UNIVERSITY OF OSLO

COMPUTATIONAL PHYSICS

Project 4

UiO : University of Oslo

Authors:

Birgitte Madsen, 66

Magnus Isaksen :14

Soumya Chalakkal, 51

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UiO : University of Oslo

Department of Physics
University of Oslo
Sem Sælands vei 24
0371 Oslo, Norway
+47 22 85 64 28
http://www.mn.uio.no/fysikk/english/

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`https://github.com/csoumya14/ForGitHub_Project4`

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Project Members:

Birgitte Madsen, 66
Magnus Isaksen
Soumya Chalakkal, 51

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ABSTRACT

This project deal with the Ising model in two dimensions without an external magnetic field. A comparative study is made on the expectation values of energy, magnetization, specific heat and susceptibility calculated using the Metropolis algorithm for different lattice sizes, temperature as well as initial spin configurations. An analysis on the behaviour of the Ising model close to the critical temperature for different lattice sizes showed an indication of phase transition.

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CHAPTER

1 INTRODUCTION

This project aims to study the phase transitions at a finite temperature for a magnetic systems using the Ising model for interacting spins in two dimensions without an external magnetic field. A canonical ensemble, which is a collection of micro systems, is considered from which the mean energy, mean magnetization and thermodynamical quantities, like susceptibility and specific heat, are derived as functions of temperature and spin lattice size. When the phase transition happens, the susceptibility and specific heat peak, and hence from these values, which can be computed, the critical temperature can be found. The main objective is to determine the critical temperature, at which the phase transition happens, for an infinitely large lattice. Since computations cannot be done for infinitely large lattices, the critical temperature for the infinitely large lattice is deduced from critical temperatures of several finite lattice sizes.

To compute the mentioned thermodynamical quantities, Monte Carlo cycles and the Metropolis algorithm is applied for the simulation of the Ising model in two dimension. The mean energy, mean magnetization, specific heat and susceptibility is initially solved both analytically and by computations for $T = 1.0$ and $N = 2 \times 2$, which is then used to test the validity of the computed Ising model for solving similar problems with different temperatures and greater spin lattices.

The number of Monte Carlo cycles needed to achieve the steady state for different temperatures and different initial spin configurations is, furthermore, studied together with the probability of the spin system having a specific energy. The dependence of the temperature on the energy of the spin system is estimated by computing this probability of appearance of specific energy states for temperatures $T = 1$ and $T = 2.4$ after reaching the steady state. These results are compared with the computed variance in energy.

Finally, the behaviour of the Ising model is studied when temperature becomes close to the critical temperature as a function of the lattice size by parallelizing the code using openMP and from the results obtained the critical temperature for an infinitely large lattice is estimated.

The main part of the report consists of two chapters: The methods and theory chapter, and the results and discussion chapter.

CHAPTER

2 METHOD

The Ising model is one of the widely studied models in statistical physics for simulations of phase transitions. It describes effectively how a magnetic material responds to thermal energy and an external magnetic field. The model consists of domains which can be considered as the poles of a bar magnet with a corresponding spin of north or south. These spins are assigned values of $+1$ or -1 to the north and south respectively. In this project an Ising model in two dimensions without an external magnetic field is considered. Here the system is represented as a canonical ensemble which exchange heat with the environment. The energy of the system in its simplest form is expressed as

$$E = -J \sum_{<kl>}^{N} s_k s_l \tag{2.1}$$

in which $s_k = \pm 1$ is the k'th spin, either up or down, $N = L \times L$ is the total number of spins in the lattice, and J is a coupling constant. The coupling constant is dependent on the strength of interaction between neighbouring spins k and l.

The source codes for the algorithms described in this chapter can be found in the Github folder `https://github.com/csoumya14/ForGitHub_Project4`.

2.1 Determining Quantities

For the canonical ensemble with probability distribution given by the Boltzmann distribution

$$P_i(\beta) = \frac{e^{-\beta E_i}}{Z} \tag{2.2}$$

with $\beta = 1/k_B T$, in which k_B is Boltzmann's constant and T is the temperature of the system, E_i being the energy of the i'th microstate, and Z being the partition function given by

$$Z = \sum_{i=1}^{M} e^{-\beta E_i} \tag{2.3}$$

for a system with M microstates. For each microstate i in a spin system with N spins $s_i = \pm 1$, the energy E_i and magnetization $\mathscr{M}_i$ are given as

$$E_i = -J \sum_{<kl>}^{N} s_k s_l \qquad \text{and} \qquad \mathscr{M}_i = \sum_{j=1}^{N} s_j \tag{2.4}$$

in which $< kl >$ means that the sum is over nearest neighbours, only, and J is the coupling constant that gives the interaction between these neighbouring spins. The expectation value of the energy, is then given as

$$\langle E \rangle = \sum_{i=1}^{M} E_i P_i(\beta) = \frac{1}{Z} \sum_{i=1}^{M} E_i e^{-\beta E_i} \tag{2.5}$$

whilst the expectation value of the magnetization, can be determined by

$$\langle \mathscr{M} \rangle = \sum_{i=1}^{M} \mathscr{M}_i P_i(\beta) = \frac{1}{Z} \sum_{i=1}^{M} \mathscr{M}_i e^{-\beta E_i} \tag{2.6}$$

From the variance of E and $\mathscr{M}$, the specific heat C_v and susceptibility χ can be found, respectively. That is

$$C_v = \frac{1}{k_B T^2} \left\langle \langle E^2 \rangle - \langle E \rangle^2 \right\rangle \qquad \text{and} \qquad \chi = \frac{1}{k_B T} \left\langle \langle \mathscr{M}^2 \rangle - \langle |\mathscr{M}| \rangle^2 \right\rangle \tag{2.7}$$

2.2 Closed Form Expressions of Quantities for the General 2×2 Spin Case

The system consisting of 2×2 spins has in total $2^4 = 16$ spin configurations. These 16 configurations are given in Fig. 2.1 below.

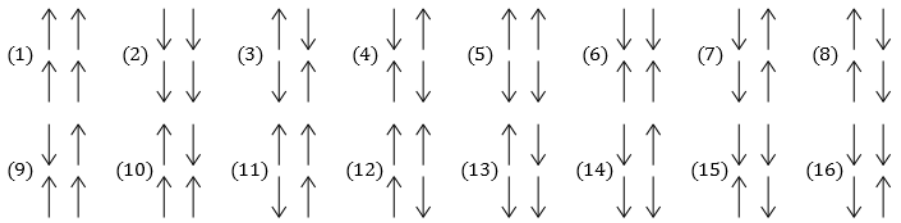

Figure 2.1. The 16 different spin configurations for the 2 dimensional case with 2 spins in each dimension. An arrow pointing upwards represents spin up with the spin value $s_{up} = +1$, whilst an arrow pointing downwards represent spin down with the spin value $s_{down} = -1$. The corresponding energies and magnetizations of each of the micro states can be found in Tab. 2.1.

The energy and magnetization for each of the 16 microstates are given in Tab. 2.1 and are calculated from Eq. (2.4). As an example, the energy and magnetization of the ninth microstate, given in Fig. 2.1 as the state with one spin down and three spin up, is calculated here:

$$\begin{aligned} E_9 &= -J \sum_{<kl>}^{2\times 2} s_k s_l \\ &= -J[((-1)\cdot 1 + (-1)\cdot 1) + (1\cdot(-1) + 1\cdot 1) + (1\cdot(-1) + 1\cdot 1) + (1\cdot 1 + 1\cdot 1)] \\ &= 0 \end{aligned}$$

and

$$\mathscr{M}_9 = \sum_{j=1}^{2\times 2} s_j = (-1) + 1 + 1 + 1 = 2$$

Table 2.1. Energy and magnetization of each of the spin configurations given in Fig. 2.1.

Configuration	Energy	Magnetization
(1)	$-8J$	4
(2)	$-8J$	-4
(3) – (4)	$8J$	0
(5) – (8)	0	0
(9) – (12)	0	2
(13) – (16)	0	-2

Hence the partition function Z defined in Eq. (2.3) for this 2×2 spin system becomes

$$Z = 12 + 2\left(e^{8\beta J} + e^{-8\beta J}\right) = 12 + 4\cosh(8\beta J) \tag{2.8}$$

The last equal sign follows from Euler's identity and the definition of $\cosh\theta$. With this partition function and the energy and magnetization for each of the 16 microstates given in Tab. 2.1, the expectation value of the energy and the magnetization becomes

$$\langle E \rangle = \frac{1}{Z}(-16Je^{8\beta J} + 16Je^{-8\beta J}) = \frac{16J}{Z}(e^{-8\beta J} - e^{8\beta J}) \tag{2.9}$$

and

$$\langle \mathscr{M} \rangle = \frac{1}{Z}(4e^{8\beta J} - 4e^{8\beta J} + 2 - 2) = 0 \tag{2.10}$$

However, the expectation value of the absolute value of the magnetization differ from zero. That is

$$\langle |\mathscr{M}| \rangle = \frac{1}{Z}\left(|4|e^{8\beta J} + |-4|e^{8\beta J} + |2| + |-2|\right) = \frac{1}{Z}(8e^{8\beta J} + 4) \tag{2.11}$$

To compute the specific heat C_v and the susceptibility, the quantities $\langle E^2 \rangle$ and $\langle \mathscr{M}^2 \rangle$ must be known. For this 2×2 spin case they become

$$\langle E^2 \rangle = \frac{1}{Z}\sum_{i=1}^{16} E_i^2 e^{-\beta E_i} = \frac{128J^2}{Z}(e^{8\beta J} + e^{-8\beta J}) \tag{2.12}$$

and

$$\langle \mathscr{M}^2 \rangle = \frac{1}{Z}\sum_{i=1}^{16} \mathscr{M}_i^2 e^{\beta E_i} = \frac{32}{Z}(e^{8\beta J} + 1) \tag{2.13}$$

The specific heat C_v and the susceptibility χ can now be determined by the expressions in Eq. (2.7), and after some manipulations with the results gained by Eq. (2.9), (2.10), (2.12) and (2.13), it is evident that

$$C_v = \frac{128J^2}{Zk_BT^2}\left[e^{8\beta J} + e^{-8\beta J} - \frac{2e^{-16\beta J} + 2e^{16\beta J} + 4}{Z}\right] \tag{2.14}$$

and

$$\chi = \frac{1}{k_BTZ}\left[32(e^{8\beta J} + 1) - \frac{1}{Z}\left(8e^{8\beta J} + 4\right)^2\right] \tag{2.15}$$

2.3 Closed Form Solutions for the 2×2 case with $T = 1.0$

In this project, the temperature is given in the units of $[k_B T/J] = [1/\beta J]$. To distinguish this from the temperature T in the ordinary unit of Kelvin, the considered temperature is, in this section, written as $\tilde{T}$. In Sec. 2.4, the c++ code for computing the expectation value of the energy and the magnetization and the specific heat and susceptibility of the 2×2 spin case with temperature $\tilde{T} = 1.0$ is introduced. The section is dedicated to find the closed form solutions for these quantities for this situation with the purpose of testing the code introduced in the mentioned section.

With $\tilde{T} = 1/\beta J = 1.0$, the partition function in Eq. (2.8) gives the value

$$Z = 12 + 4\cosh(8) \approx 5973.9 \tag{2.16}$$

The expectation value of the magnetization is still zero, whilst the expectation value of the absolute value of the magnetization becomes

$$\langle \mathscr{M} \rangle = \frac{1}{Z}(8e^8 + 4) \approx 3.9926 \tag{2.17}$$

With the temperature given in units of $[k_B T/J]$, the formulas for determining the expectation value of the energy and the specific heat and susceptibility, given in the previous section, must be slightly modified to give a value. E.g. the expectation value of the energy given by Eq. (2.9) will have to be divided by J, giving the computed expectation value in the unit of $[E/J]$. For a temperature of $\tilde{T} = 1.0$, the computed expectation value of the energy is then

$$\langle \tilde{E} \rangle = \frac{\langle E \rangle}{J} = \frac{16}{Z}(e^{-8} - e^8) \approx -7.9839 \tag{2.18}$$

This is approximately the same as the lowest energy state of the system (see Tab. 2.1), which is also what was to be expected for low temperatures. To find C_v and χ, Eq. (2.14) and (2.15) are considered, and with a temperature $\tilde{T} = 1.0$, they give the values

$$\tilde{C}_v = \frac{C_v}{J} \approx 0.12830 \qquad \text{and} \qquad \tilde{\chi} = \chi J \approx 0.03209$$

The values of the quantities gained in this section for the 2×2 spin case with $\tilde{T} = 1.0$ in units of $[k_B T/J] = [1/\beta J]$ are collected in the table below.

Table 2.2. Various quantity values for the 2×2 spin case with temperature $\tilde{T} = 1.0$ in units of $[k_B T/J] = [1/\beta J]$.

$\langle \tilde{E} \rangle$	$\langle \mathscr{M} \rangle$	$\langle \lvert \mathscr{M} \rvert \rangle$	$\tilde{C}_v$	$\tilde{\chi}$
-7.9839	0	3.9926	0.12830	0.03209

2.4 Ising model for $N = 2 \times 2$ with $T = 1.0$

The Ising model is used to study the phase transition of an element. In this case looking at a 2×2 spin system. This is done using Monte Carlo methods for estimating the changes.

Starting by making a spin matrix as seen in code below, in which 1 corresponds to spin up, and -1 corresponds to spin down. Whether the entrances of the spin matrix take the value 1 or -1 will not influence the computed expectation values as long as the number of Monte Carlo cycles are high enough. But it gives control over the energy and magnetization in the beginning.

```
mat spin_matrix(n,n);
   spin_matrix(0,0) =-1;
   spin_matrix(0,1) = -1;
   spin_matrix(1,0) = 1;
   spin_matrix(1,1) = 1;
```

The flipping of the spins happen randomly, so a random number generator is used to generate either one or zero. This allows for equal chance of the spins flipping. When finding the expected energy value, the change in energy is added up for all the Monte Carlo cycles (MC cycle). When dividing the sum of the energies in each Monte Carlo cycle by the number of Monte Carlo cycles, the most likely energy state. The magnetization is found by adding up the spins as given in Eq. (2.4).

The specific heat is found using

$$\frac{C_v}{J} = \frac{1}{MC^2_{cycles}}(\langle E^2\rangle - \langle E\rangle^2) \tag{2.19}$$

in which the expectation value of the energy is found by adding the energies for every Monte Carlo cycle and dividing by the total number of Monte Carlo cycles. The expectation value of the squared or the energy is found in a similar same way. The energy is generated individually depending on which spin is flipped.

Proceeding to generate the energy and magnetization when the spin changes. This is done using MC cycles and finding the energy change when a spin flips.

```
for (int cycles = 1; cycles <= mccycles; cycles++){
    for (int k=0; k<n; k++){
    for (int i=0; i<n; i++){
    x[i] = 1.99999*((double) rand() / (RAND_MAX)); //making sure that the row and
        column number is either 0 or 1 (randomly chosen - almost uniform)
    y[i] = 1.99999*((double) rand() / (RAND_MAX));
    //cout << "x=" << setw(5) << x[i] << setw(5) << "y=" << setw(5) << y[i] << endl;
    if (x[i]<1){
        DE_x = 4*spin_matrix(x[i],y[i])*spin_matrix(x[i]+1,y[i]);}
    else{
        DE_x = 4*spin_matrix(x[i],y[i])*spin_matrix(x[i]-1,y[i]);}
    if (y[i]<1){
        DE_y = 4*spin_matrix(x[i],y[i])*spin_matrix(x[i],y[i]+1);}
    else{
        DE_y = 4*spin_matrix(x[i],y[i])*spin_matrix(x[i],y[i]-1);}
    DE = DE_x+DE_y;
    if (DE <= 0){
        E += DE;
        M += -2*spin_matrix(x[i],y[i]);
        spin_matrix(x[i],y[i]) = -spin_matrix(x[i],y[i]);}
    else{
        w = exp(-DE/T);
        if (w > ((double) rand() / (RAND_MAX))){
            E += DE;
```

```
            M += -2*spin_matrix(x[i],y[i]);
            spin_matrix(x[i],y[i]) = -spin_matrix(x[i],y[i]);
        }}}}
    // making the energy, magnetization and the squared of them
    E_expectation += E;
    M_expectation += M;
    M_expectation2 += fabs(M);
    E_squared += E*E;
    M_squared += M*M;}
```

2.4.1 Test of one Spin Flip for 2×2 Case

A simple test is made on the algorithm by considering a 2×2 lattice having four spin values which forms the four elements of a 2 by 2 matrix. Here we calculated how the energy and magnetization of the lattice changes with one spin flip. The matrix elements are chosen to be $a_{11} = 1$, $a_{12} = -1$, $a_{21} = 1$, $a_{22} = 1$. The spin at the position $a_{12} = -1$ is selected and energy of the initial configuration is calculated by multiplying spin value at a_{12} with the neighbouring spin values and adding them that gave a result of 0. The calculated energy is tested to be less than or equal to zero or not. If it is the configuration is accepted and the energy and magnetization is updated and the configuration is changed by flipping one spin only and if its not then the value $w = exp(-\Delta E/T)$ is calculated and the probability w is compared with a random number r uniformly distributed between 0 and 1. If $w > r$ the configuration is accepted and the energy and magnetization is updated and the configuration is changed by flipping the spin. In the present case since the calculated energy of the present state is equal to 0 the present configuration is accepted and the configuration is changed by flipping the spin at position a_{12}. This gives the new configuration $a_{11} = 1$, $a_{12} = 1$, $a_21 = 1$, $a_{22} = 1$. The change in energy due to switch of spin is found to be equal to -8, which is the expected value and change in magnetization which is calculated as magnetization before spin flip +2 times the selected spin value and is equal to -2 which is also the expected value.

2.5 Ising Model for $N > 2 \times 2$

The c++ code given in Sec. 2.4 is customized for the two dimensional case with 2 spins in each of the two dimensions. To be able to find the expectation value of the energy and magnetization and the specific heat and susceptibility of a larger spin system, the code presented in Sec. 2.4 must be modified.

The first modification appear when introducing periodic boundary conditions to a lattice in which some elements are boundary elements while other elements are not. When a non-boundary element k is flipped, the change in energy will be two times the energy calculated by Eq. (2.4) with k being the flipped element, and l's being the four neighbours of that element. However, a boundary element will only have two or three neighbours. Consider the 4×4 case in Fig. 2.2 in which the boundary element in the upper leftmost corner is flipped.

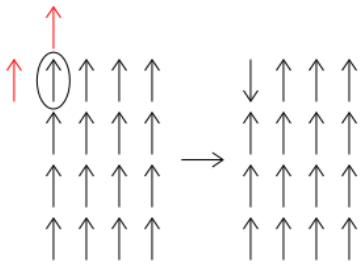

Figure 2.2. Example of spin flip for a 4×4 spin lattice. When calculating the energy change due to the flip of a corner spin, assume periodic boundary conditions, as shown with the red arrows.

When this corner element is flipped, the change in energy will depend on the two neighbours of that element *and* the last element in the same row as the flipped spin and the last element in the same column as the flipped spin due to the periodic boundary conditions. Hence, instead of calculating the change in energy using the four if-tests in Sec. 2.4, the energy change due to a spin flip at a random entrance (x[i],y[i]) of the spin matrix is computed as in the following lines of code.

```
DE = 2*spin_matrix(x[i],y[i])
   *(spin_matrix(x[i],periodic(y[i],-1,n)) + spin_matrix(x[i],periodic(y[i],1,n))
   + spin_matrix(periodic(x[i],-1,n),y[i]) + spin_matrix(periodic(x[i],1,n),y[i]))
```

The periodic function in the above c++ lines takes care of the periodic boundary condition. Consider the source code for the function *periodic*:

```
int periodic(int entrance, int pm, int spins)
//Takes care of the periodic boundary condition of lattice with "spins" number of
    spins in each direction
//pm = -1 returns the "entrance" to the left of the considered element, if the
    considered element is not a boundary element in the first row/column of the matrix.
//pm = 1 returns the "entrance" to the right of the considered element, if the
    considered element is not a boundary element in last row/column of the matrix.
{
    return (entrance + pm + spins) % spins; // "sum mod spins"
}
```

For a non-boundary element, the element spin-matrix(x[i],periodic(y[i],-1,n)) will be the element to the left of the chosen element (x[i],y[i]) in the spin matrix since $0 < y[i] < spins$ which means that the returned spin matrix element is spin-matrix(x[i],y[i]-1). If instead (x[i],y[i]) is a boundary element, say in the upper leftmost corner as in Fig. 2.2, the returned element when calling the periodic function as before is then spin-matrix(x[i],spins-1), which is the last element in the same row as the considered element, as wanted.

Since the only contributors to the change in energy when just one spin is flipped is the flipped spin itself and the four neighbouring spins, there are only 5 possible changes in energy for one spin flip. These are

$$\Delta\tilde{E} = \frac{\Delta E}{J} = \{-8,-4,0,4,8\} \tag{2.20}$$

This means that the probability function $w(E_i) = e^{-\beta E_i}$ for accepting the move can be precalculated before the actual Monte Carlo cycles, and the computational time is decreased. The inclusion of this is seen in

the source code below.

```
double w[microstates];
for (int i =0; i < microstates; i++){
    w[i] = 0;
}
for (int dE = -8; dE <= 8; dE+=4){
    w[dE+8] = exp(-dE/T);
}
for (int cycles = 1; cycles <= mccycles; cycles++){
    for (int i=0; i<n*n; i++){
    //computing row x[i] and column y[i] number as a random integer between 0 and n-1
        (almost uniformly distributed)
    x[i] = (n-0.000001)*((double) rand() / (RAND_MAX));
    y[i] = (n-0.000001)*((double) rand() / (RAND_MAX));
    DE = ....;
    if (w[DE+8] >= ((double) rand() / (RAND_MAX)))
    //comparing prop function to uniformly distributed random number between 0 and 1
    {
        spin_matrix(x[i],y[i]) = -spin_matrix(x[i],y[i]);
        E += DE;
        M += 2*spin_matrix(x[i],y[i]);
    }
    }
}
```

For the 2×2 case, the probability function is then computed as the vector

$$\mathbf{w} = \{e^{8/T}, 0, 0, 0, e^{4/T}, 0, 0, 0, 1, 0, 0, 0, e^{-4/T}, 0, 0, 0, e^{-8/T}\} \tag{2.21}$$

The value of $e^{8/T}$, $e^{4/T}$ and 1 will *always* be larger than or equal to the generated random number between 0 and 1, and hence the suggested flip will always be accepted if the flip gives rise to an energy change of -8, -4 or 0. If the energy is positive, the flip will be accepted with a probability that depends on the temperature T. Higher temperature leads to more accepted moves.

Apart from the periodic function and the probability function, the way of calculating the wanted quantities using this generalized c++ code is similar to the way given in Sec. 2.4, and that the two codes give similar results for the 2×2 case can be seen in Sec. 3.1.

2.6 Critical Temperature

The Ising model in two dimensions exhibits a critical phenomena so that below a given critical temperature T_c a spontaneous magnetization $\langle M \rangle = 0$ appears and above T_c the average magnetization is zero. This results in a phase transition between a finite magnetic and a paramagnetic phase at critical temperature T_c. The heat capacity C_v and the susceptibility χ diverge at the critical temperature only for infinitely large lattice, but since the lattices size are of finite dimensions this has little effect. A broad maximum in C_v or χ near T_c can, however, be seen, which becomes sharper and sharper as L is increased. Near T_c the physical quantities, mean magnetization, heat capacity and susceptibility exhibits a power law behaviour

as given below [1]

$$\langle \mathscr{M}(T) \rangle \sim (T - T_C)^{\beta} \tag{2.22}$$

$\beta = 1/8$ is called critical exponent

$$C_V(T) \sim |T_C - T|^{\alpha} \tag{2.23}$$

and the susceptibility

$$\chi(T) \sim |T_C - T|^{\gamma} \tag{2.24}$$

$\alpha = 0$ and $\gamma = 7/4$. An important quantity that has to be considered here is the correlation length. It defines the length scale at which the overall properties of a material start to differ from its bulk properties. It is of the order of lattice spacing for T close to T_c. Because of increase in correlation between spins, the correlation length increases as T approaches T_c. The divergent behaviour of correlation near T_c is

$$\xi(T) \sim |T_C - T|^{-\nu} \tag{2.25}$$

For a second order phase transition the correlation length becomes discontinuous at the critical point and the fluctuations spans the whole system. Since the lattice is limited in our case is proportional to the lattice size. It is possible to relate the correlation length, magnetization, specific heat and susceptibility for a finite lattice with those for an infinitely large lattice using finite scale relations. Using this relation critical temperature scales as

$$T_C(L) - T_C(L = \infty) = aL^{-1/\nu} \tag{2.26}$$

For $T = T_c$ the following relations for magnetization, energy and susceptibility becomes

$$\langle \mathscr{M}(T) \rangle \sim (T - T_C)^{\beta} \rightarrow L^{-\beta/\nu} \tag{2.27}$$

$$C_V(T) \sim |T_C - T|^{-\gamma} \rightarrow L^{\alpha/\nu} \tag{2.28}$$

$$\chi(T) \sim |T_C - T|^{-\alpha} \rightarrow L^{\gamma/\nu} \tag{2.29}$$

CHAPTER

3 RESULTS AND DISCUSSION

This chapter contains results gained by the Ising model computed in this project and related discussion for various code runs with different spin lattice sizes and temperatures. The relation between the expectation value of the energy and magnetization and the number of Monte Carlo cycles for different initial spin configurations and temperatures is discussed in Sec. 3.2, and the gained knowledge about when the steady state is reach is then used to determine the probability of energies in Sec. 3.4 for the same temperatures. Sec. 3.5 and 3.6 are dedicated to determine the critical temperature of finite and infinite spin lattices.

The results from running the codes described in Chap. 2 for computing the expectation value of the energy and magnetization and specific heat and susceptibility can be found in the GitHub folder `https://github.com/csoumya14/ForGitHub_Project4`, together with the MatLab scripts for the plots presented in this chapter.

3.1 Ising Model for the 2×2 Spin Case with $T = 1.0$

In this section, the number of Monte Carlo cycles needed to achieve acceptable values for the considered quantities from the computed Ising model for the 2×2 case with $T = 1.0$ is tested. Tab. 2.2 presents the closed form solution to this case, whilst Tab. 3.1 shows the computed values for various numbers of Monte Carlo cycles.

Table 3.1. The expectation value of the Energy, expectation value of the absolute value of the magnetization, specific heat and susceptibility for the 2×2 spin case with $T = 1.0$ for different number of Monte Carlo cycles. Data is gained by the algorithm described in Sec. 2.4.

MC-cycles	$\langle \tilde{E} \rangle$	$\langle \lvert \mathscr{M} \rvert \rangle$	$\tilde{C}_v$	$\tilde{\chi}$
10^3	-7.968	3.99	0.254976	0.0279
10^4	-7.9904	3.9966	0.0767078	0.0107884
10^5	-7.98384	3.99456	0.129019	0.0164504
10^6	-7.98421	3.99469	0.126087	0.0160518
10^7	-7.98369	3.99457	0.130192	0.0162242

The results shows a good corrolation between the closed form solution found earlier in Tab. 2.2 and the

numerical result using Monte Carlo methods in Tab. 3.1, for a large number of Monte Carlo cycles.

For the energy the accuracy is to three digits when using 100000 Monte Carlo cycles. Also the magnetization and specific heat show acceptable results with one percent or less deviation from the closed form. The susceptibility varies more from the closed-form solution, yielding computational inaccuracy in either the computation of the closed form solution or in the computation of the numerical solution.

The algorithm described in Sec. 2.4 is customized to the 2×2 spin case due to the way the change in energy is computed. However, when running the more generalized code introduced in Sec. 2.5, similar results for the considered quantities are gained (see Tab. 3.2), yielding a validity of the generalized algorithm, as well.

Table 3.2. The expectation value of the Energy, expectation value of the absolute value of the magnetization, specific heat and susceptibility for the 2×2 spin case with $T = 1.0$. Data is gained by the algorithm described in Sec. 2.5.

MC-cycles	$\langle \tilde{E} \rangle$	$\langle \lvert \mathscr{M} \rvert \rangle$	$\tilde{C}_v$	$\tilde{\chi}$
10^6	-7.98384	3.99461	0.129147	0.0161829

3.2 Dependence of Monte Carlo Cycles on Various Expectation Values

When computing the expectation value of the energy and magnetization using the Ising model presented in Sec. 2.5, the steady state will only be reached after a number of Monte Carlo cycles. Fig. 3.1 and 3.2 show the absolute value of the expectation value of the energy and the expectation value of the magnetization for the 20×20 spin case with $T = 1.0$ and $T = 2.4$, respectively. In each of the cases, the computation of the expectation values are made with both an ordered initial spin configuration with all spin ups and with a random initial spin configuration created by the for loop described in Sec. 2.5.

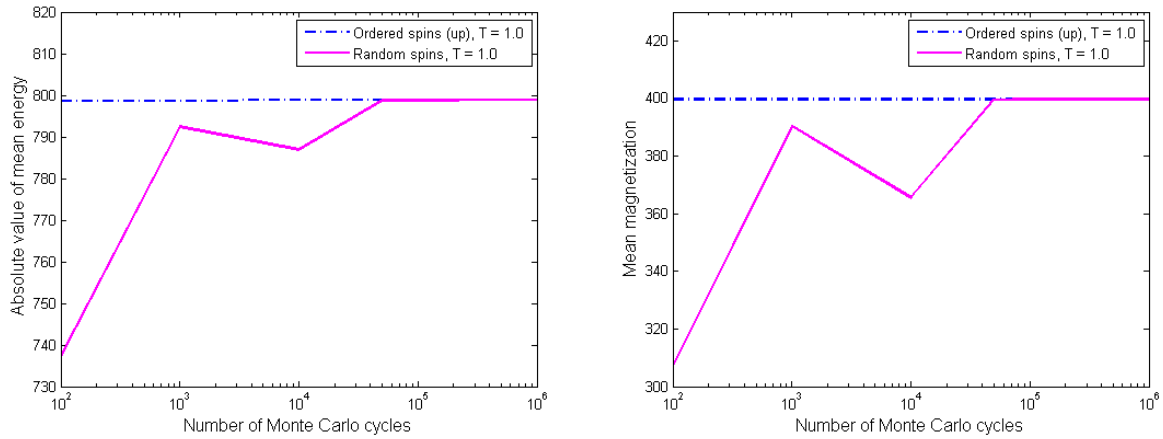

Figure 3.1. The absolute value of the expectation value of the energy and the expectation value of the magnetization as functions of the number of Monte Carlo cycles for the 20×20 spin case at $T = 1.0$ with ordered and random initial spin configurations. For the case with ordered initial spin configuration, that is all spins are up, the steady state is more or less instantaneously reached since for $T = 1.0$, since the spin configuration with all spins up (or down) is the ground state with lowest energy, as for the 2×2 spin case (see Fig. 2.1). With a random initial spin configuration, the steady state is, however, only reached after approximately 10^5 Monte Carlo cycles, at which the the mean of the energy stabilises at about -799, and the mean of the magnetization stabilises at about 400 which was to be expected for low temperatures.

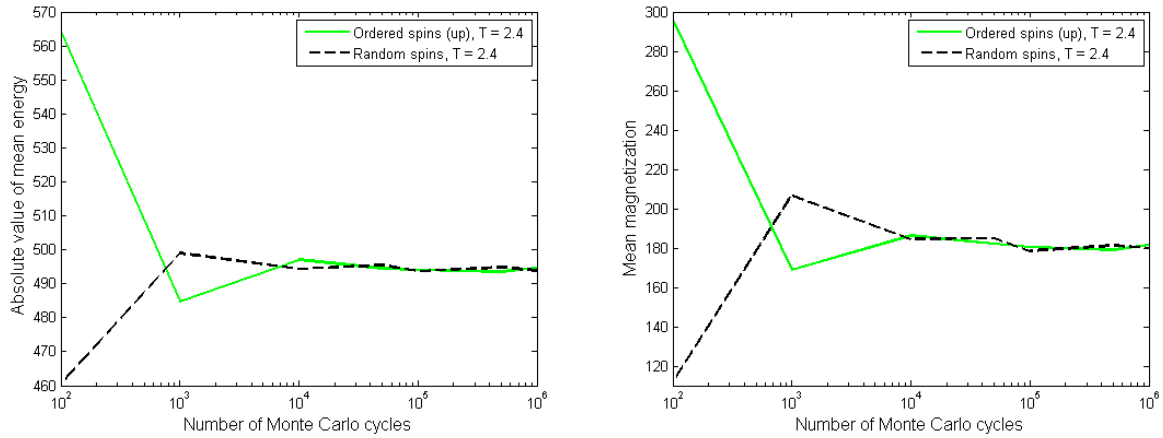

Figure 3.2. The absolute value of the expectation value of the energy and the expectation value of the magnetization as functions of the number of Monte Carlo cycles for the 20×20 spin case at $T = 2.4$ with ordered and random initial spin configurations. The steady state is for both the ordered and random initial spin configuration reached after about 10^4 Monte Carlo cycles at which the mean of the energy reaches a value of -494, and the mean of the magnetization reaches a value of about 180.

From the graphs, it is evident that if the temperature is low, it is an advantage to have an ordered initial spin configuration with all spins up (or down), which is the spin configuration with the lowest energy. This is due to the fact that if the temperature T is low, the probability $exp(-\Delta T/T)$ of jumping to a state with higher energy, which is equivalent to accepting a spin flip that causes a positive energy change ΔE, will be low. However, when the temperature increases to e.g. $T = 2.4$, the probability of accepting a flip that causes an increase in energy is greater, and hence a random initial spin configuration can be just as good as an ordered initial spin configuration.

3.3 Accepted Configurations

For every Monte Carlo cycle in the Ising model, a number, that corresponds to the number of spins in the lattice, of spin flips are proposed. These proposed spin flips give rise to a change in energy ΔE, and the proposal is only accepted if the probability $exp(-\Delta E/T)$ is greater than some random number between 0 and 1, as explained in Sec. 2.5. This gives rise to the fact that if the temperature T is increased, more flips will be accepted, since then the fraction $\Delta E/T$ will decrease, which can be seen in the figures below.

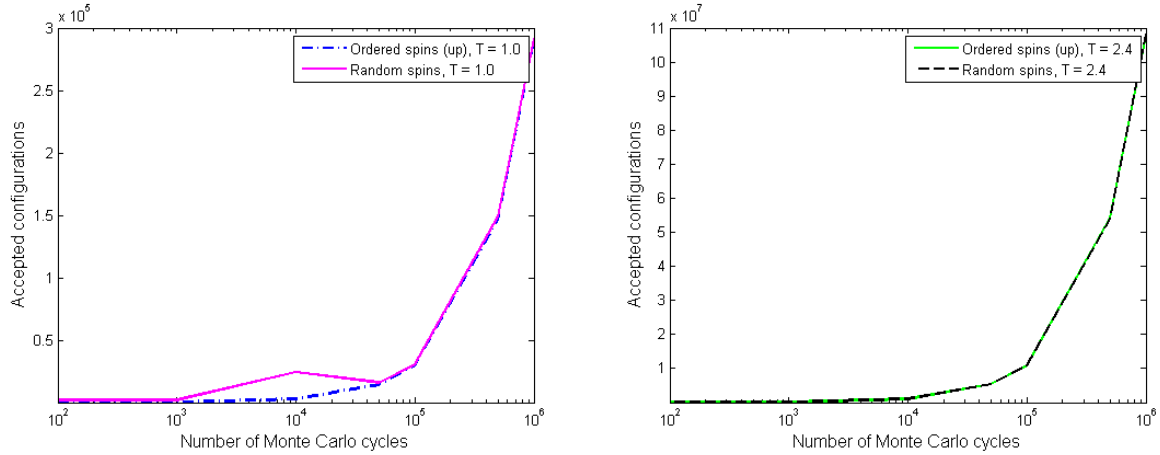

Figure 3.3. Evolution of accepted spin configuration changes with ordered and random initial spin configurations for the 20×20 spin case for both $T = 1.0$ and $T = 2.4$. For a low number of Monte Carlo cycles the number of accepted configuration for the $T = 1.0$ case is greater with the random initial spin configuration than with the ordered initial spin configuration which is in agreement with Fig. 3.1 from which it is seen that the steady state for $T = 1.0$ is reached way quicker if the initial configuration of the spins is ordered. However, a while after having reached the steady state, the number of accepted configurations is similar for the ordered and random initial spin configuration. For $T = 2.4$ the number of accepted configurations is similar for ordered and random initial spin configurations independently on the number of Monte Carlo cycles.

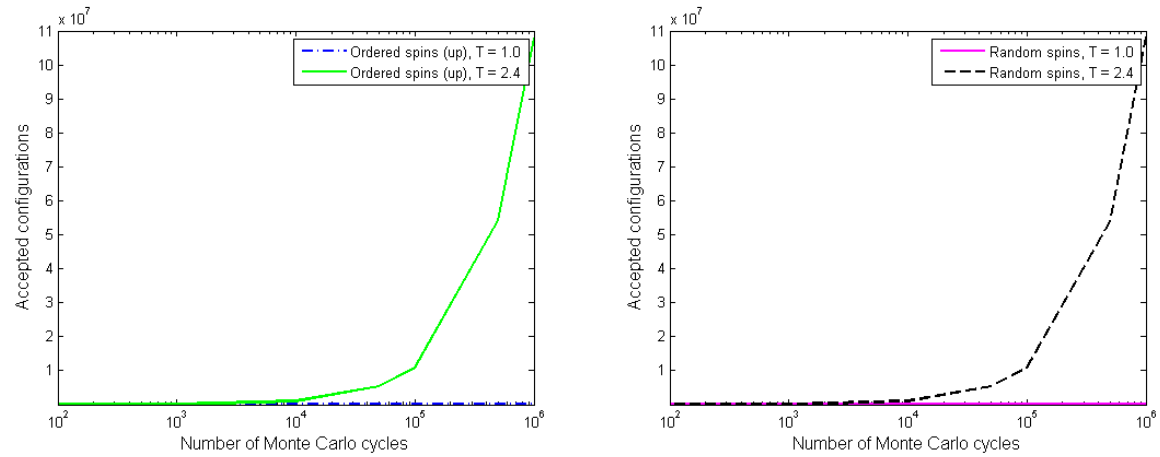

Figure 3.4. Evolution of accepted spin configuration changes for $T = 1.0$ and $T = 2.4$ plotted for both ordered initial spin configurations and random initial spin configurations. From the plots it is evident that fewer proposed spin configuration changes are accepted for low temperature than for higher temperature. This is due to the fact that the probability of accepting a spin flip that causes an increase in energy is greater for higher temperature as described in Sec. 3.2, and hence more spin flips will be made for higher temperature.

3.4 Probability of States for the 20×20 Spin Case

In the histograms below, the probability of specific energies is plotted for the 20×20 spin case with $T = 1.0$ and $T = 2.4$, respectively. The probability is computed by counting the times a specific energy appears, and normalizing the counts, after having reached the steady state.

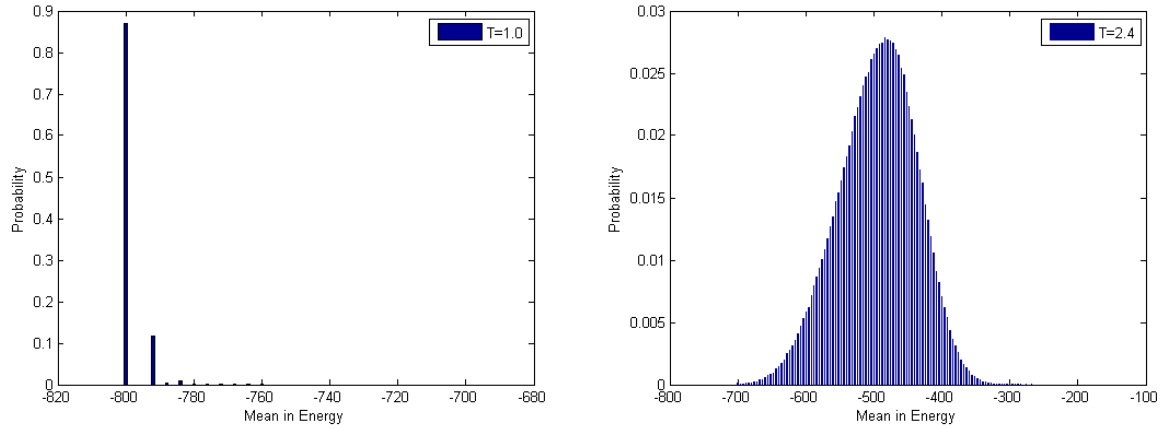

Figure 3.5. The normalized probability of energies for the 20×20 spin case after having reached steady state, that is after 10^4 Monte Carlo cycles (see Sec. 3.2), for the temperature $T = 1.0$ (the leftmost histogram) and $T = 2.4$ (the rightmost histogram), respectively. The total number of Monte Carlo cycles for each of the cases is 10^6, yielding $10^6 - 10^4 - 1$ measurements. For the $T = 1.0$ case, the initial spin configuration is ordered with all spins up, whilst the initial spin configuration for $T = 2.4$ was random.

For the two cases shown in Fig. 3.5, the computed specific heat $\tilde{C}_v = C_v/k_B$ is ultimately the constant $1/\tilde{T}^2$ multiplied by the variance in energy $\left\langle \langle \tilde{E}^2 \rangle - \langle \tilde{E} \rangle^2 \right\rangle$ in which the tilde-notation is introduced in Sec. 2.3. For the computation for $\tilde{T} = 1.0$ in Fig. 3.5, the computed value of the specific heat is

$$\tilde{C}_{v,T=1} = 9.3138$$

whilst for the $\tilde{T} = 2.4$ case, the computed specific heat is

$$\tilde{C}_{v,T=2.4} = 562.75$$

Hence, the variance of the $\tilde{T} = 1.0$ case is 9.3138, whilst the variance of the $\tilde{T} = 2.4$ case is $562.75/2.4^2 = 97.7$. For the case with $\tilde{T} = 1.0$, there is a very large probability of being in the ground state, since the probability of accepting a flip that causes an increase in the energy is low due to the low temperature. This is in agreement with the leftmost histogram in Fig. 3.5 in which the probability of being in the ground state is almost 0.9. Furthermore, the computed variance of 9.3138 for the $\tilde{T} = 1.0$ case indicates that the energy does not vary much. For the case with $\tilde{T} = 2.4$, the situation is a bit different. All flips that causes a decrease in energy will be accepted as in the $\tilde{T} = 1.0$ case, but now the probability of accepting a flip that increases the energy is increased. That shifts the mean of the energy (and magnetization), as was also seen when comparing Fig. 3.2 to Fig. 3.1, but it also increases the variance of the energy, as seen in the rightmost histogram in Fig. 3.5 and the computed value of 97.7, which is in agreement with the width of the probability distribution in Fig. 3.5.

3.5 Dependence of Spin Lattice Size on Critical Temperature

As described in Sec. 2.6, at a specific temperature, called the critical temperature T_C, the system will experience a phase transition. At this temperature, the specific heat and susceptibility will peak, and hence by investigation these quantities, the critical temperature can be determined for different spin lattice sizes $N = L \times L$. The plots in Fig. 3.6 and 3.7 are made by computing the quantities with a temperature step length of $T_{step} = 0.05$

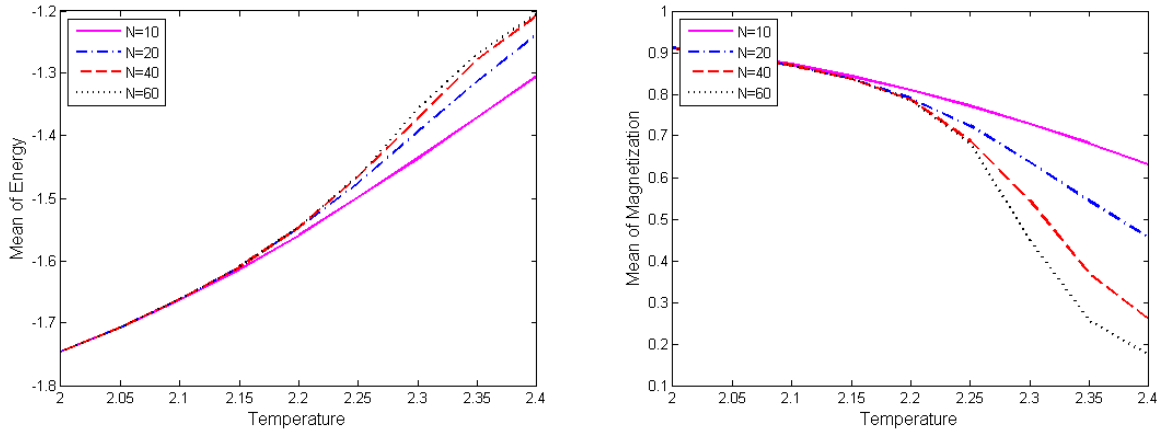

Figure 3.6. Expectation value of the energy and magnetization plotted against the temperature for different spin lattice sizes: 10×10, 20×20, 40×40, 60×60. The expectation values are normalized to show the expectation values of each spin in the lattice by dividing by the total number of spins when plotting the data, meaning that the ground state for all lattice sizes has an energy of -1, whilst the magnetization of the ground state is 1. This is done to make the plots for different spin lattice sizes comparable.

The plots in Fig. 3.6 show, in agreement with the plots in Sec. 3.2 that is the temperature is increased, the expectation value of the energy will increase, as well, whilst the expectation value of the absolute value of the magnetization will decrease. Furthermore, the plots show that an increase in lattice size decreases the expectation value of the absolute value of the magnetization, as predicted by Eq. (2.27). This is also in agreement with the statement given in Sec. 2.6, that at the critical temperature the expectation value of the magnetization goes to zero.

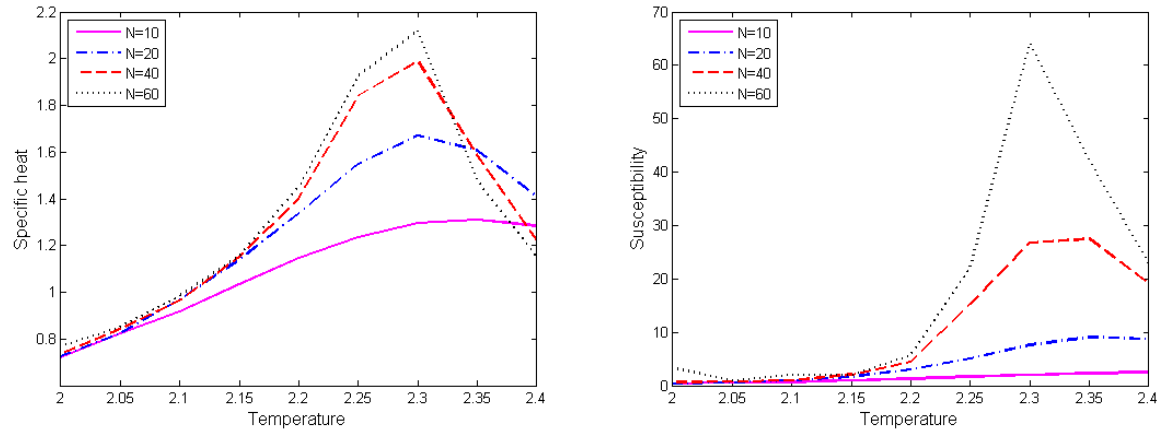

Figure 3.7. Specific heat and susceptibility plotted as functions of the temperature for the same spin lattice sizes as in Fig. 3.6. From the plots is it evident that a phase transition happens around a critical temperature that is slightly shifted when varying the spin lattice size as predicted by Eq. (2.28) and (2.29).

Fig. 3.7 clearly shows the peak in specific heat and susceptibility at the critical temperature, and that this peak is shifted slightly to the left when the spin lattice size is increased. This yields that for an infinitely large spin lattice, the critical temperature will be below 2.29 which seems to be the approximate critical temperature for the 60×60 case.

3.6 Determining Critical Temperature for Infinitely Large Spin Lattice

From the finite spin lattices, it is possible to deduce the critical temperature for an infinitely large spin lattice. This is done by considering the theory presented in Sec. 2.6.

Table 3.3. Critical temperature for various spin lattice sizes. The values of the critical temperature i found by identifying the approximate critical temperature from Fig. 3.7, in which the temperature step length is 0.05, and computing the specific heat and susceptibility around that approximate critical temperature for smaller step lengths $T_{step} = 0.01$, for the spin lattices 10×10, 20×20, 40×40. The critical temperature is then identified directly from the computed data as the temperature at which the value of the specific heat and susceptibility is greatest. For the 60×60 spin case, the critical temperature is estimated directly from the plots in Fig. 3.7.

Spins	Critical temperature
10×10	2.35
20×20	2.32
40×40	2.31
60×60	2.29

The data displayed in Tab. 3.3 can now be used to determine the critical temperature for an infinitely large spin lattice by Eq. (2.26) from which it is evident that the critical temperature for an infinitely large spin lattice $T_C(L = \infty)$ can be determined from the critical temperature of a finite spin lattice $T_C(L)$ by the relation

$$T_C(L) = T_C(L = \infty) + aL^{-1} \tag{3.1}$$

in which L is the number of spins in each direction. In Eq. (3.1) ν in Eq. (2.26) is set equal to 1. Hence, by making a linear regression of the data in Tab. 3.3 with the the critical temperature as a function of L^{-1}, that is $T_C(L^{-1})$, the intersection of the line with the y-axis ($L^{-1} = 0$) will then be the critical temperature for a infinitely large lattice. This is done in Fig. 3.8 using MatLab to produce the linear regression.

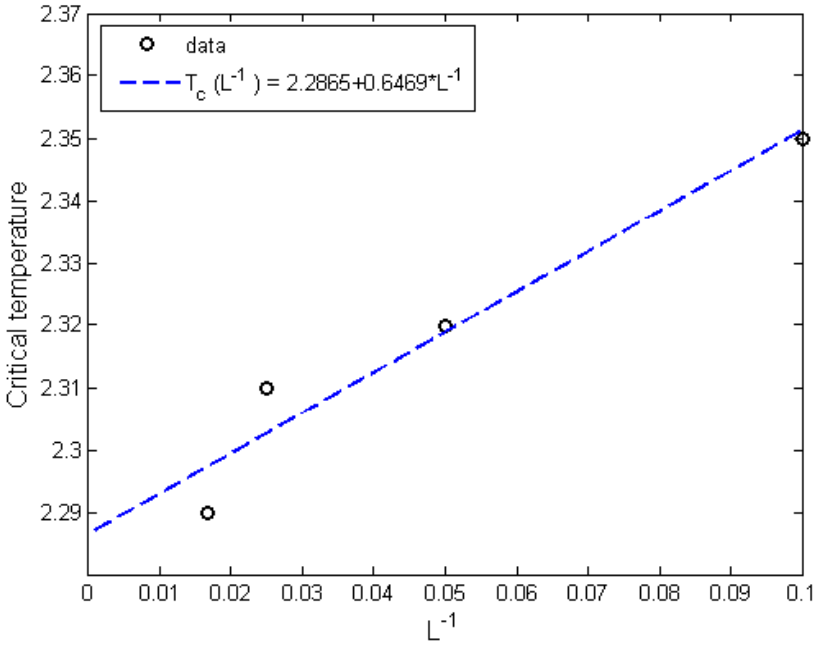

Figure 3.8. Linear regression of the data presented in Tab. 3.3 for the critical temperature as a function of the inverse value of the number of spins in each direction. Since the independent variable is the *inverse* of the number of spins in each direction, $L^{-1} = 0$ corresponds to an infinitely large spin lattice, and hence $T_C(0) = T_C(L = \infty)$.

From the linear regression shown in Fig. 3.8, the estimated critical temperature for an infinitely large spin lattice is

$$\tilde{T}_C(L = \infty) \approx 2.29 \tag{3.2}$$

The exact result is in the project description given to be 2.269. Hence, the deviation of the computed result to the exact result is

$$\text{Deviation} = \frac{2.29 - 2.269}{2.269} \cdot 100\% = 0.93\% \tag{3.3}$$

which is an acceptable deviation considering the fluctuation around the linear regression of the data points in Fig. 3.8. To gain a better result, more data points should be included in Fig. 3.8. Preferably, the data for larger spin lattices that 60×60 should be included, as well.

CHAPTER

4 CONCLUSION

The Ising model in two dimensions without an external magnetic field is in this project studied explicitly. At first, only two spins in each dimension was considered and the closed form solution of the partition function and expectation values for energy, magnetization, specific heat and susceptibility as functions of temperature was calculated. These values were then compared with the computed results for a temperature $T = 1$ using metropolis algorithm, as a test of the computed Ising model. Both values were found to be in good agreement with each other after 1000 Monte Carlo cycles.

The computed Ising model was then used to compute the expectation values for energy, magnetization, specific heat and susceptibility for a lattice with 20 spins in each direction for a temperature $T = 1.0$ and $T = 2.4$ using both ordered and random spin orientation as initial configuration. It was found that for a low temperature ($T = 1$), the steady state is immediately reached with an ordered initial configuration of all spins up, but with a random initial spin orientation, it takes in the order of 10^4 Monte Carlo cycles to reach the steady state. With an increase in temperature ($T = 2.4$) it is found that both ordered and random initial configuration require in the order of 10^4 Monte Carlo cycles to reach the steady state.

Study on the behaviour of accepted configuration as a function of temperature showed that for a low number of Monte Carlo cycle the number of accepted configuration, for the $T = 1.0$ case, is greater with the random initial spin configuration than with the ordered initial spin configuration. However, after reaching the steady state the initial spin configuration has no influence on the number of accepted spin flips, as was to be expected. For $T = 2.4$, the number of accepted configurations is found to be similar for ordered and random initial spin configurations independently on the number of Monte Carlo cycles.

The of temperature on the energy is estimated by computing the probability of appearances of specific energy states for temperatures $T = 1$ and $T = 2.4$ after reaching steady state.

Finally an analysis is made on the behaviour of the Ising model in two dimensions close to the critical temperature as a function of the lattice size $L \times L$. Different plots of the expectation values of energy and magnetization, the specific heat and susceptibility as a function of T in the range 2.0 to 2.4 for various lattice sizes, namely 10×10, 20×20, 40×40, and 60×60 show an indication of phase transition near the critical temperature. From these results the critical temperature for an infinite lattice is computed to be 2.29 which deviates about 1% from the exact result of 2.269, with the help of finite scaling relations.

BIBLIOGRAPHY

[1] M. Hjorth-Jensen, “Computational physics - lecture notes fall 2015,” August 2015.