FYS3150 Project 4

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Abstract

1 Introduction

Many systems in nature can be modelled as being binary, in the sense that the individual components that make up the system can only assume one of two states. For example, neuronal activity in the brain can be modelled by assuming that each "neuron" can be either on, or off. However, it is by allowing these simple components to interact, that interesting behaviour emerges. For the neuronal example, an interaction can be that different nodes in a network excite each other, causing spike trains of activity. In this text, we will explore the so-called Ising model, which is typically used to describe a system of particles on a lattice. Each of these particles has so-called spin, either up or down, and interact magnetically. For all its simplicity, the Ising model still manages to capture some of the complex properties of real magnetic materials, such as phase transitions.

We will begin our investigation by outlining the Ising model for spins on a lattice interacting magnetically, and consider the specific case of a 2×2 lattice. Using the Boltzmann distribution, and some statistical physics, we arrive at analytical expressions for the expected values for the absolute magnetization, energy, heat capacity at constant volume, and magnetic susceptibility in the 2×2 case. After describing the Ising model, we move on to the Metropolis Algorithm, a Monte Carlo simulation strategy for computing the behaviour of the Ising model over time, at different temperatures. We then address how to implement the Metropolis algorithm as part of a Monte Carlo simulation of the Ising model.

2 Theory

2.1 The Ising Model

While usually used to model the magnetization of simple solids in terms of particle spins [2], the Ising model can in general be said to describe a system of particles on a lattice, where each particle can take on one of two values. The particles are coupled by some interaction, and may also interact with their environment. For the magnetic case, these values are taken to be the dimensionless particle spins, which can be either up (1), or down (-1), and the external interaction may be in the form of an applied magnetic field. As each particle in a way acts like a small bar magnet, they also interact magnetically with each other, the effect of which depends on the material we wish to investigate. In this text, we will consider the simplest case, in which only nearest neighbours interact, and there is no applied magnetic field. In that case, the total energy of a configuration of spins is given by

$$E = -J \sum_{<k,l>} s_k s_l, \tag{1}$$

where s is the spin of a particular particle, while the indices $\langle k, l \rangle$ indicate that we only sum over nearest neighbours. J is a coupling constant reflecting the strength of particle-particle interactions, with unit energy. The actual value of J depends on the situation we are modelling. Note also that we have to sum over the entire lattice in order to obtain the total energy.

When modelling materials, spins can for example tend to interact in such a way that they align, and strengthen an applied magnetic field. As a famous example, *ferromagnetic* iron not only strengthens any magnetic field it is exposed to, it also retains its magnetization for some time afterward, MORE, + CITE. From (1) we can see that a positive value of J implies that the energy is minimized when spins align. For this simple reason, our model will be mimicking the behaviour ferromagnetic materials, as we will only consider the $J > 0$. However, we will as stated not apply a magnetic field, we will only consider *spontaneous* magnetization.

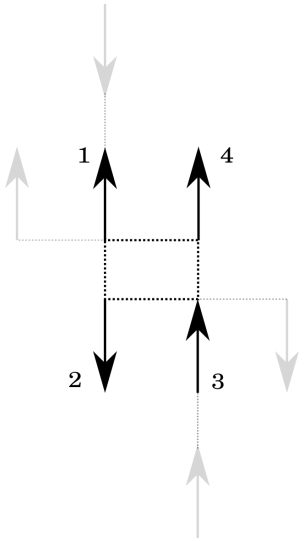

Figure 1: Illustrated 2×2 lattice of spins, with periodic boundary conditions.

As stated previously, we will only sum over nearest neighbours, and we will also only count a contribution to the energy once. What this, and (1) in essence leads to, is that we count the number of *bonds* in the lattice. To see how this works in practice, and also find some useful analytical expressions, we are going to consider a grid of only 2×2 spins. We will also limit ourselves to so-called periodic boundary conditions, where we say that the spins along the boundaries, actually "sees" a spin outside the boundary, whose spin value is taken to be equal to the that of the spin on the opposite side of the lattice. By doing so, we can create a slightly more realistic dynamic in our system, as opposed to just having free ends, and neglecting possible boundary effects. Note that for large system, and certainly in the thermodynamic limit when the number of spins go to infinity, there is little no distinction between these two types of boundary conditions.

In order to visualize how we may find the energy of a finite grid of spins, illustrates Fig. 1 a lattice of 2×2 spins arranged on a square grid. We treat the particles as distinguishable, as they can be identified by their position, and denote the particles with subscripts 1 through 4, going counterclockwise. We have also attempted to illustrate the periodic boundary conditions, shown as shaded spins outside the actual lattice. Note how these spins take on the spin value of the particle on the other side of the lattice.

To find the energy associated with the configuration in Fig. 1, and guarantee that we don't count terms twice, we can position ourselves at spin sites 1 and 3 (or 2 and 4), and simply follow the prescription in (1). Doing so, we find that the total energy is

$$E = -2J(s_1 s_2 + s_1 s_4 + s_3 s_2 + s_3 s_4), \tag{2}$$

where s denotes a spin value, and the factor two comes from the periodic boundary conditions. It should be pointed out that this not only tells us the energy of the specific configuration in Fig. 1, it gives us a way of finding the energy for *any* 2×2 spin configuration. Plugging in $s_1 = s_3 = s_4 = 1$, and $s_2 = -1$, we find $E = 0$ for the case in Fig. 1.

As we are going to simulate our Ising model using a Monte Carlo method, it would be very useful to know the *expected* behaviour of the simplest case, our 2×2 grid. To determine any expectation values for the system, we first need to know that it actually follows a probability distribution, and if so, which one. As it turns out, we can model this system as a collection of particles in thermal equilibrium with their surroundings. From thermodynamics, such systems tend to obey the Boltzmann distribution CITE SCHROETER.

$$P_i(E_i) = \frac{1}{z} e^{-\beta E_i}, \tag{3}$$

where z is the so-called partition function of the system, while E is the energy associated with the particular spin configuration of state i. $\beta = 1/k_B T$ is simply a measure of the system temperature, (times the Boltzmann constant k_B. However, since these are probabilities, we know that they must necessarily obey the normalization condition

$$1 = \frac{1}{z} \sum_i e^{-\beta E_i}, \tag{4}$$

where we sum over all possible states, which in the 2×2 gives us $2^4 = 16$ different possibilities. Fortunately, (4) tells us that we can quite easily determine the partition function of a system, if we know the energy E_i associated with a given state. Inserting from (1), we get

$$z = \sum_{i=1}^{16} e^{2\beta J(s_1+s_3)(s_2+s_4)},$$

where we have rewritten the energy expression in a somewhat more suggestive form. To simplify matters, we can use a bit of combinatorics, and the fact that the number of different energies is limited. If only there is only one spin up, or one down, for example, the exponent goes to zero, something which can be accomplished in $\binom{4}{1} + \binom{4}{3} = 8$ different ways. We can also have all spins down or up, which can only be done one way each, accounting for two more possibilities, both with energy $-8J$. Finally, we can have two spins up, and and two down, which gives an energy of either $E = 0$, or $E = 8J$. The final option can occur in $\binom{4}{2} = 6$ ways, which completes our set of 16 possibilities. Putting this together, we end up with

$$z = 2e^{8\beta J} + 8e^0 + 2e^{-8\beta J} + 4e^0,$$

where we have used the fact that we can only obtain $(s_1 + s_3)(s_2 + s_4) = -8$ in two ways (s_1 and s_3 must point up, and the rest down, or vice versa). Tidying up, we find

$$z = 4\cosh(8\beta J) + 12, \tag{5}$$

in the 2×2 case.

Another interesting quantity we can determine quite easily, is the average absolute magnetization, $\langle |M| \rangle$. For a certain state i, the magnetization is just $M_i = \sum_{i=1} s_1 + s_2 + s_3 + s_4$ for the 2×2 lattice.

Since the magnetization of the system is precisely determined by its spin configuration, the probability of getting a certain magnetization is given by (3), and the average value is

$$\langle |M| \rangle = \frac{1}{z} \sum_i^{16} |M_i| e^{-\beta E_i}, \tag{6}$$

where we once again sum over all possible configurations of the four spins. We can also use the fact that the magnetization of a given state M_i, is uniquely determined by the number of spins pointing up (or down), as we know the total number of spins. As such, we know that the absolute magnetization can be only 4, 2, or 0. The first case is simple, and achieved by either arranging all spins up, or all spins down. The second occurs when all but one particle have spin up or down, and the last when all spins cancel. We can however use this to find a neat expression for (6). As there are four particles, there is a grand total of $2^4 = 16$ possible states, which means that the sum over all states must contain 16 terms. However, as we noted, there are only three possible (absolute) values of the magnetization, one of which is zero, and therefore does not contribute to the sum. For the remaining states, there are only two ways of obtaining the maximum magnetization of 4, with corresponding energy $-8J$. The final possibilities are those with one spin up, or one spin down, which can occur in $\binom{4}{1} = \binom{4}{3} = 4$ ways each. If we once again write the energies in the more suggestive fashion $E_i = -2J(s_1 + s_3)(s_2 + s_4)$, we can see that both these possibilities carry $E = 0$. Putting all of this together, we find that

$$\langle |M| \rangle = \frac{1}{z}\left(4\left(e^{2\beta J\cdot 4} + e^{2\beta J\cdot 4}\right) + \binom{4}{1}2e^0 + \binom{4}{3}2e^0\right),$$

or that

$$\langle |M| \rangle = \frac{8}{z}\left(e^{8\beta J} + 2\right). \tag{7}$$

As for the squared magnetization, the probabilities (and possibilites) remain the same as for the absolute value case, we only need to square the actual value of the magnetization. Therefore, we can adapt our earlier expression, and obtain

$$\langle M^2 \rangle = \frac{32}{z}\left(e^{8\beta J} + 1\right) \tag{8}$$

We are also going to need the expected value of the actual magnetization, which is fortunately quite simple in this case. Due to symmetry, we can, for each possible value of the magnetization, simply flip all spins, and obtain the same absolute spin, with an opposite sign. Therefore, we must have that the sum over all states cancels, and

$$\langle M \rangle = 0. \tag{9}$$

We can also determine the expected value for the energy of the system, in the usual manner:

$$\langle E \rangle = \frac{1}{z}\sum_{i=1}^{16} E_i e^{-\beta E_i},$$

where we would have to sum over all states once again. But, the experienced reader might have noted another possibility, by observing that

$$\frac{\partial z}{\partial \beta} = \sum_{i=1}^{16} -E_i e^{-\beta E_i},$$

which should not be problematic, as z only consists of well-behaved exponentials. Therefore,

$$\langle E \rangle = -\frac{1}{z}\frac{\partial z}{\partial \beta} = -\frac{32J}{z}\sinh(8\beta J). \tag{10}$$

We can also find the expected squared energy, $\langle E^2 \rangle$ using the same approach, and differentiating z twice, which gives

$$\langle E^2 \rangle = \frac{256J}{z}\cosh(8\beta J). \tag{11}$$

Now that we have some essential building blocks, we can formulate a few more useful quantities, namely the specific heat at constant volume, C_V, and the magnetic susceptibility, χ. The specific heat tells us how much energy is required to heat a specific amount of substance by one degree. For our purposes, it can be defined as

$$C_V = \frac{1}{k_B T^2} \left(\langle E^2 \rangle - \langle E \rangle^2 \right). \tag{12}$$

CITE LECTURES Note that we can use (12) only as long as we keep the volume, or size of our system, which is the case for a fixed-sized lattice of spins, which we will focus on. Inserting for the expected squared energy, and squared expected energy, we get

$$C_V = \frac{256}{k_B T^2 z^2} \left(z \cosh\left(8\beta J\right) - 4 \sinh^2\left(8\beta J\right) \right).$$

The magnetic susceptibility is a measure of the degree to which a material is *susceptible* to being magnetized, and can be defined as

$$\chi = \beta \left(\langle M^2 \rangle - \langle M \rangle^2 \right), \tag{13}$$

and for our 2×2 lattice, we find

$$\chi = \frac{32\beta}{z} \left(e^{8\beta J} + 1 \right)$$

As a last, tantalising aspect of the Ising model, we will consider how it acts close to the critical temperature T_C, at which a phase transition occurs. For a two-dimensional model, this transition takes the form of a sudden discontinuity of the magnetic susceptibility and the heat capacity. As the temperature of the system approaches the critical point, the so-called correlation length of the system, tends toward infinity. The correlation length is, roughly speaking, a measure of the distance that can separate spins on the lattice, and still have them affect each other. CITE LECTURES. However, if we are to investigate the behaviour of the Ising model near the critical temperature, we first need to know what it might be. One possible way of doing so is by simply simulating different sized lattices, and extracting the temperature at which a discontinuity appears in the value of the magnetic susceptibility, for instance. However, it turns out that the critical temperature of the Ising model scales with the lattice size l as

$$\hat{T}_c(l) = aL + \hat{T}_c(\infty), \tag{14}$$

[1]where $\hat{T}_c(\infty)$ is the critical temperature of an infinite lattice of spins, and a some constant. Therefore, if we can determine the critical temperature for different gridsizes, we can also approximate the critical temperature for the infinite case, by performing a linear regression for different values of $\hat{T}_c(l)$. The exact value of $\hat{T}_c(\infty) = 2/\ln(1+\sqrt{2})$ is actually known, and is due to Norwegian mathematician Lars Onsager [2].

2.2 The Metropolis Algorithm

As we can see from the 2×2 lattice, finding analytical solutions describing the Ising model can be difficult, even in the very simplest case. Motivated by this, we will attempt to use a Monte Carlo method to analyze a system of $l \times l$ spins. Specifically, we will attempt to outline and apply the Metropolis algorithm, a Monte Carlo algorithm tailored to the Ising model.

The general strategy of the Metropolis algorithm is to first "position ourselves" randomly at some spin site on the $l \times l$ lattice. We then try to see what happens to the energy of the system if we flip the selected spin, and if the change in energy is negative, we automatically accept the new configuration. If the change in energy is non-negative, however, we need some selection rule to determine if the flip should be approved or not.

While it is tempting to simply reject any positive change in energy, as physical systems tend to move toward lower energy states, this approach can bias our model, and we may never, for example,

find all interesting energy states. As a general example, we can imagine a situation where we end up in a local energy minimum. To escape such a minima, we may need to make moves which increase the energy locally. Therefore, we require that our system is ergodic, or in other words that every possible state is accessible to the system, given enough time.

As we have already seen, the spins that make up the lattice follow the Boltzmann distribution, with probability density of being in a certain energy state given by (3). While we do not know the probability of transitioning from one state to another, we can model the probability of moving from a state with energy E_i to one with energy E_j as

$$p_{i\to j} = P(E_i)T_{i\to j}A_{i\to j},$$

where $A_{i\to j}$ is the probability of accepting a transition, while $T_{i\to j}$ is the probability of said transition occuring. Simply put, our model is then that for a transition to occur, we need for the system to be in a state with energy E_i, *and* have that a transition from state i to j occurs, *and* that we accept the transition. We are also going to require that we have so-called detailed balance, which means that $p_{i\to j} = p_{j\to i}$. EQUILIBRIUM SITUATION, CITE CHEMLIBRE?. In this text, we will also assume that the transition probabilities are equal at equilibrum, and therefore that

$$\frac{A_{i\to j}}{A_{j\to i}} = e^{-\beta(E_j - E_i)},$$

where we have simply equated $p_{i\to j}$ and $p_{j\to j}$, and inserted the respective probabilities from the Boltzmann distribution. While we do not know the acceptance probability, we have already mentioned that we automatically accept changes which lead to lower energies. In other words, if we consider two states i and j, and the j-state carries a greater energy, we must set $A_{j\to i} = 1$, as such a move would lower the energy. The acceptance probability of performing the oppsite transition must then be

$$A_{i\to j} = e^{-\beta(E_j - E_i)}, \tag{15}$$

and in the opposite case, where $E_i > E_j$, the acceptance probability is simply 1. Now that we have a selection rule for our Monte Carlo simulation, we can, for each proposed spin flip, find the resulting change in energy, and calculate the acceptance probability according to (15). In order to accept or reject a move, we can simply draw a random uniform number between 0 and 1, and compare this to the acceptance probability, which we can call w. If the drawn number is smaller than w, we accept the move, if not, we reject it. The reason it should be smaller, is simply due to the fact that we wish that large increases in energy should be accepted more rarely than small ones.

3 Methods

The Ising model was implemented in c++ using Monte Carlo simulation, according to the Metropolis algorithm. For all simulations, a scaled, dimensionless temperature $\hat{T} = k_B T/J$ was used. The spins were in all cases required to be on a $l \times l$ square grid, and the system was initialized using either an ordered, all spin up- or down state, or a random configuration. For the random initialization, the spin value at a given site was determined by drawing a pseudorandom uniform number between 0 and 1, using the c++ standard library function rand(). If the drawn number was less than 0.5, the spin was set to -1, and 1 otherwise.

A Monte Carlo cycle (MC cycle) was taken to be $l \times l$ suggested steps using the Metropolis algorithm, such that all spin sites were likely to be visited, for a sufficient number of MC cycles. As the total number of steps might be quite large, the coordinates of a suggested spin site were drawn (pseudo)randomly from a uniform integer distribution, generated using the c++ mt19937 Mersenne Twister random number generator (RNG). For each step, the energy associated with a selected spin s_i was found according to (1). To save computations, only the resulting change in energy due to flipping

s_i to $-s_i$ was found, as

$$\Delta E = 2s_i \sum_{k=1}^{4} s_k,$$

where s_k is the value of a neighbouring spin. In accordance with the discussion on the acceptance probability of (15), negative changes in energy were automatically accepted. If an increase in energy was found, a pseudorandom, uniform random number between 0 and 1 was generated using the Mersenne Twister RNG, and compared to the acceptance probability of (15). If the drawn number was smaller than the acceptance probability, the spin flip was accepted, otherwise it was rejected. For each accepted spin flip, the change in energy was logged, and the magnetization was updated according to

$$M_2 = M_1 + 2s_2,$$

where the subscripts 1 and 2 denote the values of magnetization before and after the spin flip, respectively. The above simply entails that flipping a spin must necessarily change the magnetization by 2, as the spin is not removed, but reversed. For all simulations, natural units were used, by setting $J = 1$, and $k_B = 1$. By doing so, the computed expectation values were actually scaled according to $\langle E \rangle / J$, $\hat{C}_V = C_V / k_B$, and $\hat{\chi} = J \cdot \chi$, which are all dimensionless. Note that the magnetization was already dimensionless before scaling.

In order to verify the Ising model implementation, a simulation of a 2×2 lattice of spins at dimensionless temperature $\hat{T} = 1.0$ was run for $n = 10^5$ MC cycles. The average energy, absolute magnetization, magnetic susceptibility, and heat capacity per spin was then computed, and compared with the analytical results of (10), (7), (2.1) and (12), respectively. The comparison was performed by determining the logarithmic absolute relative error. In addition, unit tests were implemented, which compared results from the implemented model with the 2×2 lattice analytical results. These unit tests verified, for a 2×2 model, that initial energies were calculated correctly, to a tolerance of 10^{-16}, and that the magnetization tended towards zero after 10^6 MC cycles, to a tolerance of 0.01.

To investigate the equilibration time of the Ising model at different temperatures, a 20×20 spin lattice was simulated for $n = 10^6$ MC cycles, and the absolute magnetization, as well as the scaled mean energy was logged. Simulations were performed for $\hat{T} = 1.0$, and $T = \hat{} 2.4$, and in both cases both an ordered, as well as a random initial spin configuration was used. For the ordered configuration, all spins were taken to be up. For all these cases, the average values were inspected visually, and the equilibration time was approximated as the MC cycle at which the average value appeared to have stopped changing. For these simulations, the number of accepted spin flips was also logged at the end of each MC cycle.

For the 20×20 lattice simulations, the current energy of the system was logged at the end of each MC cycle. Using these energies, the discrete probability distribution of the system energy per spin was approximated. This was done simply by counting the number of times a given energy appeared during simulation, and normalizing with respect to the number of MC cycles and spins. Note that for $\hat{T} = 1.00$, the results using an ordered spin configuration was used, and the first 1000 MC cycles were not included, to ensure that equilibrium had been reached. For $\hat{T} = 2.40$, the results for a random initialization was used, and the first 2000 MC cycles were not included.

In order to uncover the behaviour of the Ising model near the critical temperature $\hat{T}_c$, the model implementation was parallelized using the external Message Passing Interface (MPI) library. This was done in order to run multiple instances of the Ising model simultaneously, at different temperatures. As a verification of parallelism, timing was performed on some trial runs, with and without vectorization compiler flags. Using the parallelized Ising model, simulations were performed for 40×40, 60×60, 80×80, and 100×100 lattices, at temperatures ranging from $T = \hat{} 2.0$ to $\hat{T} = 2.6$, with a temperature step of 0.025. For each of these simulations, a random initialization was used, and all simulations were performed using $n = 10^6$ MC cycles.

Using results from the parallel computations, the critical temperature for an infinite sized lattice was approximated by performing a linear regression of critical temperature versus lattice size, in

accordance with (14). Note that the critical temperature was taken as the temperature at which the scaled heat capacity and magnetic susceptibility had their maximum values.

4 Results

Fig. 2 shows the absolute relative error ($\log_{10}$) of the scaled thermodynamic quantities, i.e. the average energy, absolute magnetization, as well as magnetic susceptibility and heat capacity at constant volume, per spin for a 2×2 lattice of spins, using periodic boundary conditions at scaled temperature $\hat{T} = 1.0$. It appears that the scaled average energy, absolute magnetization and heat capacity reach their equilibrium value after around 10^4 MC cycles, after which point they appear to oscillate around the exact value, which was found to be approximately 1, -2, 4, and 0.03 for the absolute magnetization, energy, magnetic susceptibility, and heat capacity, respectively. For the magnetic susceptibility, no oscillation is observed, and and apparent equilibrium is reached only after approximately $2 \cdot 10^4$ MC cycles. It is worth noting that the average energy and absolute magnetization appear to be, neglecting oscillations, correct to around the third digit, while the heat capacity and magnetic susceptibility only appear to be correct to around the first or second digit.

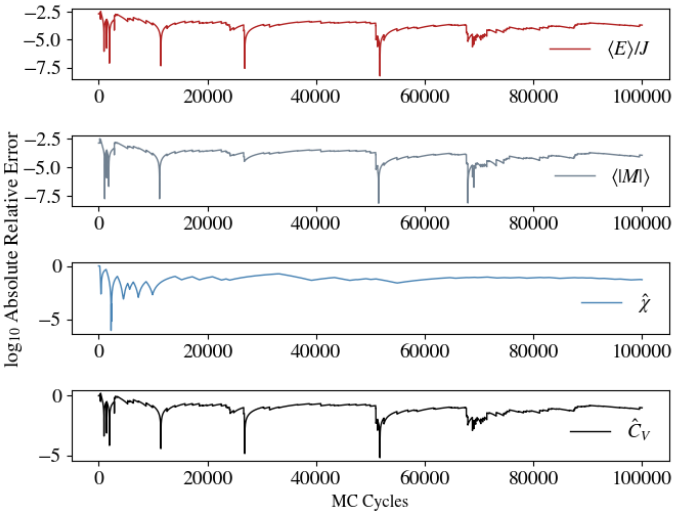

Figure 2: $\log_{10}$ absolute relative error of the scaled average energy, average absolute magnetization, magnetic susceptibility, and heat capacity at constant volume, for an Ising model of lattice size 2×2, simulated using $n = 10^5$ Monte Carlo cycles at scaled temperature $\hat{T} = 1.0$, using the Metropolis algorithm

Fig. 3 shows the scaled average energy and absolute magnetization per spin, as a function of simulation length in terms of the number of MC cycles, for an Ising model of lattice size 20×20. Results are indicated for both ordered, as well as random spin initializations, for scaled temperatures $\hat{T} = 1.0$ and $\hat{T} = 2.4$. For the $\hat{T} = 1.0$ case, we can see that both the average absolute magnetization, and the scaled average energy appear to stabilize after approximately 1000- 2000 MC cycles for an ordered initialization. For the random initialization, the results appear to converge more slowly, and the absolute magnetization only appears to begin to settle after approximately 10^4 MC cycles, towards a value just below unity, which is also the case for the ordered case. The scaled average energy appears converge to more quickly, requiring approximately 4000 MC cycles to get close to the equilibrium value of around -1.997, as found for the ordered case. For the $\hat{T} = 2.4$ case, we can see that both solutions converge, taking roughly 1000 MC cycles for the scaled energy to converge to a value of approximately

-1.23, both for the ordered and random cases. For the magnetization, however, the ordered simulation appears to take approximately 5000 MC cycles to settle to a value of approximately 0.45, while the random initialization appears to do so after approximately 2500 cycles.

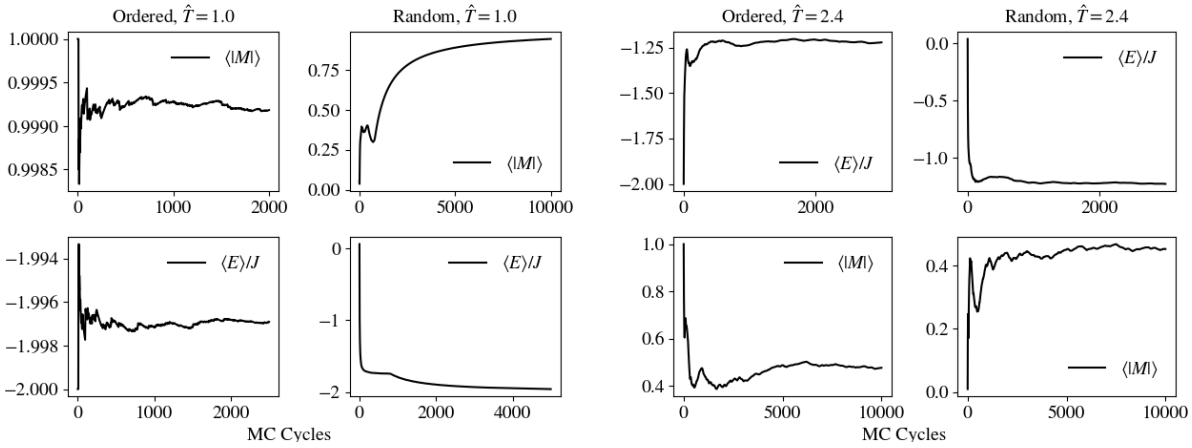

Figure 3: Average values of absolute magnetization $\langle|M|\rangle$, and scaled energy, $\langle E\rangle/J$, for an Ising model of lattice size 20×20 spins. Shown are simulations for scaled temperatures of both $\hat{T} = 1.0$ and $\hat{T} = 2.4$, for different numbers of Monte Carlo cycles. For each temperature, both random and ordered (all spin up), initial spin configurations were used, as indicated.

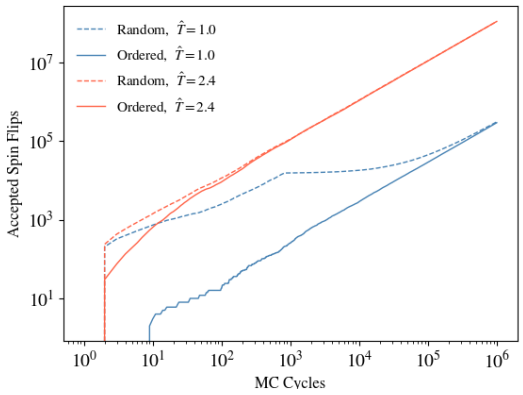

Figure 4: log-log plot of the total number of accepted spin flips, versus the total number of Monte Carlo cycles. Inset are the number of accepted moves using both random and ordered (all spin up), initial spin configurations, simulated using scaled temperatures $\hat{T} = 1.0$ and $\hat{T} = 2.4$.

Fig. 4 shows a log log-plot of the total number of accepted spin flips, as a function of the number of MC cycles for the same simulation as in Fig. 3. We can see that the number of accepted moves in all cases increases steadily with the number of MC cycles, but that is generally lower for a lower temperature of $\hat{T} = 1.0$. For the $\hat{T} = 1.0$, ordered case, we see that the number of accepted flips stabilizes at around 1000 MC cycles, indicating that equilibrium is reached, which is also in agreement with the finding from Fig. 3. We also see that the random initialization takes much longer to stabilize, as the number of accepted flips only approaches that of the ordered initialization after approximately 10^5 MC cycles. For $\hat{T} = 2.4$, we observe that the number of accepted flips is much greater for a given

MC cycle, but that the random configuration appears to stabilize more quickly (and equilibrium may have been reached), which is also in agreement with what is observed in Fig. 3. We can also note that after equilibrium is reached, the number of accepted increases linearly with the number of MC cycles, as the slope of loglog curve is approximately 1.

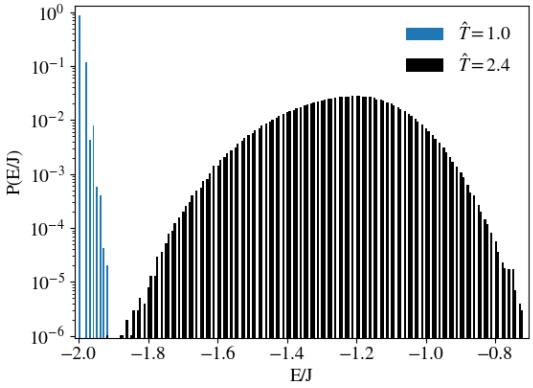

Figure 5: Approximate probability distribution of scaled energy states per spin, for an Ising model of lattice size 20×20. Shown are the relative number of appearances of a given scaled energy per spin, after system equilibration. Shown are the approximate probability distributions for a scaled temperature of $\hat{T} = 1.0$, and $T \hat{=} 2.4$. Note that the total simulation time was 10^6 Monte Carlo cycles, but the first 1000, and 2000 cycles were discared for the $\hat{T} = 1.0$, and $\hat{T} = 2.4$ case, respectively, to ensure that equilibrium had been (approximately) reached.

Table 1: Execution time for Ising Model, for various lattice sizes, $l \times l$, for $n = 10^4$ Monte Carlo cycles, in the temperature range $T \in [2.0, 2.6]$, with temperature step $\Delta T = 0.05$. Values are tabulated for the baseline run, with no added compiler flags, and only one process, as well as parallel runs, with 8 parallel processes. Also shown is the same parallel processes, compiled with the -02 compiler flag. Lastly, the speedup of the -02 run compared with the baseline is shown.

Execution time $[s]$				
L	Baseline	Parallell	Parallel -02	Speedup $[s/s]$
40	73.4	27.2	9.5	7.73
60	167.7	61.5	21.6	7.76
80	305.3	106.9	37.4	8.16
100	474.1	170.0	59.9	7.91

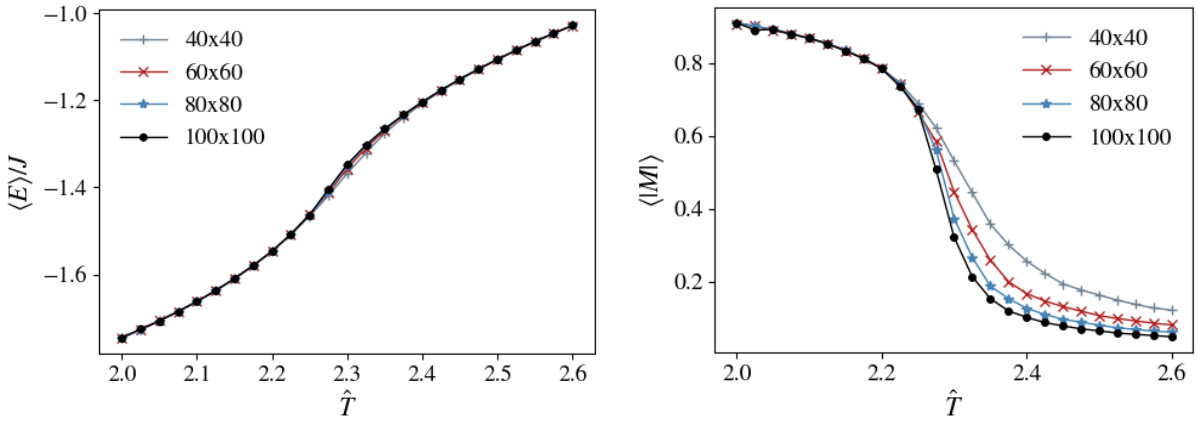

Figure 6: Scaled average energy per spin (left hand side), and average absolute magnetization per spin, for Ising models of lattice sizes 40×40, 60×60, 80×80, and 100×100, as a function of scaled temperature $\hat{T}$. Each data point represents the final average value of the quantity in question, extracted after the simulation was run for 10^6 Monte Carlo cycles.

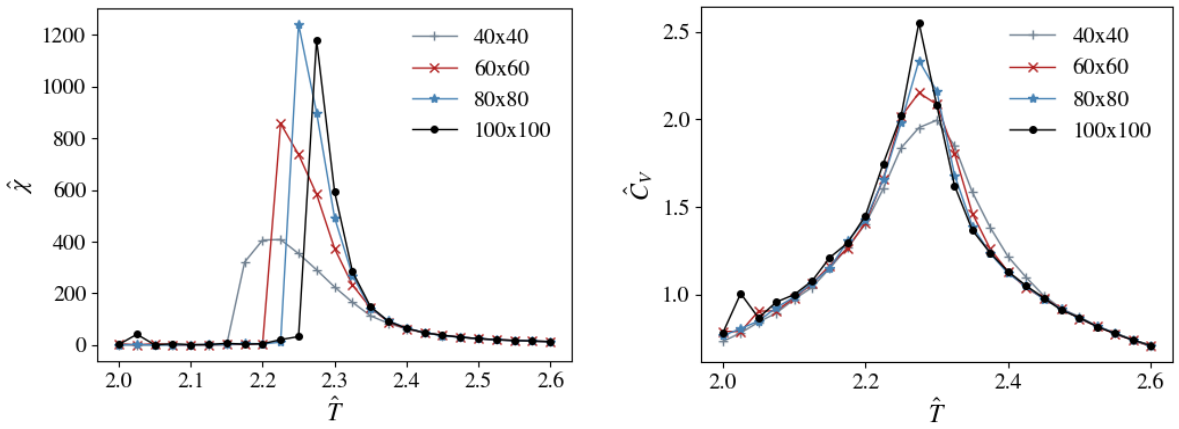

Figure 7: Scaled magnetic susceptibility per spin (left hand side), and scaled heat capacity per spin, for Ising models of lattice sizes 40×40, 60×60, 80×80, and 100×100, as a function of scaled temperature $\hat{T}$. Each data point represents the final average value of the quantity in question, extracted after the simulation was run for 10^6 Monte Carlo cycles.

5 Discussion

https://nanohub.org/resources/4127/download/02-28-08-forweb.pdf

Execution time does not show best-case scenario. Chose random init. based on prelim. findings.

6 Conclusion

References

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