Metastability and the Ising model

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Abstract

The way the magnetisation for an Ising model of interacting spins changes with magnetic field strength at two different temperatures is investigated. The observed behaviour is rationalised by determining the free energy as a function of the magnetisation.

1 Introduction

Many of the physical systems that appear in the real world can adopt one of multiple metastable states. This behaviour cannot be described using the models that appear in textbooks on statistical mechanics. There is no way that an ideal gas, two-level system or harmonic oscillator would get trapped in a particular part of phase space. For a system to exhibit metastable states there must be interactions between the particles that the system is composed of.

This report presents the results of Monte Carlo (MC) simulations that have been performed on a simple system of interacting spins that interact with a magnetic field. We use this simple model to explain how two metastable configurations can arise and how the relative stability of these two states is affected by the strength of the field and the temperature.

The report is laid out as follows. We introduce the Hamiltonian under study and the Monte Carlo simulations that have been performed in section 2. This section also provides information on what we have done to ensure that the averages are converged. In section 3 we then perform simulations to illustrate how the average magnetisation depends on the field strength and the temperature. Free energies as a function of the magnetisation for a number of different temperatures are then computed in section 4. The conclusion in section 5 then explains why these surfaces can be used to rationalise the results in section 3.

2 Methods

This paper presents simulations on the two-dimensional Ising model. As illustrated in figure 1, L^2 spins sit on a square lattice with period boundary conditions in this system. Each of

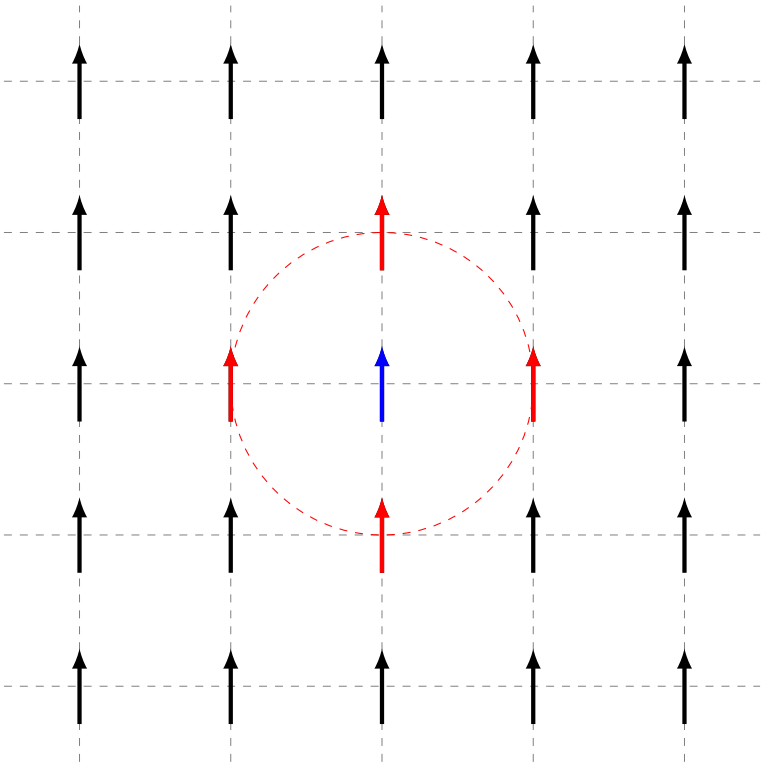

Fig. 1. An illustration of the system of Ising spins that has been simulated in this work. The spins are all aligned in the microstate that is shown but they can point either up or down in our model. The coloured arrows indicate how the spins interact. The spin that is shown in blue interacts with its four closest neighbours that are highlighted in red.

these spins has a coordinate σ_i that can be $+1$ or -1. The Hamiltonian is then:

$$H(\sigma) = -H \sum_j \sigma_j - J \sum_{\langle i,j \rangle} \sigma_i \sigma_j$$

The first sum above runs over all the spins. The second sum then runs over the pairs of spins that are adjacent in the lattice. As illustrated in figure 1 each spin thus interacts with its four immediate neighbours. We operate in a system of natural units in all the work that follows and thus set J equal to one. All energies are thus given in units of J.

Average properties for this system at a range of different temperatures and different field strengths were calculated by performing Monte Carlo simulations. The Metropolis algorithm was used to draw sample configurations in thermal equilibrium at each temperature. Trial moves were generated by either randomly-selecting a single spin and flipping its value or by flipping the values of all the spins at once. The relative probabilities for generating these two types of move were $\frac{L^2}{L^2+1}$ and $\frac{1}{L^2+1}$ respectively, where L^2 is the number of spins.

The magnetisation per spin for a microstate of the Ising model was computed using:

$$\overline{M} = \frac{M}{L^2} = \frac{1}{L^2} \sum_j \sigma_j$$

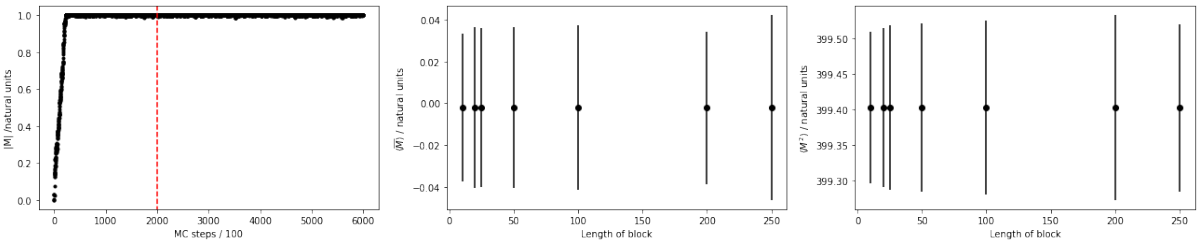

Fig. 2. Results from benchmarking calculations that were performed to check that the averages we are calculating were converged. The left panel shows the value of the absolute magnetisation took during a 600000 step MC simulation at a temperature of 1.0 natural units. You can see that the system is equilibrated after the first 200000 steps of the simulation. The middle panel shows the dependence of the error for a 95% confidence limit on the average magneitisation depends on the sizes of the blocks that averages are computed from. The right panel offers a similar analysis for $\langle M^2 \rangle$, where M in this case is the unormalised sum of the spins.

where the sum runs over the L^2 spins in the system. The left panel of figure 2 shows how the absolute value of $\overline{M}$ changes over the course of a short simulation of a 20 by 20 lattice spins in the absence of a magnetic field at a temperature of 1.0 natural units. Statistics were collected every 100 steps in this and every other simulation we perform. You can see that the system takes 200000 steps to equilibrate . After this point the magnetisation oscillates around a constant value. When taking averages we thus discard the first 200000 steps of every simulation we perform.

To calculate averages and errors in the following sections we use block averaging to account for the correlations in the series of random variables that we get from our simulations. The right two panels of figure 2 show how the errors for a 95% confidence limit on $\langle \overline{M} \rangle$ and $\langle M^2 \rangle$ depend on the block size. You can see that the size of the error for both of these quantities stabilises once blocks of 100 configurations are employed. We thus blocks with a length of 100 when calculating averages in what follows.

3 Response to magnetic field

MC simulations were performed to calculate $\langle \overline{M} \rangle$ for a 20×20 lattice of Ising spins at temperatures of 2 and 5 natural units and a range of different magnetic field strengths. The averages from these simulations are shown in the left column of figure 3. Errors for a 95% confidence limit on all averages are also shown in this figure but many of these errors are smaller than the size of the dots.

The top left panel of figure 3 shows that the system rapidly switches from negative to positive magnetisation when the temperature is 2 natural units when the field changes sign. The bottom panel shows that this change still occurs at the lower temperature. However, at the lower temperature the change is more gradual.

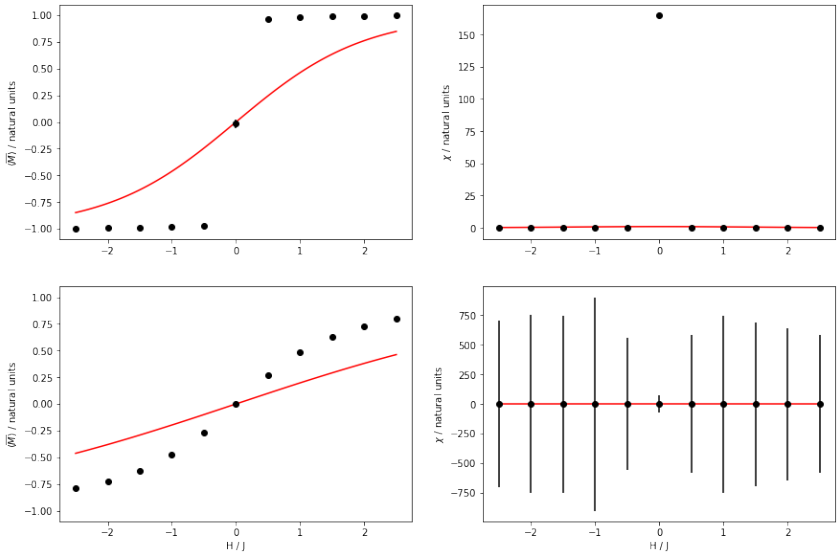

Fig. 3. The dependence of the average magnetisation $\langle \overline{M} \rangle$ (left) and susceptibility (right) on the strength of the magnetic field at temperatures of 2 (top) and 5 natural units (bottom). The black dots show the results from MC simulations of the Ising model. Errors that indicate a 95% confidence limit on the average are shown for all quantities. The red lines show how the values of these quantities change for a system of non-interacting spins.

In figure 3 the behaviour of the Ising model is contrasted with the behaviour of a system of non-interacting spins. The Hamiltonian for the non-interacting spins is:

$$H = -H \sum_j \sigma_j$$

where the sum runs over all the spins. The canonical partition function for this spin Hamiltonian is given by:

$$Z = 2^N \cosh^N(\beta H)$$

The ensemble average for the magnetisation is thus:

$$\langle M \rangle = \left(\frac{\partial \ln Z}{\partial (\beta H)} \right) = N \tanh(\beta H)$$

You can clearly from figure 3 see that the change from negative to positive magnetisation for the non-interacting is gradual at both temperatures. There does not appear to be the (almost) discontinuous change in magnetisation that is observed for the Ising spins.

The fact that there is this rapid switch from positive to negative magnetisation is further evidenced by the left column of figure 3. These two panels show how the susceptibility:

$$\chi = \frac{1}{L^2} \left(\frac{\partial \langle M \rangle}{\partial H} \right)$$

changes with field at the two temperature of interest. We calculate the susceptibility from our MC simulations using:

$$\chi = \frac{1}{L^2}\frac{\langle M^2\rangle - \langle M\rangle^2}{k_B T}$$

where T is the temperature and k_B is Boltzmann's constant, which is set equal to one in this work. You can see that there is a sharp peak in the susceptibility at the lower temperature and that there is no similar peak at the higher temperature. This peak is further evidence of the rapid (almost discontinuous) transition between the negative magnetisation and positive magnetisation states that only seems to take place at the lower temperature.

The red lines in these right panels of figure 3 show the susceptibility for the non-interacting spins. There is no peak in the susceptibility for this system and hence no evidence of a rapid transition for the system of non-interacting spins.

4 Free energy surface

To understand the behaviour of the Ising system that was described in the previous system we estimated the free energy as a function of the magnetisation using:

$$F(\overline{M}') = -k_B T \ln P(\overline{M}')$$

In this expression k_B and T are Boltzmann's constant and the temperature respectively. Meanwhile, $P(\overline{M}')$ is the following ensemble average:

$$P(\overline{M}') = \frac{1}{Z}\int \mathrm{d}x \delta(\overline{M}(x) - \overline{M}') e^{-\beta H(x)}$$

where Z is the canonical partition function and δ is a Dirac delta function. This integral cannot be calculated exactly. We thus estimated $P(M')$ from MC simulations. Errors on these estimates of $F(\overline{M}')$ were then determined by block averaging. Figure 4 shows how the average error on the estimate of the free energy depend on the size of the blocks for a simulation of a 20×20 lattice of Ising spins in the absence of a field at a temperature of 2.0 natural units. In subsequent calculations we use blocks of 200 configurations when calculating averages as figure 4 shows that the error on the free energy is maximal for this block size.

Figure 5 shows estimates of the free energy as a function of magnetisation for two different temperatures and three different magnetic field strengths. You can clearly see that there are two minima in the free energy when the temperature is low. These two minima have the same energy when there is no field present. However, this degeneracy is broken once a field is present. When the field is turned on the system will occupy the state that has the lower free energy rather than the metastable state. The fact that the state with the lowest free energy changes when we move from positive to negative magnetisation explains the discontinuous change in magnetisation that is observed in the upper-left panel of figure 3.

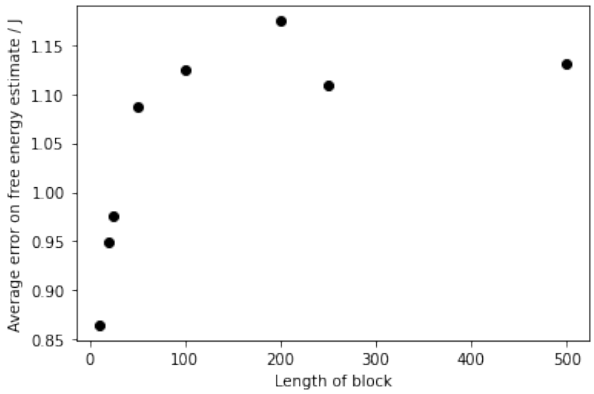

Fig. 4. Average error on the estimates of the free energy as a function of block size for a simulation of a 20×20 lattice of Ising spins in the absence of a field at a temperature of 2 natural units.

The behaviour observed for the lower left panel of figure 3 is explained by the free energy surfaces in the bottom row of figure 5. At the higher temperature the free energy surface only has one minimum. The average magnetisation changes continuously in response to the magnetic field as does the position of minimum in the free energy.

5 Conclusions

Simulations of a 20×20 lattice of Ising spins were performed. We found that there are two minima in the free energy landscape for this system when the temperature is low and that there is only one minimum when the temperature is high. The way this system responds to a magnetic field is thus dependent on temperature.

Notice that the free energy surfaces we drew in figure 5 are useful because the order parameter on the x-axis is able to distinguish between the two minima in the energy landscape. Figure 6 shows the free energy as a function of the internal energy in the absence of a field at a temperature of 2 natural units. This free energy surface was prepared in the same way as the free energy surfaces in 5. However, there is no evidence here of the two minima in the energy landscape that we know are present from the middle-top panel of figure 5 because the order parameter on the x-axis cannot distinguish between these two configurations.

It is easy to find an order parameter that can distinguish the two states of the Ising model. For more complicated systems it is much more difficult to identify these order parameters. There is thus a great deal of current research work on this topic. Much of this research involves using machine learning and artificial intelligence.

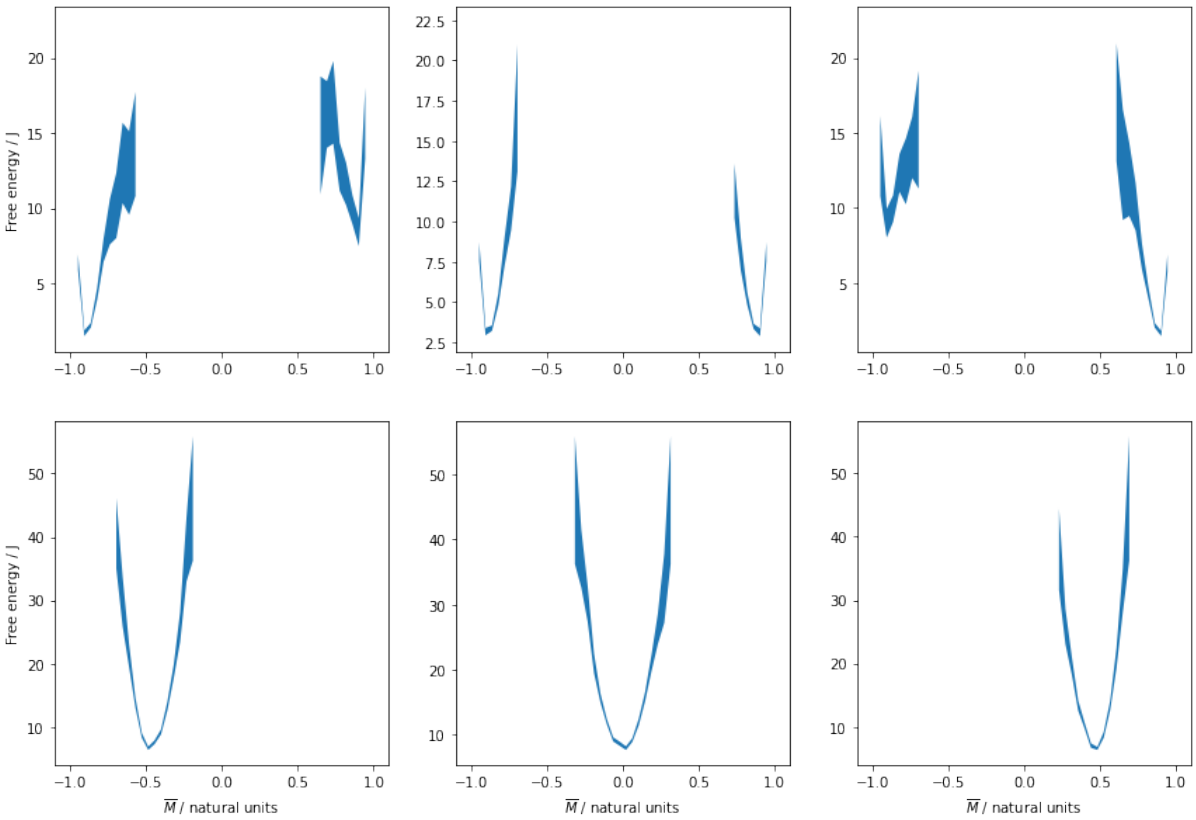

Fig. 5. The free energy as a function of $\overline{M}$ for a 20×20 lattice of Ising spins under various conditions. The top row shows free energies surfaces at a temperature of 2 natural units. The bottom row shows these surfaces at a temperature of 5 natural units. The middle column are the free energy surfaces that are obtained in the absence of a field. The surfaces in the left column are for fields of -0.01 J (top) and -1 J (bottom). The surfaces in the right column are for fields of $+0.01$ J (top) and $+1$ J (bottom). The width of the lines illustrate the 95% confidence limit on our estimates of the free energies.

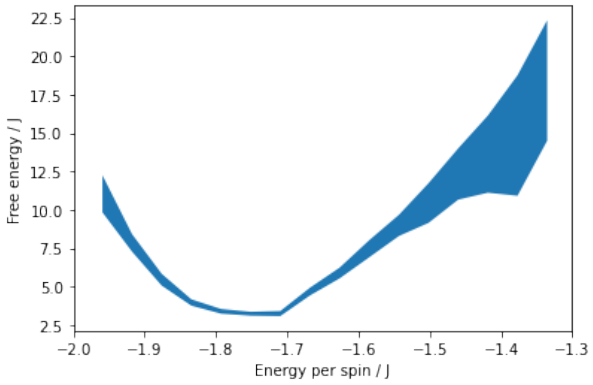

Fig. 6. Free energy as a function of internal energy for a 20×20 lattice of Ising spins. This free energy surface was calculated in the absence of a magnetic field at a temperature of 2 natural units.The width of the lines illustrate the 95% confidence limit on our estimates of the free energies.