FYS3150 Project 4

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Abstract

The statistical physics of a simple Ising model is used to gain isnight into temperature dependent characteristics of a system of binary spins. The Ising model is implementet with periodic boundary conditions, using multi threading and post steady state data collection. For small 2×2 lattices, the steady state is found after about 100 cycles, with mean energies corresponding to Lars Onsager's analutical results for T=1 and T=2.4. For bigger lattices, on a temperature gradient $T \in [2, 2.6]$ with $\Delta T = 0.02$, the critical temperature is found at T = 2.3, where the magnetic susceptibility and specific heat peaks. After T = 2.3, the mean absolute magnetic moment drops quickly, indicating a phase change.

1 Introduction

In material science and statistical physics, macroscopic phenomena of matter is explored through simulating microscopic interactions many times, and produce statistics which characterizes the macroscopic behaviour of the system. If successful, this can be used to understand how macroscopic behaviour works, and gain insight into new materials.

To achieve this, a numerical Monte Carlo method based on the Ising model and metropolis algorithm is developed. The method produces statistics which explores the mean energy and magnetic moment of the system, as well as the magnetic susceptibility and specific heat for a range of temperatures. The systems consists of binary spins arranged in a lattice with periodic border conditions and a range of sizes from L=2 to L=100.

Through analysis of the produced statistics, insight into critical temperature and phase change phenomena can be explored.

2 Theoretical background

The equations here are obtained from the lectures, lecture notes and assignment document.

For a 2×2 lattice, where N is given as $N = L \times L$, for $L = 2$ we obtain $N = 4$, such that with 2 different spins the number of states is $2^4 = 16$. The partition function Z is all the possible states summed such that

$$z = \sum_{i=1}^{16} e^{-\beta E_1'} \tag{1}$$

Resulting in expected energy

$$E[E] = \frac{1}{z}\sum_{i=1}^{16} E_i e^{-\beta E_i} \tag{2}$$

The specific heat C_V, is a function of the variance σ^2, the energy E and the temperature T where k_B is the Boltzmann constant such that

$$C_V = \frac{\sigma^2 E}{k_B T^2} = \frac{1}{k_B T^2}\left[\frac{1}{Z}\sum_{i=1}^{16} E_i^2 e^{-\beta E_i} - E[E]^2\right] \tag{3}$$

Which is a quantity that can be measured experimentally.

The expected value for the magnetic moment is

$$E[M] = \frac{1}{z}\sum_{i=1}^{16} M_i e^{-\beta E_i} \tag{4}$$

WHere the variance of the magnetic moment is

$$\sigma_M^2 = \frac{1}{2}\sum_{i=1}^{16} M_i^2 e^{-\beta E_1} - E[M]^2 \tag{5}$$

With susceptibility

$$X = \frac{\sigma^2 M}{k_B T} \tag{6}$$

2.1 Configurations

In a 2×2 lattice of spins, we get the following structure:

$$\begin{matrix}\uparrow\uparrow \\ \uparrow\uparrow\end{matrix}$$

Where, with periodic boundaries, for every given spin, the spin over and under will be the same, and the spin left and right will be the same, because the "end" of the lattice just mirrors the neighbour on the opposite side. With such a small lattice, this limits the total number of possible energies, but when the lattice becomes bigger, this boundary inaccuracy becomes smaller.

Up	Down	Spin sum	Old E	New E	ΔE
4	0	4	-4J	4J	8J
3	1	2	-2J	2J	4J
2	2	0	0	0	0
1	3	-2	2J	-2J	-4J
0	4	-4	4J	-4J	-8J

Table 1: Possible configurations of neighbouring spins, where sums to +1 and down sums to -1. The energy difference is the difference before and after the "middle" spin is flipped from up to down.

The energy og a specific energy of a microstate when summing over the nearest neighbours is given by

$$E_i = -J \sum_{<kl>}^{N} s_k s_l \tag{7}$$

In *Table* 1, we see all the possible energy differences of the microstates when summing over the nearest neighbours. Now that all the energy differences are known, they can be pre-calculated and stored in an array or matrix. If we know the "Old E", as in *Table* 1, then we know that there is only one corresponding energy difference for that microstate if the spin is flipped, so if the previous energy is known, then we can flip without calculating the new energy difference. This assumes that the spin of the closest neighbourhood is updated in this energy, otherwise the number of up spins would have to be known to find the new energy difference. If the spin goes from down to up, then it's the same energy difference just with a change of sign. Regardless, the point still stands that

$$e^{\Delta E \beta}$$

does not have to be calculated every flip, however it ends up being implemented.

3 Setting up Ising the model

The Ising model works by setting up an $L \times L$ lattice of spins, either up(+1) or down(-1). The system can be initialized with either random, or uniform, spin directions. Every cycle of the simulation, a spin can either be flipped, or not, depending on a random process determined by the spins energy and the systems temperature. The system favours reaching a steady state, which is the most likely state. The system will eventually converge to the most likely state. For the exact implementation used here, please see the code.

3.1 Periodic boundary conditions

One problem with modelling the real world, with essentially infinite latice size, is what to do at the boundaries? Here we will implement the periodic boundaries, which means that the spin coming after the last spin in the lattice will return the first one, and the one before the first one will return the last one. When summing over the close neighbourhood in

$$E_i = -J \sum_{<kl>}^{N} s_k s_l$$

We can simply implement an if statement for when the index is the first or last. However, if statements are inefficient inside loops, and since we know that the last and first spin per row and column always has this problem, we can simply do these operations outside of the for loop. This will add more lines to the code, but will be much more efficient.

For the 2×2 lattice, we always have this problem for every spin, so the loop with the "normal" sums can be avoided entirely.

3.2 OpenMP multithreading and compiler flags

When creating a temperature gradient, to see how the system behaves as a function of T, it is helpful to implement multithreading so that the program can calculate the statistics for different vales of T simultaneously. In *Table* 2 we see three levels of optimization. While multi threading

proves to drastically imrpve runtimes, the compiler flag -O3 does not seem to do so. This may be either be because the code is so simple that it really can't be optimized much more, or because the code is so bad and complicated that it can't be optimized more. As the author of the program, I hope it is the former rather than the latter.

	-O	OpenMP	-O3 + OpenMP
runtime [s]	12.8726	2.4252	2.4851

Table 2: A run with teperature gradient $\Delta T = 0.02]$ for $T \in [2, 2.6$ with 5000 mcs, compiled with no optimization, OpenMP and OpenMP + -O3 level optimization.

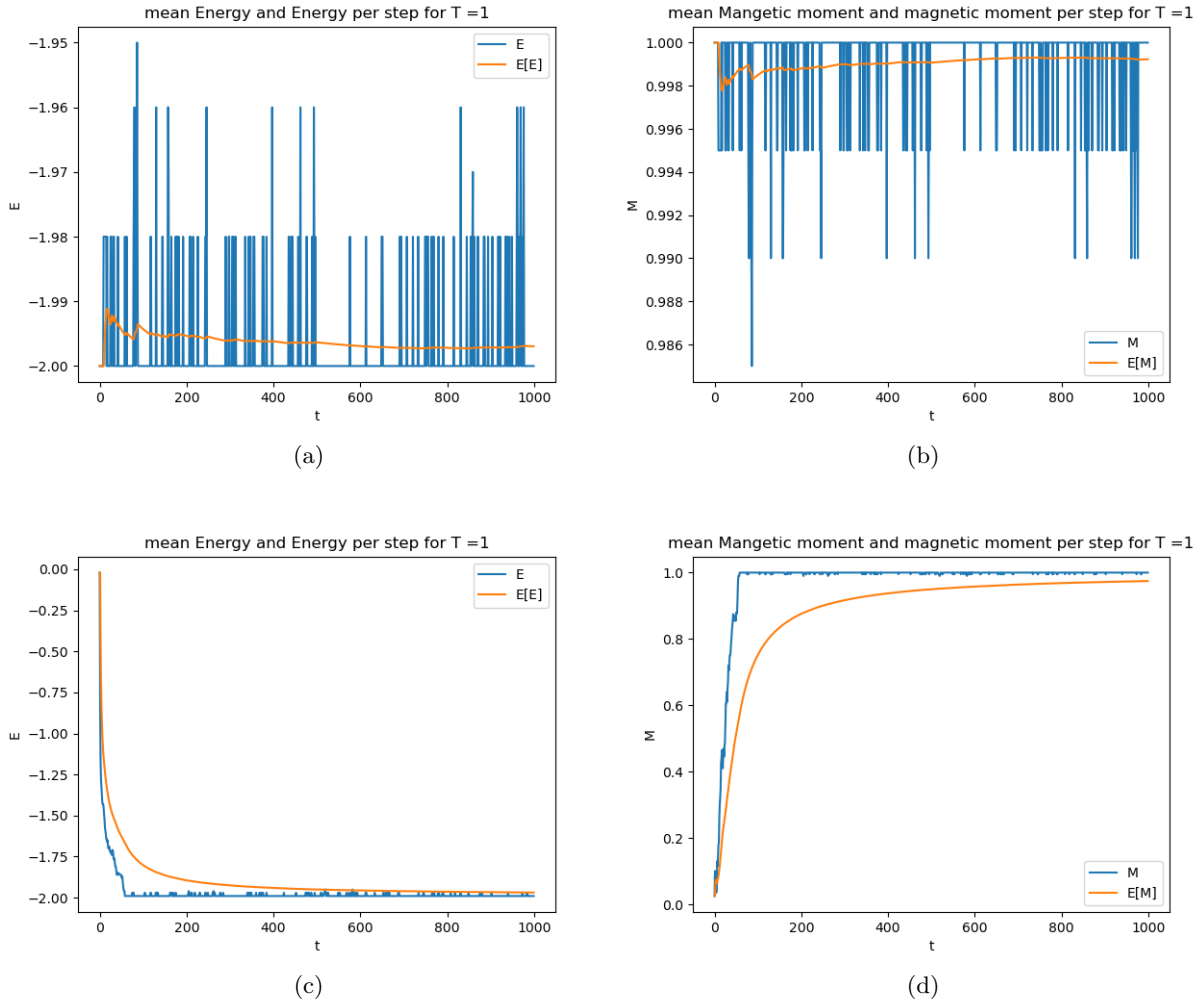
4 Single temperature results

Here, results of the Monte Carlo simulation with only one temperature per run is discussed. We will mainly be working with lattice size L=2 and L=20, and temperatures T=1 and T=2.4.

4.1 2×2 Lattice

The first, and most simple scenario studied is the 2×2 lattice. Although very simple, it can be used to understand how the system works, by comparing it to analytical values as shown in the theoretical section and in *Table* 4. The first objective is to see when the steady state has been achieved, both with starting at all spins up and with random spins.

In *Figure* 1, at T = 1, starting with all spins up, we see that the system is already in its steady state, with very little changes over the 1000 cycles. The random spin runs quickly converge to the steady state with all spins up.



(a) (b)

(c) (d)

Figure 1: Mean magnetic moment per cycle and total magnetic moment per total amount of cycles for a spin up (b) and random spin (d). Mean energy per cycle and total energy per total cycle for spin up start (a) and random spin start (b). The temperature is T = 1 over 1000 cycles.

In *Figure* 2 however, with T=2.4, the neither the random spin start or the all spins up start seems to be the same as the steady state, so the system converges to the steady state. With the average $E[E]$ and $E[M]$, we see that the energy stabilizes, while the magnetic moment tends to fluctuate for T = 2.4.

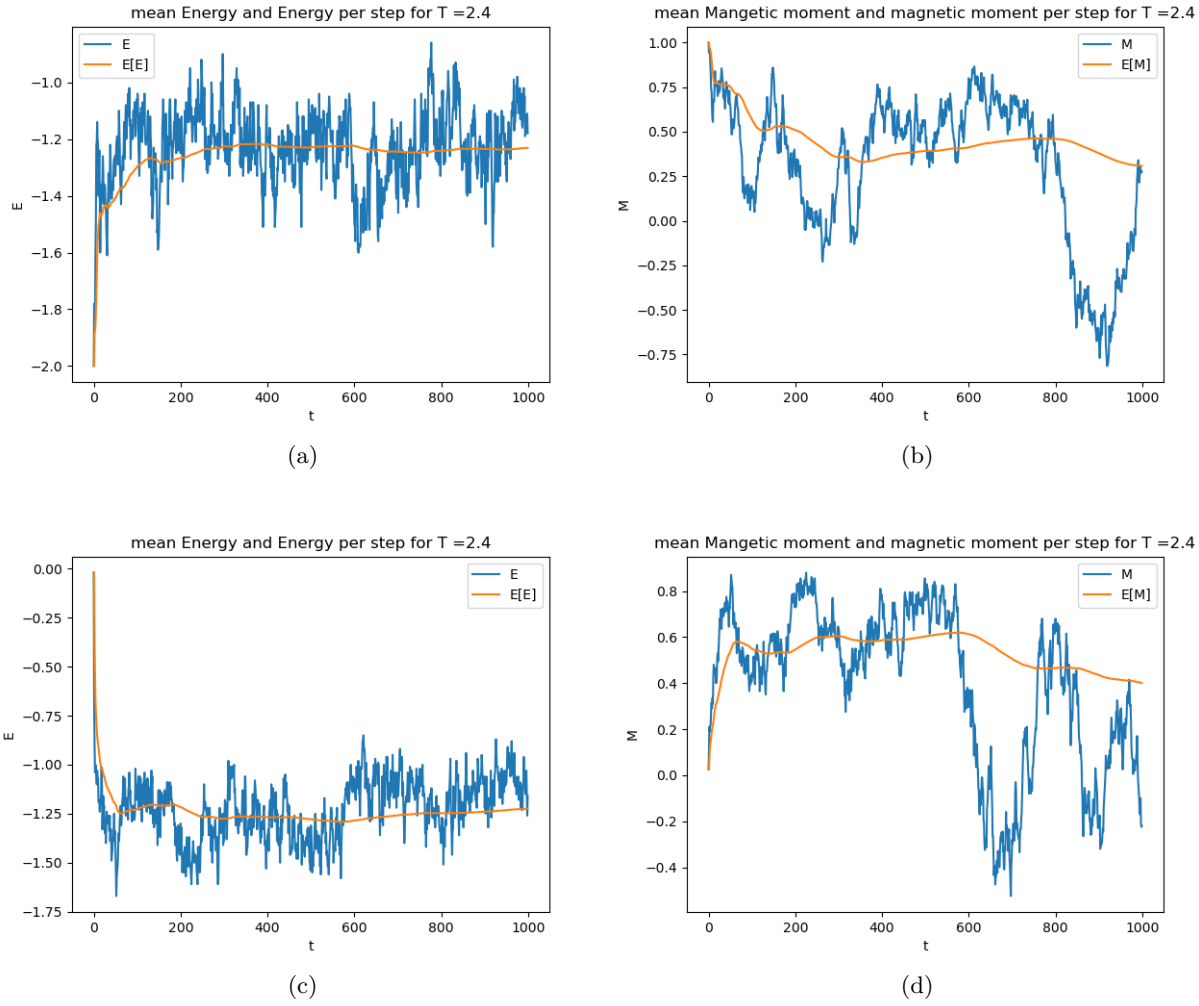


Figure 2: Mean magnetic moment per cycle and total magnetic moment per total amount of cycles for a spin up (b) and random spin (d). Mean energy per cycle and total energy per total cycle for spin up start (a) and random spin start (b). The temperature is T = 2.4 over 1000 cycles.

In both *Figure* 1 and 2, it is assumed that the steady state is reached when the mean energy stabilizes, which occurs somewhere around 100 cycles. From here on, when finding statistics, sampling values only happens after 150 or 200 cycles in similar runs. Also, to prevent cases where the initial condition is the steady state, random spin initial conditions are preferred.

4.2 Energy probability distribution

The energy probability distribution can be studied by counting the number of times any of the 5 possible energies occur. The total should always sum to 1, and the mean of the distribution should correspond to the mean found for the whole system over the whole run.

In *Table* 3, the energy distribution of T=1 and T=2.4 is shown. If we compare the probability distribution with the variance and mean energy in *Table* 4, we see a clear correlation where the low variance occurs in both data sets, and the mean is approximately the same. This is reassuring,

T	P(-4)	P(-2)	P(0)	P(2)	P(4)
1	0	0.998997	0.00066875	0.000334375	0
2.4	0	0.460425	0.259256	0.280319	0

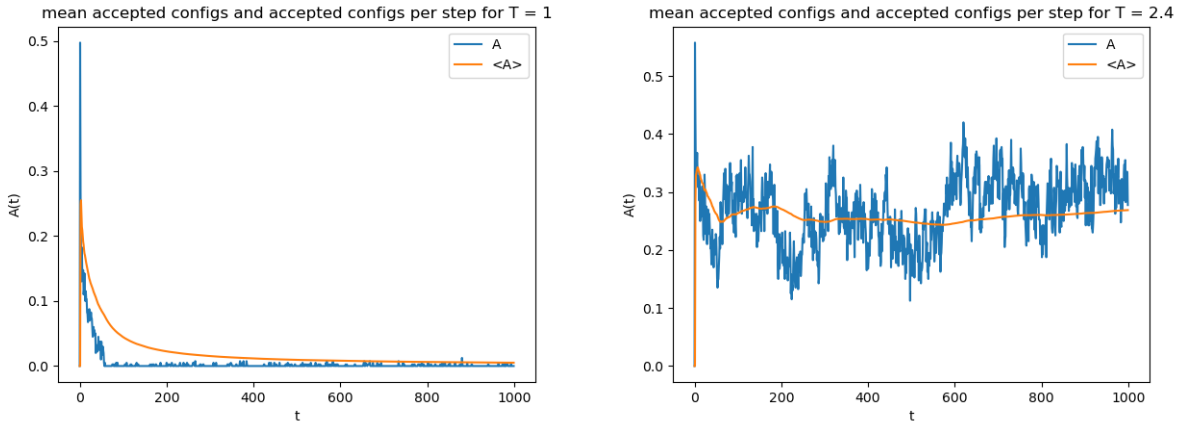
Table 3: The energy probability distribution in a L=20 simulation with 1000 mcs that started sampling at 200 cycles.

as the mean energy of the whole system should correspond to the probability distribution of the single spin energies. This also shows how a distribution of discrete energies can create any energy in between the discrete energies as a mean energy of a big system.

One thing to note is that higher temperature also causes a wider distribution, and greater variance.

4.3 Accepted new configurations

Another thing that is related to temperature, is the number of accepted new configurations. To some extent, this measures how dynamic or static a system is.



(a) (b)

Figure 3: Mean accepted new configurations and accepted new configurations per msc for a system starting with random spins in a 20×20 lattice for T=1 (a) and T=2.4 (b) for 1000 mcs.

In *Figure* 3, we see that initially, after starting at a random configuration, the system accepts a high number of new configurations. After reaching the steady state, the system accepts a constant number of new configurations. The higher temperature system in (b), accepts many more new configurations, causing it to be more dynamic compared to (a) which accepts almost no new configurations after reaching the steady state.

4.4 When to start sampling?

In order to maximize the statistical accuracy of the computed means and variances, one wants to have as much good data as possible, and as little bad data as possible. We want to collect statistics after the system has reached its steady state, as before that there is an unusually high number of new configurations, different mean energy and different magnetic moment than after the system has

reached it's steady state. Unusually high or low values, and an unusually dynamic system, leads to a high variance, which results in a higher standard deviation, which can be interpreted as our error of the mean.

mcs	T	start sampling	σ_E^2	σ_E	computed $< E >$	Analytical$< E >$
1000	1	0	0.0279	0.1670	-1.99659	-1.99598
		150	0.0797	0.2823	-1.990	
1000	2.4	0	8.7060	2.9510	-1.26517	-1.64356
		150	5.3058	2.3034	-1.2326	

Table 4: Statistics produced for simulation runs with L=20 at 1000 Monte Carlo cycles, starting sampling for statistics at 0 and 150 cycles (when steady state is reached), for temperatures 1 and 2.4. The analytical values are for 2×2 lattice, and used for reference only, not a direct comparison.

In *Table* 4, the same simulation as in *Figure* 1 and 2 where the steady state was found is run, starting sampling values for the statistics immediately and after 150 cycles. The error σ, is much lower when sampling starts after reaching the steady state, even though it has fewer values for the statistics. We also see that the mean energy is closer to the analytical values for a 2×2 lattice.

As a result, the sampling for the following section on temperature gradient discards the first 20% of the data to improve statistics. It may be a bit much, but it's better to discard a bit too much than too little, as finding the steady state for each lattice size and temperature and fine tuning it is not practically feasible.

Another strategy can be to calculate local variance, or locally get accepted new configurations, and try to detect when it stabilizes. However this assumes we are even able to effectively implement this, and may slow things down or not work all the time, so it is not done here. As such the blunt strategy of discarding the first 20% is favored.

5 Temperature gradient results

As seen already, the variance of the various statistics changes with respect to temperature. Now, given that we know that energetic and magnetic variance also changes the susceptibility and specific heat, that means that temperature also changes it.

In order to gain insight into this, and how it affects the system, the statistical values mean energy $< E >$, mean absolute magnetic moment $< |M| >$, specific heat C_V and susceptibility X is calculated in steps as seen in *Figure* 4.

The mean energy increases as the temperature increases, seemingly increasing faster before T = 2.3 and slower after T = 2.3. This is to be expected as temperature is a measure of average kinetic energy, so higher temperatures should mean more average energy.

5.1 Evidence of phase change

The mean magnetic moment is somewhat constant, yet decreasing a little before dropping to zero at around 2.3. This can be an indication of ferromagnetic phase transitions, where all magnetic moment is zero after a certain point, and as such the "magnet" stops working when heated up to a critical point.

According to critical phenomena, the magnetic susceptibility and critical heat should peak around the critical temperature. In *Figure* 4, we see peaks at around T=2.3, which is the same temperature as the ferromagnetic phase transition discussed already. As a result, there is strong evidence for a critical temperature and phase transition happening.

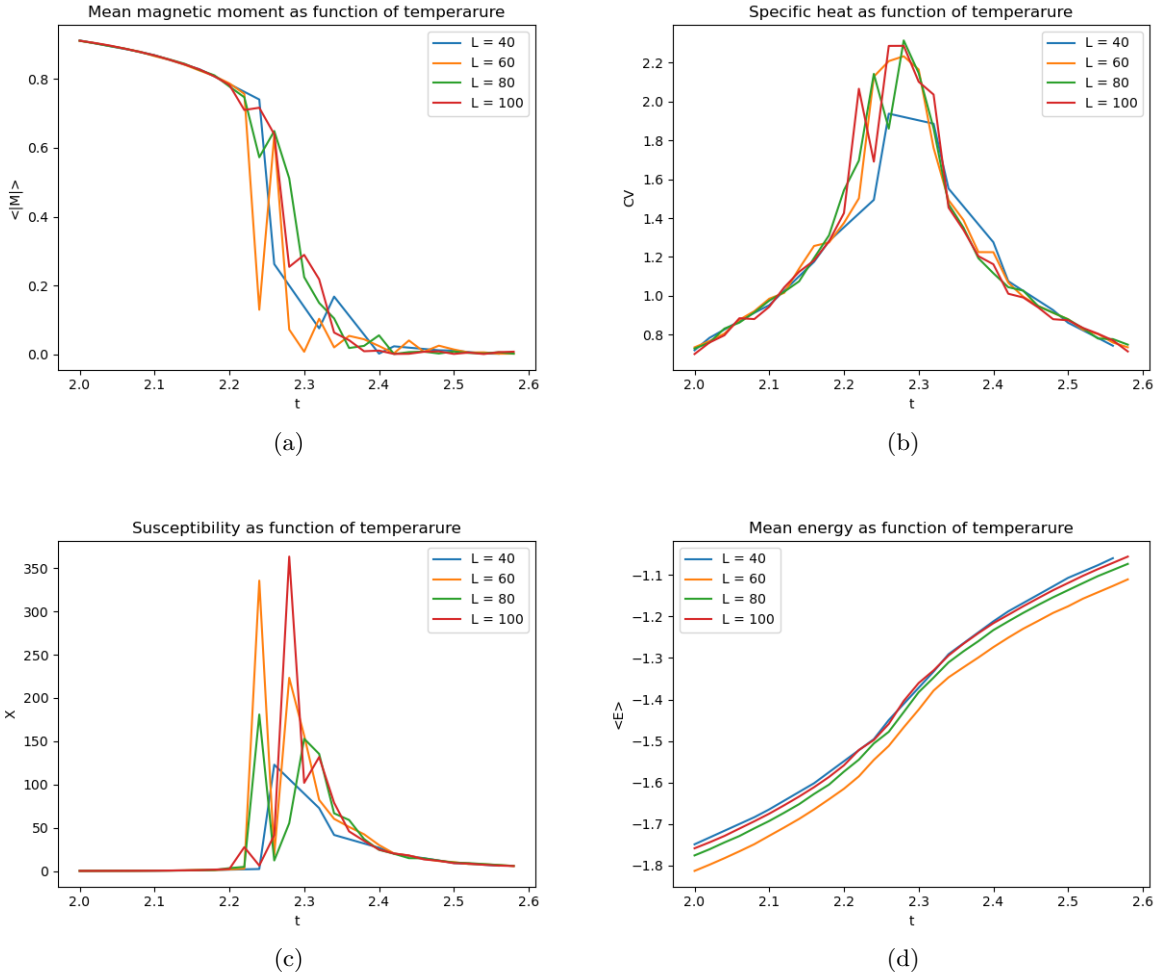


Figure 4: This simulation is ran at 50 000 Monte Carlo cycles per T, with a $\Delta T = 0.2$ on the domain $T \in [2.0, 2.6]$ for square lattices $L \times L$ with L=40, L=60, L=80 and L=100. In (a), the mean absolute magnetic moment is shown as a function time, decreasing after around 2.2-2.3. The mean energy is seen in (d), steadily increasing as the temperature increases. The specific heat (b) and susceptibility (c) peaks a little before 2.3.

5.2 Estimation of critical temperature

From the plots in *Figure* 4, a crude estimate of the critical temperature can be made to be somewhere between 2.2 and 2.3. Any further estimates would need better figures. However, the simulations in *Figure* 4 took approximately 10 minutes to complete with OpenMD and compiler flag optimization, and increasing the accuracy would lead to computing times becoming unpractical for the type of average laptop used. The known value, after Lars Onsager, is 2.269, which is within that interval.

5.3 Lattice size's effect on the statistics

In *Figure* 4, the lattice size doesn't really seem to have a huge effect on the accuracy of the peaks, drops and other characteristics described. Perhaps the number of monte carlo cycles used is too great, so the dominating factor here is mcs and not L. Perhaps the code is bad, and other results should be expected. The curves seem to be somewhat smoother, and peaks somewhat higher, for higher L, but this is inconclusive.

6 Discussion and conclusion

The Monte Carlo method of using the Ising method and the metropolis algorithm for exploring a lattice of binary spins (up or down), proves particularly well suited for numerical methods due to it's analytical solutions for 2×2 lattices, efficient implementation and being limited to only 5 energy levels. In particular, only having 5 energies makes it possible to pre-calculate them, saving a lot of computing time.

The simple 2×2 lattice, with its analytical solutions, gains insight into the validity of our model, helping us find an estimated time for the number of cycles needed to obtain a steady state, which is the most likely state with corresponding mean energy to the anlytical values. Our model did indeed agree with anylitical values of mean energies, meaning that the validity of the model is proven. Additionally, both initializing the system with all spins up, and randomized spins are explored. It turns out that one might accidentally start the simulation in the steady state when all spins are the same, so the random initialization is preferred.

Further, after gaining insight into when the steady state is reached, starting the collection of values from the simulation after the steady state is reached is explored. The σ values for energy and magnetic moment are much lower when waiting for the steady state to be reached before calculating the statistics.

To explore phenomena such as phase transitions and and critical temperature, a temperature gradient with mean energy, mean magnetic moment, specific heat and magnetic susceptibility is generated. Evidence of a phase transition is found, with an estimated ciritcal temperature of T = 2.3. The plots are generated with L=40, L=60, L=80 and L=100, but appear jagged at time, and not smooth. Additionally, the L=100 data was not significantly better, or sharper, or more insightful, than the L=40 data. The reason for this is unknown, perhaps a computational error, or not sufficient cycles or ΔT.

To conclude, the Ising model and metropolis algorithm for a lattice of spins is used to investigate the properties of mean energy, mean magnetic moment, phase transitions and critical temperature phenomena in simulated materials. The analytical solutions of the 2×2 lattice is used to check whether our methods are viable or not. OpenMD and multithreading is implemented for temperature gradients, giving a singificant performance boost.

Acknowledgements

Thank to the developers of "OpenMP" at `https://www.openmp.org//`, and "armadillo" `http://arma.sourceforge.net/` for their cpp tools for linear algebra and multithreading.

References

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[3] "Computational Physics Lecture Notes Fall 2015" by Morten Hjorth-Jensen, Department of Physics, University of Oslo