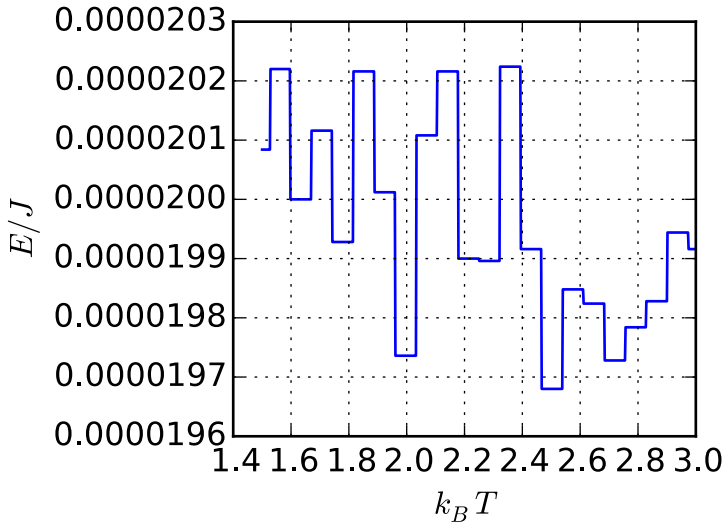
The Ising model in two dimensions

FYS3150

Ivar Haugaløkken Stangeby

November 13, 2015



A Metropolis skyline as a function of temperature for 100000 MC-cycles.

Abstract

In this project we look at the Ising model in two dimensions. There are a set of physical quantities related to magnetic systems that are interesting to examine. We implement the Metropolis algorithm and compute various expectation-values for these quantities. For a 2×2 Ising model we derive the analytical expressions for these values and compare them with the numerically computed ones. We also examine what happen when we reach the thermodynamical limit, as the lattice size of the model increases. All source code can be found on my GitHub page:

github.com/qTipTip

Contents

1 The Ising model

We first start by discussing the Ising Model in its most general form. We later specialize the model to our specific needs.

1.1 The general Ising model

The *Ising Model* is a model in statistical physics that describe phase transitions in ferromagnetism[1]. In this model we represent magnetic dipole moments of

[1] Ferromagnetism is the basic mechanism by which certain materials form permanent magnets, or are attracted to magnets. Ferromagnetism is the strongest type of magnetism.

atomic spins that can be in one of two states, $\uparrow$ or $\downarrow$. The spins are arranged in a *lattice*, which enables us to relate one spin to its neighbors.

We first introduce some notation. Let Λ be a set of lattice positions, where each element in Λ is assigned a set of neighboring sites. The lattice then forms a graph. We assign for each $k \in \Lambda$ a variable σ_k which takes the value 1 or -1, representing the site's spin, $\uparrow$ or $\downarrow$, respectively. We can now create a *spin configuration* σ which is a specific configuration of this lattice. For two sites $i, j \in \Lambda$ one can talk about the *interaction* J_{ij}. Generally, for each $i \in \Lambda$ one also has an *external magnetic field* h_i interacting with i.

We can talk of the *energy* of a specific configuration, which is given by the Hamiltonian

$$E = H(\sigma) = -\sum_{\langle ik \rangle} J_{ij}\sigma_i\sigma_j - \mu \sum_j h_j\sigma_j \tag{1}$$

where the notation $\langle ij \rangle$ just means that we sum over adjacent spins only.

In order to calculate relevant physical quantities for such a system, we need an appropriate probability that describe the probability of finding the system in a certain configuration. The *configuration probability* is given by the Boltzmann distribution

$$P_\beta(\sigma) = \frac{e^{-\beta H(\sigma)}}{Z_\beta} \tag{2}$$

where Z_β is a normalization constant. We call Z_β the *partition function* for the *canonical ensemble*. It is interesting to note that when increasing the temperature T, the probability $P_\beta(\sigma)$ of finding the system in a specific configuration σ *decreases*. This is essentially due to the fact that when we increase the temperature the probability of finding states in an unfavorable configuration become probabilistically feasible in comparison with the most common configurations.

When modeling a magnetic physical system there are certain physical quantities that we are interested in. Firstly, the *mean energy* given by

$$\langle E \rangle = \sum_{i=1}^{M} E_i P_\beta(\sigma) = \frac{1}{Z} \sum_{i=1}^{M} E_i e^{-\beta E_i}. \tag{3}$$

The *mean magnetization* is given by

$$\langle \mathcal{M} \rangle = \sum_{i=1}^{M} \mathcal{M}_i P_\beta(\sigma) = \frac{1}{Z} \sum_{i=1}^{M} \mathcal{M}_i e^{\beta E_i}, \tag{4}$$

where $\mathcal{M}_i = \sum_{j \in \Lambda} \sigma_j$ for all configurations σ and M denotes the number of possible configurations. We are also interested in the *magnetic susceptibility* χ which tells us how much an extensive parameter changes when an intensive parameter increases. It is given by

$$\chi = \frac{1}{k_B T} \left(\langle \mathcal{M}^2 \rangle - \langle \mathcal{M} \rangle^2 \right). \tag{5}$$

The *specific heat* C_V, which tells us how much the energy changes by increasing the temperature, is given by

$$C_V = \frac{1}{k_B T^2} \left(\langle E^2 \rangle - \langle E \rangle^2 \right). \tag{6}$$

If we can make some assumptions about the interaction J_{ij} we can classify the Ising model. If for all $i, j \in \Lambda$ we have

i) $J_{ij} > 0$, we call the interaction *ferromagnetic*;

ii) $J_{ij} < 0$, we call the interaction *antiferromagnetic*;

iii) $J_{ij} = 0$, the spins are non-interacting.

1.2 Ising model specialized to our project

We can make some simplifications to the general Ising model in order to tailor it to our specific needs. First of all, we wish to examine the system with no external magnetic field[2]. We can therefore, due to $h_j = 0$ for all $j \in \Lambda$, rewrite eq. (1) as

$$E = H(\sigma) = -\sum_{\langle ik \rangle} J_{ij} \sigma_i \sigma_j. \tag{7}$$

[2] This specific system was solved analytically by Lars Onsager in 1944.

We also assume that the coupling constant J_{ij} that describe the interaction between neighboring spins as constant J for all $i, j \in \Lambda$. Equation (7) can then be read as

$$E = H(\sigma) = -J \sum_{\langle ik \rangle} \sigma_i \sigma_j \tag{8}$$

In this project we wish to examine a ferromagnetic system, $J > 0$. This in turn, means that it is favorable for neighboring spins to be parallel, as this leads to a lower energy. This can be seen from the fact that $\sigma_i \sigma_j = 1$ whenever spin i and j have the same sign.

1.3 A 2×2 Ising model

In order to get a feel for what these systems look like we examine a two dimensional Ising model with lattice dimensions $L = 2$ and periodic boundary conditions. Our model has $M = 2^4$ different configurations σ. The energy for any arbitrary configuration is given by

$$E_i = -J \sum\nolimits_{\langle kl \rangle}^{4} \sigma_k \sigma_l.$$

Based on this expression we see that whenever all spins are parallel we have a configuration energy of $E_i = -8J$. In the cases where one single spin is anti-parallel to the other three we have a configuration energy of $E_i = 0$. If we have two parallel and two anti-parallel, the configuration energy is $E_i = 0$ or

$E_i = 8J$. Each energy state E_i has a *degeneracy* $\Omega(E_i)$ which corresponds to the number of configurations with the same energy state. The ground state for this system has degeneracy 2, so we can either start with all spin up or all spin down and still be in the lowest energy state possible. For a small 2×2 system such as this one, it is not unlikely that we can transition from a configuration with all spin up to a configuration with all spin down (although keeping the same energy level), however this is unlikely for large lattices.

We are now interested in examining the physical quantities of interest introduced above. For the 2×2 Ising model these quantities have closed form expressions. The work needed to show these relations are given in Appendix A. The partition function for this particular system is given by

$$Z = \sum_{i=1}^{16} e^{-\beta E_i} = 4\cosh(8\beta J) + 12.$$

We can now compute the mean energy of the system. This gives

$$\langle E \rangle = 8J \frac{\sinh(8\beta J)}{\cosh(8\beta J) + 3}$$

Differentiating once more gives us an expression for the specific heat C_V

$$C_V = -\frac{64J^2}{k_B T^2(\cosh(8\beta J) + 3)} \left(\cosh(8\beta J) - \frac{\sinh^2(8\beta J)}{\cosh(8\beta J) + 3} \right)$$

Similarly, we have a closed form expression for the susceptibility:

$$\chi = \frac{8\left(e^{8\beta J} + 1\right)}{\cosh(8\beta J) + 3} \frac{1}{k_B T}.$$

We will later refer back to these specific values for the 2×2 Ising model when we compare the analytical results to the numerically computed values.

2 The Metropolis-Hastings Algorithm

In this project we need random samples from a probability distribution $P_\beta(\sigma)$ associated with the physical system we wish to model. However, direct sampling can be difficult due to the fact that we need to compute the partition function in order to express the probability distribution in its entirety.

The Metropolis-Hastings algorithm is very well suited for this type of problem because in order to sample from a specific distribution $P_\beta(\sigma)$ all we need is a function f proportional to the distribution density.

2.1 The Metropolis Algorithm

Under the assumption that the proposed probability distribution function is symmetric, we can make some simplifications to the Metropolis-Hastings algorithm. This is what we call the Metropolis Algorithm. The general procedure can be described as follows:

1. Initialization: We pick an initial sample.
2. For every iteration:
   (a) We generate a new candidate for the new sample by picking a random element in the sample.
   (b) We calculate the acceptance ratio, which decides whether to reject or accept the new candidate. (This is why the Metropolis algorithm is good for this sort of problem. When computing the acceptance ratio, we divide out the normalization factor Z, which is the computationally heavy bit.)
   (c) If the acceptance ratio is greater than one, we automatically accept the candidate. Otherwise, we accept the candidate with a probability equal to the acceptance ratio. In the case of a rejection the new sample is set to the previous one.

3 Implementation

In this section we take a closer look at some of the implementation specific details in this project. The Ising model was implemented in C++ and the class `Ising.cpp` contains all the methods needed for simulating the model.

3.1 The Ising class

I chose an object-oriented approach to this implementation because I wanted the possibility of having class instances that represented a physical system at any given time. By wrapping all the methods in a class I could easily rerun a similar simulation for a different temperature by re-initializing the system and keeping any values from the previous temperature.[3] I also had a boolean flag for checking whether the system had been previously thermalized for a previous temperature - in that case, one could skip the thermalization.

[3] If I managed to pull any of this through by any stretch of the imagination can be discussed.

I did not manage to figure out a way of outputting data that would satisfy the demands of all the text-problems in the project at once, so I did have to do some monkey-patching for some of them.

The computationally heavy methods are the `simulate` and `metropolis`-methods, where `simulate` calls `metropolis` once for each Monte-Carlo cycle. If we let L denote the grid dimension and M the number of Monte-Carlo cycles, then each call of the `metropolis` method constitutes a complexity of $\mathcal{O}(L^2)$. The `simulate` method calls `metropolis` M times, hence the total complexity for one simulation for one temperature is $\mathcal{O}(ML^2)$.

3.2 Main method

The main method is fairly simple, given a temperature range $[T_1, T_2]$ it assigns a subinterval based on the number of nodes running in parallel to each node.

Each node then proceeds to simulate the system for its assigned temperature range, and outputs its data the same data-file. The sorting of the data is done by `Python`. The parallelization is done using OpenMPI.

3.3 Errors

My program gives correct values for certain systems, and very wonky values for other systems. I have not been able to determine whether this is an artifact of running too few simulations, whether my temperature resolution should have been higher, or whether it is an artifact introduced by the stochastic nature of the algorithms or (most probable) there is a bug somewhere in my program.

Based on the plots produced, all the weird behavior occurs in the quantities directly dependent on the magnetization, which might indicate that that is where the problem lies.

4 Simulations

In this section we simulate the Ising model with various properties and examine the properties of interest as functions of temperature T and as functions of lattice dimension L.

4.1 2×2 Ising with $T = 1$

We assume we have a grid size of 2×2 as in section 1.3. We wish to consider these for a fixed temperature $T' = 1.0$ in units of Tk_B/J. We can therefore make the following algebraic manipulations: Let E' be the energy scaled by the coupling constant J, that is $E' = E/J$. Similarly let $C'_V = C_V/k$ and $\chi' = \chi J$. Let N denote the number of Monte-Carlo cycles.

We can now easily compute the quantities using the closed form solutions given in section 1.3. The results are given in Table 1. If we look at the error in the numerical approximation, by means of the ratio between numerical and analytical results we should expect a convergence towards 1. However, for the specific heat, this is not the case, as the numerical results converge fairly slowly. In fig. 1 we see that the magnetization and energy converge quickly, after only two thousand cycles, the susceptibility follows suit after some 10000 cycles while the specific heat never seem to converge, even after a million cycles.

4.2 20×20 Ising

We now consider a 20 by 20 lattice. We are interested in examining the number of Monte-Carlo cycles needed to establish an equilibrium situation where it is feasible to start calculating the expectation values. We start by plotting the various expectation values as functions of the number of Monte-Carlo cycles. We consider both an initial random configuration and an initial ordered configuration for both the temperature $T = 1$ and $T = 2.4$.

Table 1: Comparing numerical results to closed form analytical solutions for a 2×2 Ising model.

N	$\langle E \rangle$	$\langle \mathcal{M} \rangle$	C_V	χ
100	-2	1	0	0
1000	-2	1	0	0
10000	-1.9964	0.67935	0.0287482	2.14783
100000	-1.99654	0.0276321	0.0276321	3.98085
1000000	-1.99611	0.05832	0.0310754	3.97991
Analytical	-1.99598	0	0.03208	3.99330

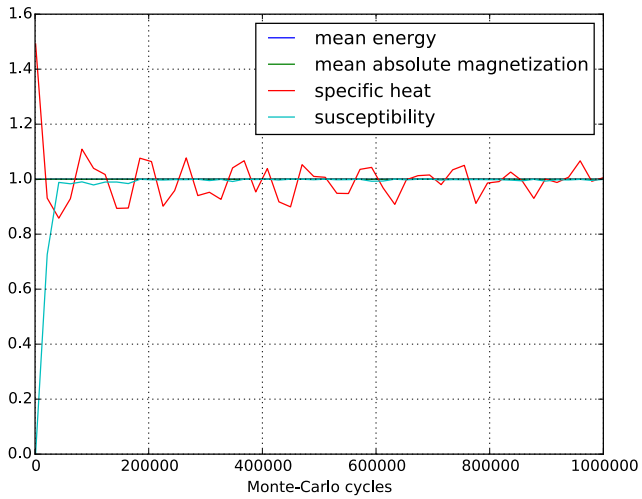


Figure 1: This plot shows the convergence rate of the four quantities of interest. The magnetization and the energy converges after 2000 cycles, while the susceptibility is slightly slower at 10000 cycles. The specific heat fails to converge, even for a million cycles.

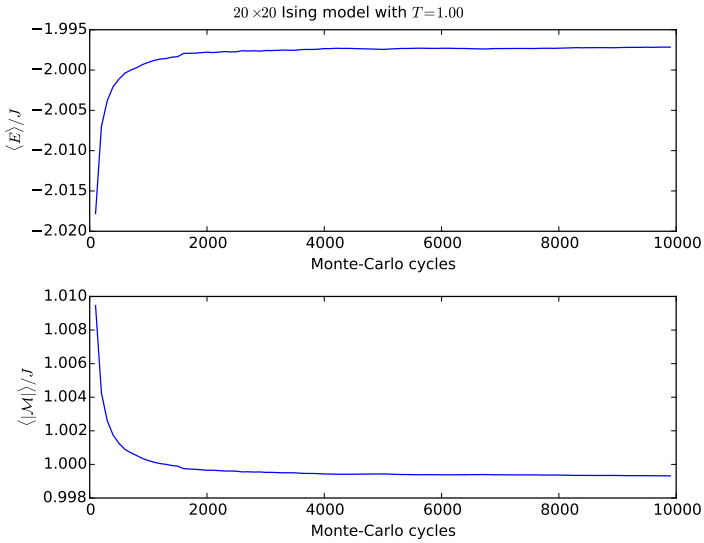


Figure 2: Plotting the expected energy and expected absolute magnetization as functions of the number of Monte-Carlo cycles. This system has a temperature of $T = 1$ and an ordered initial configuration. In this situation the values seem to stabilize around 2000 cycles.

While we're at it, we also keep track of the number of accepted configurations and plot this as a function of temperature. We see that for both random and ordered initial conditions, the system with a temperature of $T = 1$ stabilizes fairly rapidly as can be seen in fig. 2 and fig. 3 With a temperature of $T = 2.4$ however, the expectation values are a bit jittery at first, and seem to somehow converge for upwards of 4000 cycles. This can be seen in fig. 4 and fig. 5.

When we consider the number of accepted states as a function of temperature, we see that it increases drastically as the temperature increases. This is of course in accordance with what we would assume if we were to just look at the probability of any given state. As the temperature increases, the probability of any arbitrary state becomes close to the probability of the most likely state. You can view this as "unlocking" more possible states as the temperature increases. The results are shown in fig. 6.

We also want to look at the probability $P(E)$ for this same system for both temperatures of $T = 1$ and $T = 2.4$. These are given in fig. 7 and fig. 8. If we compare these results to the computed energy variance σ_E^2 which for $T = 1$ is evaluated to $\sigma_E^2 \approx 9.34$ and for $T = 2.4$ is evaluated to $\sigma_E^2 \approx 3229$ we see that the plots seem reasonable.[4] For $T = 1$ the standard deviation $\sigma_E \approx 3.06$ and for $T = 2.4$ it is $\sigma_E \approx 56.8$. The physical interpretation of this is that when increasing the temperature we accept more possible states as previously discussed. We therefore see more energy states appearing further from the most likely state.

[4] These are not per spin as the other quantities discussed.

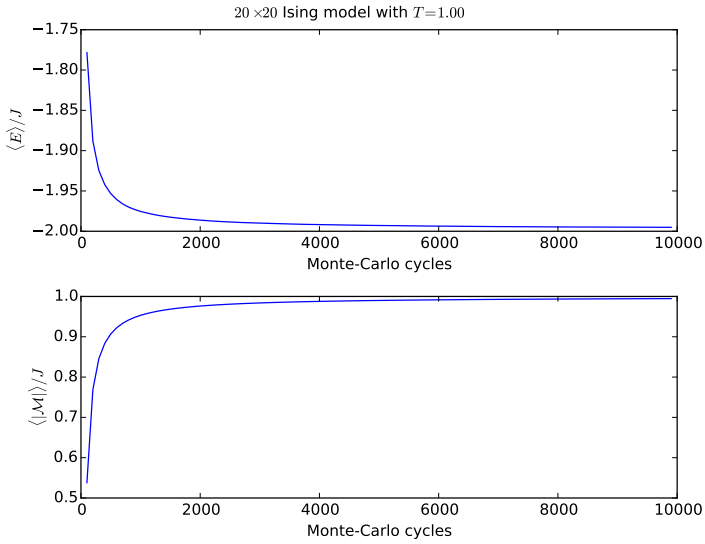


Figure 3: Plotting expected energy and expected absolute magnetization as functions of the numbers of the number of Monte-Carlo cycles. System has a temperature of $T = 1$ with a random initial configuration. The system stabilizes around 2000 cycles.

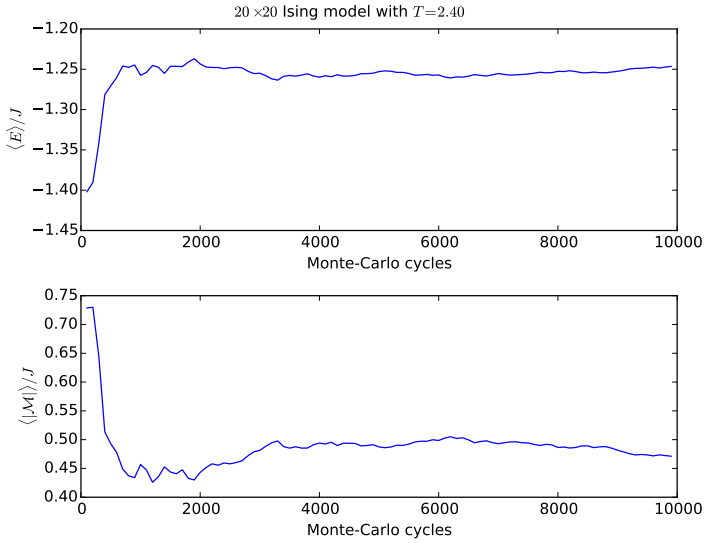


Figure 4: Plotting expected energy and expected absolute magnetization as functions of the numbers of the number of Monte-Carlo cycles. System has a temperature of $T = 2.4$ with a random initial configuration. The system stabilizes around 4000 cycles.

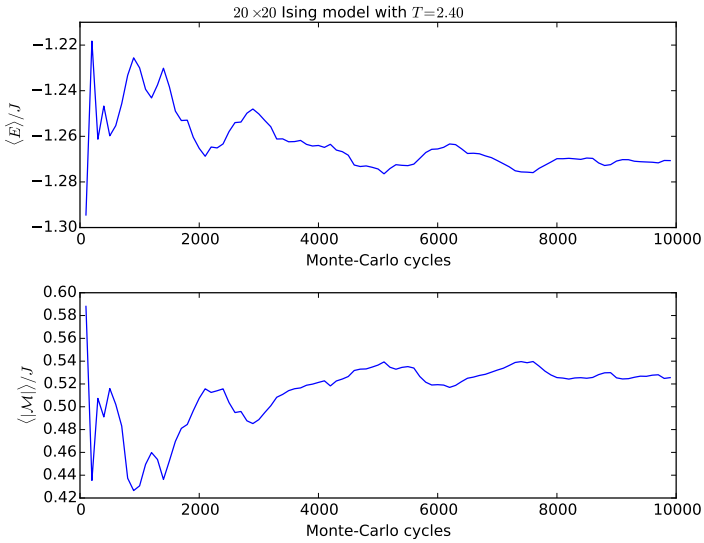


Figure 5: Plotting expected energy and expected absolute magnetization as functions of number of Monte-Carlo cycles. System has a temperature of $T = 2.4$ with a random initial configuration. The values seem to stabilize around 4000 cycles.

4.3 The critical temperature T_C and the thermodynamical limit.

In this section we examine the properties of the Ising model for various grid sizes, and we fix our attention specifically to the temperature interval $[2.0, 2.4]$ as we know that the system undergoes a phase transition for $T \approx 2.3$.

If we look at the plots given in fig. 9, fig. 10, fig. 11 and fig. 12 we see that increasing the grid size changes the behavior of the system close to the critical temperature. Firstly, we see that the susceptibility χ dramatically increase. As far as I have understood, this means that near critical temperature, any change in intensive parameters that does not depend on the number of particles in the system constitutes a large change in magnetization. We also see that as the absolute magnetization converges to zero for increasing grid size near critical temperature which definitely indicates that the system is undergoing a phase transition. I used python to visualize this phase transition for a 200×200-model. A `GIF` can be found in the `animations`-folder.

Near the critical temperature it turns out we can look at the behavior of certain physical quantities by means of a power law. For $\beta = 1/8$, $\alpha = 0$ and $\gamma = 7/4$ we see that the mean magnetization, specific heat and susceptibility as

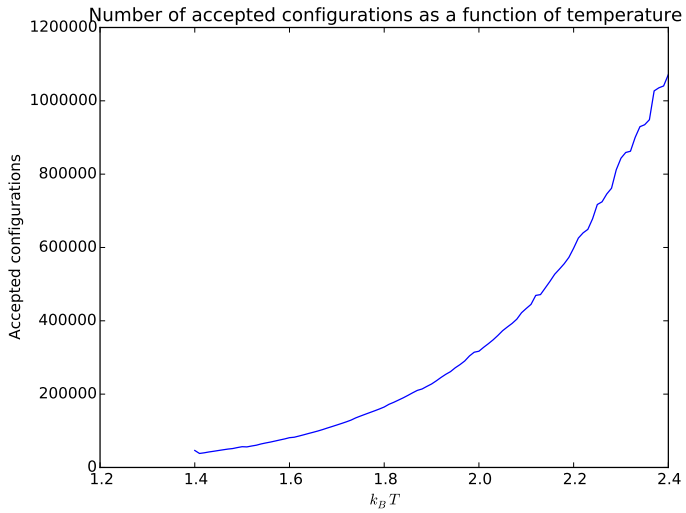


Figure 6: Number of accepted configurations as a function of temperature. The results are in accordance with the mathematical expression for the probability of any given state. This number is probably more interesting when divided by total number of configurations looked at. We then get a graph converging to some number $t \in [0, 1]$ which corresponds to the probability of a configuration being accepted.

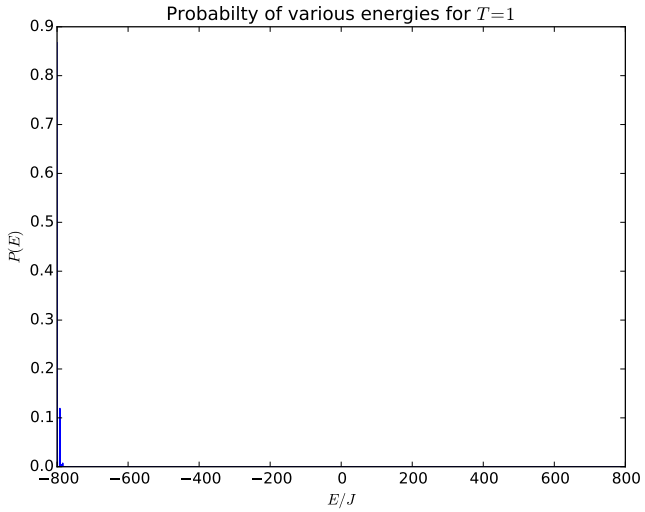


Figure 7: The probabilities of various energy levels in a Ising model with a temperature of $T = 1.0$. The energy states with a high probability are squashed all the way to the left which seems reasonable, since we start with an initially ordered configuration already in its ground state. Under low temperatures, the chance of escaping this ground state is very slim.

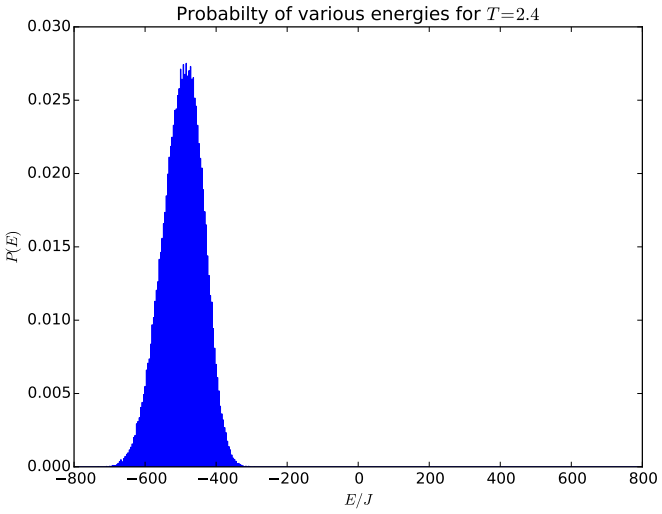


Figure 8: The probabilities of various energy levels in a Ising model with a temperature of $T = 2.4$. Here the energy states of interest are distributed more evenly with the distribution centered at about $-500J$.

functions of temperature T closely follows the following relations:

$$\begin{aligned}\langle \mathcal{M}(T) \rangle &\sim (T - T_C)^{\beta} \\ C_V(T) &\sim |T_C - T|^{\alpha} \\ \chi(T) &\sim |T_C - T|^{\gamma}\end{aligned}$$

We can also look at the relation between a quantity computed for a finite lattice size and the corresponding quantity in the thermodynamical limit. We now wish to see whether we can approximate the thermodynamical limit using our simulations of finite grids. The critical temperature as a function of lattice size satisfies the following relation:

$$T_C(L) - T_C(L = \infty) = aL^{-1/v},$$

where for $v = 1$ the exact result for critical temperature is $kT_C/J = 2/\ln(1 + \sqrt{2})$ which evaluates to approximately 2.269. Rearranging the equation gives us

$$T_C(L = \infty) = T_C(L) - aL^{-1/v}. \tag{9}$$

We can now look at our simulations and see if we can approximate the critical temperature in the thermodynamical limit. My simulations are not sufficiently good for me to be able to point out the differences in critical temperature for the various grid sizes, so all I know is that it is located between $T = 2.25$ and $T = 2.30$. That being said, the only reasonable assumption based on the results my simulations produced is that T_C is 2.275 for all lattice sizes. However, this renders us unable to calculate the factor a in the following relations:

$$\begin{aligned}T_C(L = \infty) &= T_C(20) - a20^{-1} = 2.275 - \frac{a}{20} \\ T_C(L = \infty) &= T_C(40) - a40^{-1} = 2.275 - \frac{a}{40} \\ T_C(L = \infty) &= T_C(60) - a60^{-1} = 2.275 - \frac{a}{60} \\ T_C(L = \infty) &= T_C(80) - a80^{-1} = 2.275 - \frac{a}{80}\end{aligned}$$

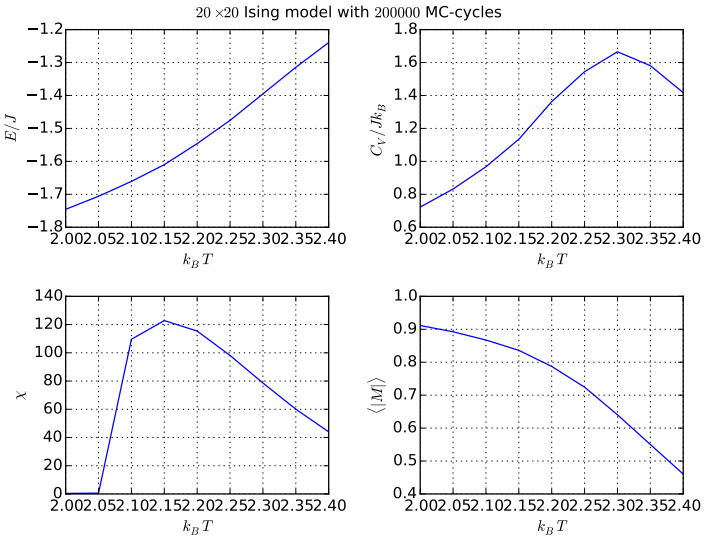


Figure 9: Physical quantities near the critical temperature T_C for a grid size of 20.

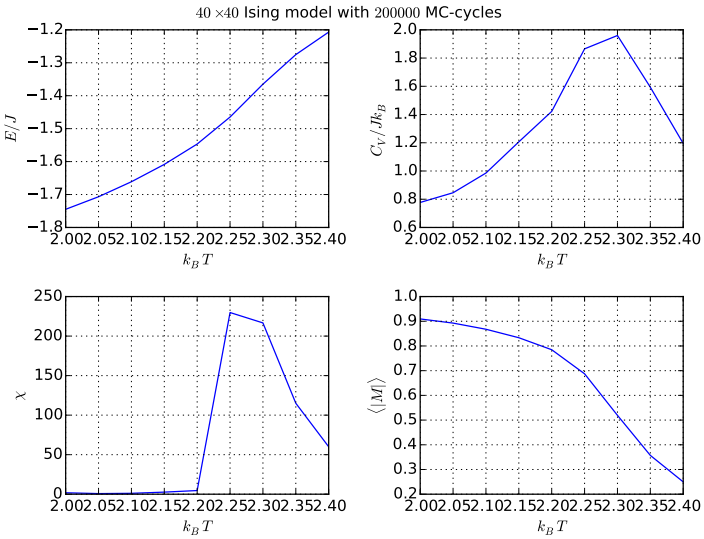


Figure 10: Physical quantities near the critical temperature T_C for a grid size of 40.

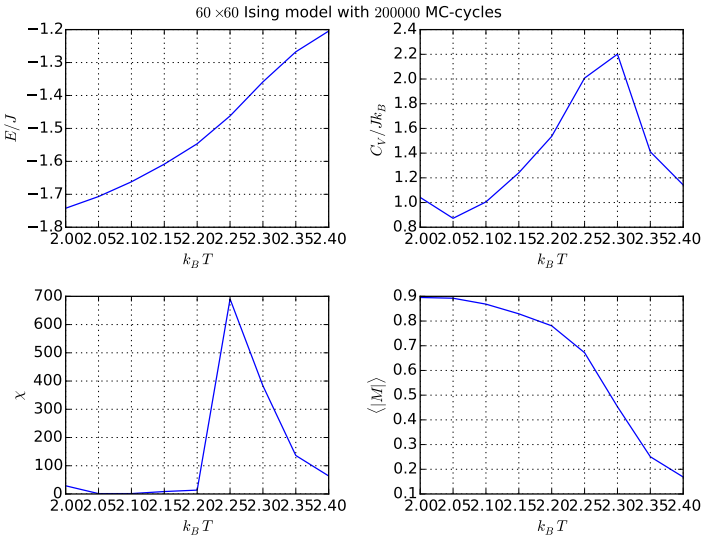


Figure 11: Physical quantities near the critical temperature T_C for a grid size of 60.

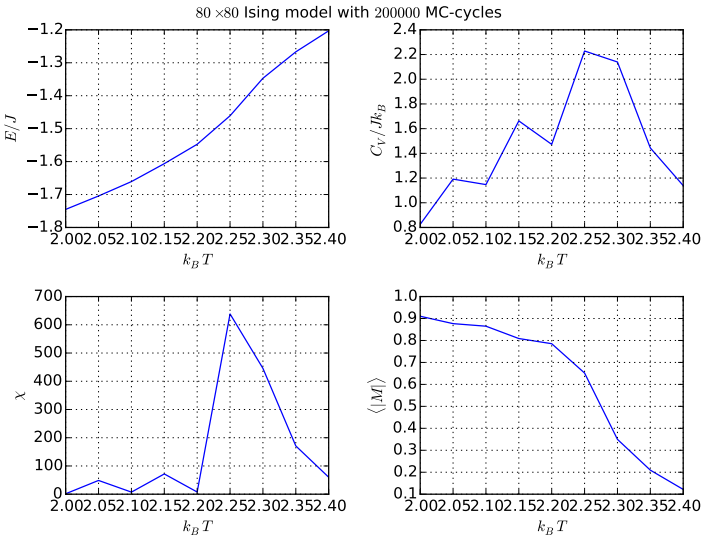


Figure 12: Physical quantities near the critical temperature T_C for a grid size of 80.

5 Conclusion

In this project we implemented the Metropolis algorithm in an effort of simulating the Ising model for varying sizes of finite lattices. My simulations gave me accurate results for certain models and results that did not converge properly for others. This is extra apparent in the plots for varying grid sizes when looking for the critical temperature. Despite these issues I feel that I was able to answer most the questions asked in the problem text.

A Analytical derivations

In this section we derive the closed form analytical expressions for the physical quantities for a 2×2 Ising model. The mean energy and specific heat of a thermodynamical system can be expressed in terms of the partition function.

$$\langle E \rangle = -\frac{\partial}{\partial \beta} \ln Z; \qquad \langle C_V \rangle = \frac{1}{kT^2} \frac{\partial^2}{\partial \beta^2} \ln Z.$$

We recall that the partition function for a 2×2 model is given by $Z = 4\cosh(8\beta J) + 12$. The mean energy then becomes

$$\langle E \rangle = -\frac{\partial}{\partial \beta} \ln\left(4\cosh(8\beta J) + 12\right) = -8J \frac{\sinh(8\beta J)}{\cosh(8\beta J + 3)},$$

and the mean specific heat becomes

$$\begin{aligned} \langle C_V \rangle &= -\frac{1}{kT^2} \frac{\partial}{\partial \beta} \left(-8J \frac{\sinh(8\beta J)}{\cosh(8\beta J + 3)} \right) \\ &= \frac{1}{kT^2} \frac{64J^2}{\cosh(8\beta J) + 3} \left(\cosh(8\beta J) - \frac{\sinh^2(8\beta J)}{\cosh(8\beta J) + 3} \right). \end{aligned}$$

The magnetization of a configuration is given by the sum of all spins. In order to examine the mean magnetization of a system of a given lattice size, we simply sum over all possible magnetizations multiplied by the probability of the system being in each such configuration. Mathematically, this translates into

$$\langle \mathcal{M} \rangle = \frac{1}{Z} \sum_{i=1}^{M} M_i e^{-\beta E_i}.$$

For a simple 2×2 lattice this simply reduces to counting all the possibilities and this gives us that the mean magnetization is

$$\langle \mathcal{M} \rangle = \frac{1}{Z} \left(-4e^{8\beta J} - 8e^0 + 8e^0 + 4e^{8\beta J} \right) = 0.$$

If we were to consider the mean of the absolute magnetization $|\mathcal{M}|$, then this simply becomes

$$\langle |\mathcal{M}| \rangle = \frac{1}{Z} \left(4e^{8\beta J} + 8e^0 + 8e^0 + 4e^{8\beta J} \right) = \frac{4 + 2e^{8\beta J}}{\cosh(8\beta J) + 3}.$$

The susceptibility χ of a thermodynamical system can be calculated if we know the variance $\sigma^2_{\mathcal{M}}$ of the magnetization and is given by

$$\chi = \frac{1}{kT}\sigma^2_{\mathcal{M}}.$$

We first start by computing the variance of the magnetization:

$$\sigma^2_{\mathcal{M}} = \langle \mathcal{M}^2 \rangle - \langle \mathcal{M} \rangle^2 = \frac{32}{Z}\left(e^{8\beta J} + 1\right) - 0 = \frac{8\left(e^{8\beta J} + 1\right)}{\cosh(8\beta J) + 3}.$$

The susceptibility then reads

$$\chi = \frac{8\left(e^{8\beta J} + 1\right)}{kT(\cosh(8\beta J) + 3)}.$$