cluster has reached its final size, which is highly dependent on the temperature. When the final size is reached, that is when the algorithm is back on the first base position and has visited all neighbours, a new random position is selected and the whole procedure starts over again.
In order to avoid flipping back to the former spin value of created clusters, a boolean matrix with the same length and width as the lattice is introduced, which we call 'blacklist'. Before the cluster creation starts, all positions on the blacklist are 'True'. When a position is flipped, it's position on the blacklist becomes 'False'. When selecting a neighbour to be flipped in step two, only neighbours that are 'True' may be considered. Lastly, in order to let the system find an equilibrium magnetization for a certain temperature and external magnetic field, the procedure of selecting a new random position and growing a cluster must be performed many times. The number of times is controlled by 'Niter' in our script.
In order to measure observables, information about the total magnetization m and the energy E is needed. The total magnetization is simply obtained by summing all spins of the lattice after equilibruim has been reached. The total energy is obtained according to **??**.

$$E = -J \sum_{<ij>} \sigma_i \sigma_j - h \sum_j \sigma_j \tag{2}$$

To find critical temperature, magnetic susceptibility and heat capacity, one wants to observe how the magnetization and energy vary with varying temperature. Changing the temperature in the same lattice is done as follows, all spins are aligned and the temperature is set far below the theoretical critical temperature. The Wolff algorithm is applied and a equilibrium lattice configuration is found. Afterwards, the whole lattice is flipped and the temperature is raised a little bit. The Wolff algorithm is applied again, resulting in a new equilibrium lattice configuration. This procedure is repeated for a temperature range starting below the critical temperature to one above the critical temperature. We took $K_b = 1, J = 1$ So that the theoretical critical temperature should be $T_c = 2.2727$.

IV. Results

I. Critical Temperature

According to the theory, we expect the following exponential behaviour around the critical temperature 3.

$$m \sim (-T_c + T)^{\beta}; T < T_c \tag{3}$$

Where $\beta = \frac{1}{8}$. For 200 steps in temperature between $1.3 < T < 2.7$ and averaged over 100 runs, for a $100x100$ sized lattice, the following plot 1 could be made.

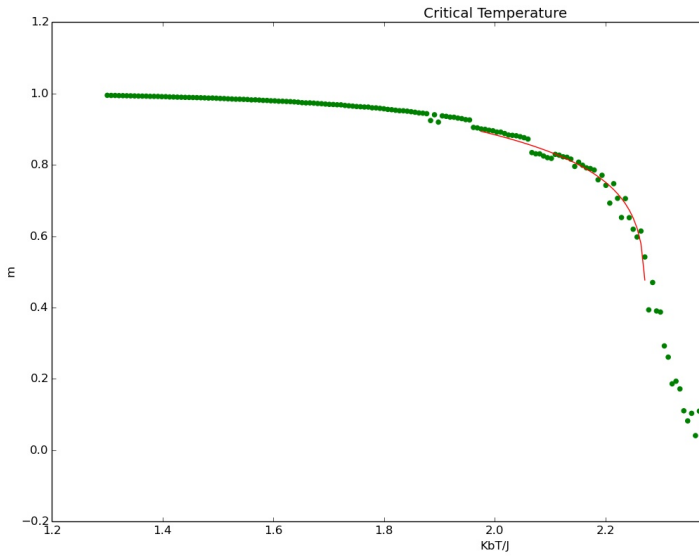

Figure 1: *Critical temperature, red line is fit for β.*

It is clear that close to the critical temperature, the magnetization starts to drop rapidly.

The exponential behaviour compares very well tot the theoretical value close to the critical temperature.

II. Magnetic Susceptibility

The magnetic susceptibility can be found easily by making use of the fluctuation dissipation theorem. For a lattice of $100x100$, 200 Temperature steps between $1.3 < T < 4.7$ and averaged over 20 runs, the following plot is made.

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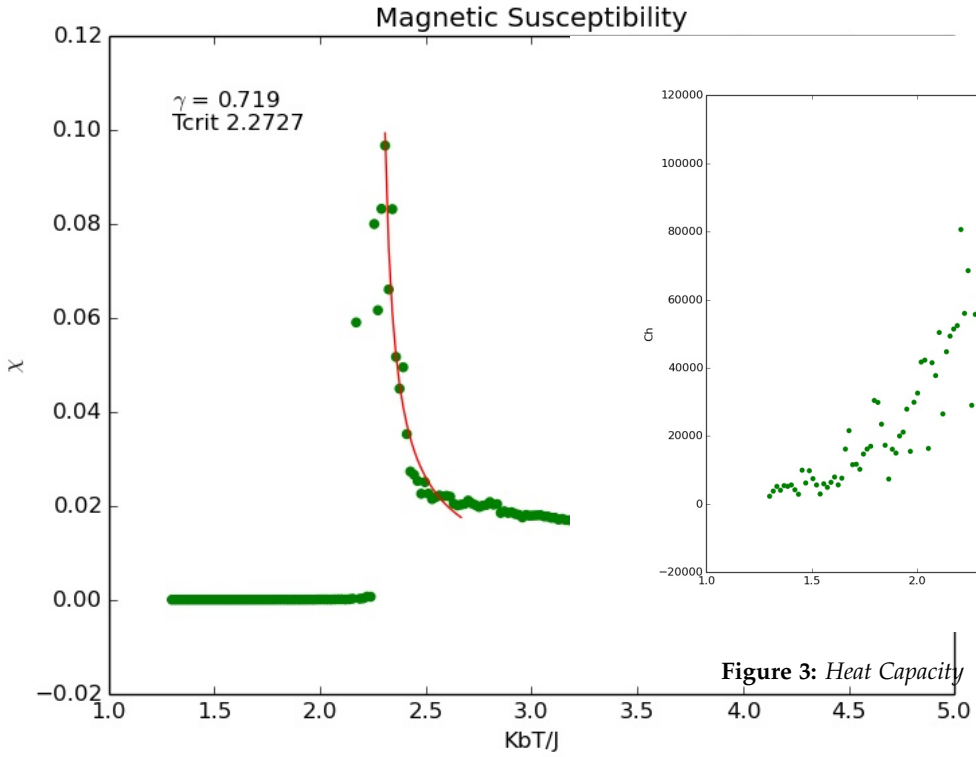

Figure 2: *Magnetic Susceptibility, red line is fit for γ.*

Theoretically we expect the following exponential behaviour close to the critical point 4.

$$m \sim |T - T_c|^{-\gamma} \tag{4}$$

The theoretical value of $\gamma = \frac{7}{4}$. We observe that for temperatures just below the critical point, the magnetic susceptibility has a very steep increase, however it was not possible to fit the exponential behaviour there. For temperatures just above the critical temperature, the critical behaviour could be fitted. The results vary significantly from the theoretical value.

III. Heat Capacity

The heat capacity was also found by making use of the fluctuation dissipation theorem. For a lattice of $100x100$, 200 Temperature steps between $1.3 < T < 4.7$ and averaged over 20 runs, the following plot is made.

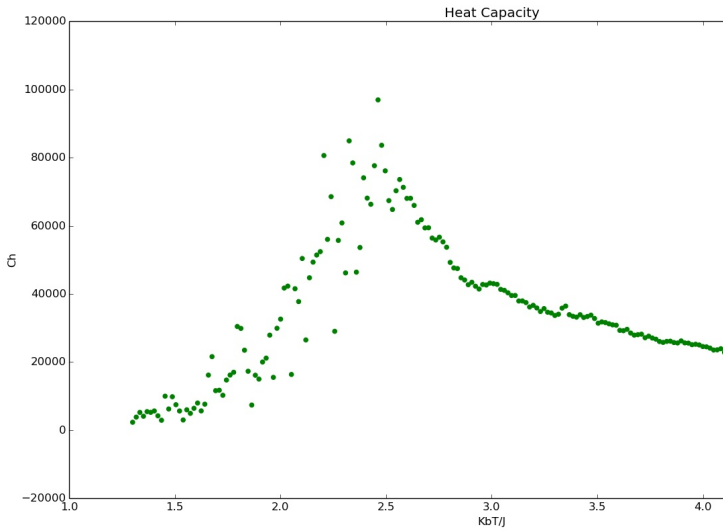

Figure 3: *Heat Capacity*

Because of the spread of the datapoint close to the critical point it was not possible to obtain a reasonable fit. According to the theory, the critical behaviour around the critical temperature for the heat capactity can be described by 5.

$$m \sim |T - T_c|^{-\alpha} \tag{5}$$

Where $\alpha = 0$. The latter suggests that we do not expect a sharp peak close to the critical point, which is in agreement with the figure.

IV. magnetisation with varying small magnetic field at the critical temperature

To find the magnetisation with varying small magnetic field at the critical temperature 'MVMF', we have a fixed temperature, but a varying external magnetic field. To find this parameter, the same method as for the other observables is utilized, where the varying temperature is replaced by a varying external magnetic field.
According to the theory, the critical behaviour is as follows 6

$$m \sim h^{\frac{1}{\delta}} \tag{6}$$

Where h is the external magnetic field. The theoretical value of $\delta = 15$. The following plot is made for $100x100$ lattice, the difference between the graphs lies in the number of steps between the smallest and biggest value of h. Information on the latter is summarized in the following table **??**

var comp Niter.jpeg

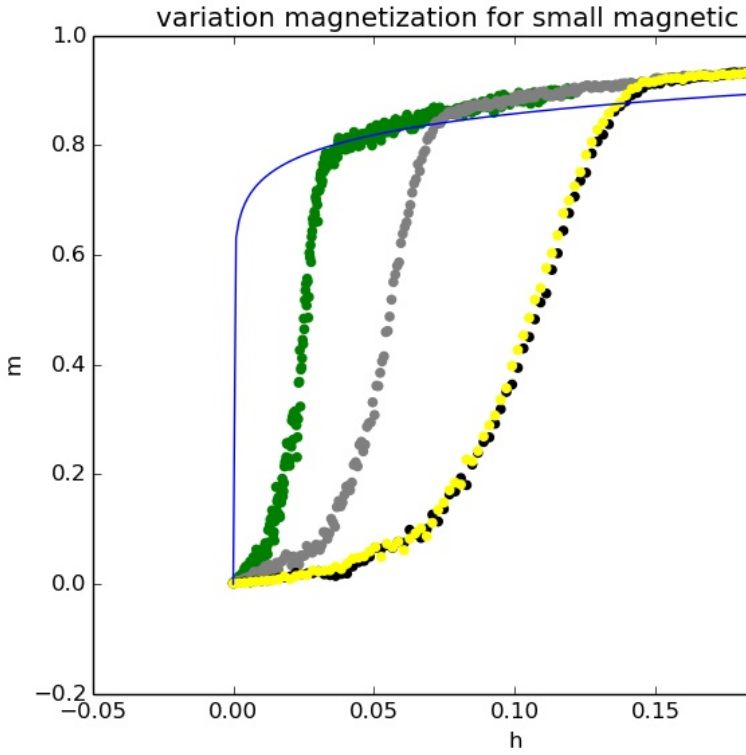

Figure 4: *MVMF for different plot parameters, blue line is theoretical*

From figure 4 it becomes clear that mainly the number of steps has a great influence on the MVMF. The figure suggests that if the number of steps goes to infinity, the theoretical value will be approached. For reasons of calculation time this was not tested. Another fact that can be obtained from the difference between the black and the yellow graph is that increasing *Niter* - that is, giving the system more time to find its equilibrium setup - does hardly influence the magnetization. This suggests that the system is to a good approximation in a equilibrium configuration for $Niter = 300$.

V. Discussion and Conclusion

What we think of the results.

Colour	*Niter*	minimum h	maximum h	steps
green	500	0	1.2	600
grey	300	0	2	300
yellow	1000	0	2	100
black	300	0	2	100

Table 1: *Information on plot parametersfor MVMF plot.*

References

[http://fluidos.eia.edu.co/] *Fluidos, Carlos Toro s.*

[http://www.windows2universe.org/] *Becca Hatheway*

[http://meteorologia.pucp.edu.pe/] *Hernan Castillo, Pedro Ríos*

[http://www.ammonit.com/Manuales] *Ammonit Measurement GmbH*

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