FYS4150 H20 - Project 4: The 2-Dimensional Ising Model and Monte Carlo Simulations

Olav Fønstelien

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Abstract

This report gives presents a solution to the Ising model in two dimensions applied on a magnetic material. The model is interpreted as a reversible Markov process which is evolved using Monte Carlo simulation with the Metropolis algorithm as acceptance criteria. We show that the Markov process reaches its most likely state independently of initial state, and that these therefore may be selected freely – however with a cost to equilibration time.

We use a 2×2 lattice to show that the model approximates the expectation values and variances of magnetic energy and moment with precision up to 10^{-3}, but that this requires $\geq 10^6$ Monte Carlo cycles. We also show that the model can be used to estimate the probability distribution of the lattice energy, and that it correctly reproduce the phase transition phenomena. The critical temperature of the infinite lattice, T_C, is approximated with an error of with an error of 0.31 %.

Please visit my GitHub repository `https://github.com/fonstelien/FYS4150/tree/master/project4` for the source code developed for this report.

1 Introduction

In this report we will study the Ising model and how this can be solved by statistical methods. The model describes the binary state of the particles in a quadratic lattice. The state of each particle or *spin* is either *up* or *down*, and the preferred state of each spin is to equal that of its four nearest neighbors in the lattice. The ground state is up, and one could maybe conclude that a lattice filled with ups makes for a dull model, but when applying an outer influence, like increasing the temperature, transitions away from the state of the neighbors become more likely. We would start to see scattered areas of downs in the lattice, a tendency which would only increase towards a complete random configuration as $T \to \infty$.

We will develop a simulation model for solving the Ising model in two dimensions. Even if an analytical solution to the two-dimensional model exists, the simulation model is easily extended beyond this. In this report we will study the Ising model applied on a magnetic material. We will use it to show steady state conditions and phase transitions by changing the temperature and extent of the lattice.

However, the Ising model can also be used to solve problems in the social sciences, where the *state* of one individual is heavily influenced by the state of its nearest neighbors. As such, our study in this report could serve as an introduction to a more general method of solving problems of this nature.

The model that we will develop uses the Monte Carlo method in combination with the Metropolis algorithm to simulate the distribution of ups and downs in an $L \times L$ lattice at a given temperature. We pick spins from the lattice by a stochastic process and decide whether to flip it or not – *yes* if the new state corresponds better to that of its neighbors; *maybe* if not – to be decided by the Metropolis algorithm. We will see that this process, when repeated some tens to some hundred times over the lattice, forms a Markov process, with the lattice reaching its most likely state independently of its initial condition.

We will start with a review of the mathematics needed to develop our model in Section 2, where we also give the outline of an efficient implementation in a computer program. Then we present results from the simulations of different lattice sizes and temperatures, including the effects of initial conditions, and an approximation of the probability distribution of the spin configuration in Section 3. We end by summarizing our findings and drawing conclusions with some thoughts about future work in Section 4.

2 Methods

The magnetic energy of the spins in a lattice depends on their neighbors. The total energy E of a lattice $\mathcal{L}$ is given by

$$E = -J \sum_{\langle kl \rangle} s_k s_l, \tag{1}$$

where $\langle kl \rangle$ denotes all neighboring pairs of spins $s_k, s_l \in \{-1, +1\}$ in the lattice. J is the coupling constant and tells how strong the interrelation between the spins is. In this report we will assume that $J > 0$. The magnetic moment of the lattice is

$$\mathcal{M} = \sum_k s_k; \tag{2}$$

a simple sum over all spins in the lattice.

If we now let the lattice $\mathcal{L}$ be quadratic with $L \times L$ spins, the likelihood of any spin configuration $\mathcal{L}_i$ at a temperature T is given by the Boltzmann probability distribution as

$$P_i = \frac{e^{-\beta E_i}}{Z}, \quad \text{where} \quad \beta = \frac{1}{k_B T}. \tag{3}$$

E_i is $\mathcal{L}_i$'s magnetic energy in this configuration, as given by Equation (1), and Z is the partition function for the canonical ensemble (see [1]). The partition function is defined as

$$Z(\beta) = \sum_{i=1}^{M} e^{-\beta E_i}, \tag{4}$$

where $M = 2^{L^2}$ and $i = 1, 2, ..., M$ denotes each of the possible configurations $\mathcal{L}_i$ that $\mathcal{L}$ may have.

We see from Equations (1), (3) that if we let -1 denote a spin's *down* state and +1 denote its *up* state, the most likely state will be all ups, since this gives the lowest energy and hence highest probability, and at absolute zero temperature, this is how $\mathcal{L}$ will remain.

However, increasing temperature will make other states more likely. Increased kinetic energy will cause individual spins to flip, giving the lattice a new state $\mathcal{L}_j$ with energy E_j. This process can be described by a Markov chain

$$\mathbf{w}_{t+1} = \mathbf{W}\mathbf{w}_t, \tag{5}$$

where $\mathbf{w}_t = \{w_i\} = \{P_i\}$ denotes $\mathcal{L}$'s (discrete) probability distribution at time t. $\mathbf{W} = \{W_{i\to j}\}$ denotes the transition probabilities for all possible transitions $\mathcal{L}_i \to \mathcal{L}_j$, and is unknown. To overcome this, we will re-phrase $W_{i\to j}$ as a stochastic process, where the likelihood $T_{i\to j}$ of a spin to be a *candidate* for the flip is equal for all, and the likelihood that we *accept* this spin to flip is $A_{i\to j}$. That is;

$$W_{i\to j} = T_{i\to j} A_{i\to j}. \tag{6}$$

Transition the other way, $\mathcal{L}_j \to \mathcal{L}_i$, is also allowed. We let $W_{j\to i} = T_{j\to i} A_{j\to i}$ denote the reverse process, and by taking the right side of Equation (5) we get the so-called detailed balance;

$$\frac{W_{i\to j}}{W_{j\to i}} = \frac{T_{i\to j} A_{i\to j}}{T_{j\to i} A_{j\to i}} = \frac{A_{i\to j}}{A_{j\to i}} = \frac{w_j}{w_i} = \frac{P_j}{P_i} = e^{-\beta \Delta E_{i\to j}}. \tag{7}$$

Here, $\Delta E_{i\to j}$ denotes the change in energy between state $\mathcal{L}_i$ and $\mathcal{L}_j$, $\Delta E_{i\to j} = E_j - E_i$.

We will use the Metropolis algorithm to establish the two unknowns $A_{i\to j}$ and $A_{j\to i}$. The Metropolis algorithm states that if $\Delta E_{i\to j} \leq 0$, we flat out accept the transition, such that $A_{i\to j} = 1$. The likelihood that we accept the reverse then becomes $A_{j\to i} = e^{-\beta \Delta E_{j\to i}}$, which gives us the general form of the Metropolis algorithm;

$$A_{i\to j} = \begin{cases} 1 & \text{if} \quad \Delta E_{i\to j} \leq 0 \\ e^{-\beta \Delta E_{i\to j}} & \text{otherwise} \end{cases}. \tag{8}$$

The decision whether to accept the flip on not is then made in another stochastic process. In each iteration we draw a new random number $r_i \sim \mathcal{U}(0, 1)$

and apply it to the Metropolis algorithm. The outcome is then summarized by the following rules:

$$\begin{aligned} r_i < A_{i\to j} &\to \text{accepted} \\ r_i \geq A_{i\to j} &\to \text{not accepted} \end{aligned} \quad . \tag{9}$$

The transition probability $\mathbf{W}$ is a stochastic matrix, which means that it has a single largest eigenvalue $\lambda_{max} = \lambda_1 = 1$, and $\lambda_i < 1$ for the remaining [1]. If we let $\mathbf{v}_i$ denote the corresponding eigenvectors, we can write the initial probability distribution $\mathbf{w}_0$ as

$$\mathbf{w}_0 = \sum_i \alpha_i \mathbf{v}_i. \tag{10}$$

After the first iteration we get

$$\mathbf{w}_1 = \mathbf{W}\mathbf{w}_0 = \sum_i \lambda_i \alpha_i \mathbf{v}_i, \tag{11}$$

and if we continue to the pth iteration, $\mathbf{w}_p = \mathbf{W}^p \mathbf{w}_0 = \sum_i \lambda_i^p \alpha_i \mathbf{v}_i$, it becomes obvious that we reach a limit where

$$\mathbf{w}_q \approx \lambda_1^q \alpha_1 \mathbf{v}_1 = \alpha_1 \mathbf{v}_1. \tag{12}$$

Since the sum of the probability distribution in $\mathbf{v}_1$ must be equal to 1, $\sum_i P_i = 1$, we must have $\alpha_1 = 1$. We then get that

$$\mathbf{w}_t = \mathbf{v}_1, \quad \text{for} \quad t \geq q, \tag{13}$$

which means that after sufficient iterations, the probability distribution vector $\mathbf{w}_t$ becomes independent on the initial conditions $\mathbf{w}_0$. $\mathbf{w}_t$ will reach $\mathbf{v}_1$, which is the Boltzmann probability distribution for the defined partition function $Z(\beta)$ [2], a quantity depending on temperature and the lattice itself. This means that if we allow ourselves enough time, the initial configuration of $\mathcal{L}$ can be selected freely since its probability distribution is bound to reach its most likely state from any initial configuration.

From Equation (8) we see that the Metropolis algorithm lets us simulate the spin distribution of the lattice without knowing the partition function $Z(\beta)$. Evaluating this is not complicated, but it would require us to sum over all the possible configurations $\mathcal{L}_i$ of the lattice. The number of configurations is given by $M = 2^{L^2}$; a factor which very quickly becomes unwieldy. However, to derive any useful quantities for the lattice at a given temperature, it would still be necessary do sum over all configurations, unfortunately.

The expected magnetic energy and moment of the lattice are given by the

equations

$$\begin{aligned} \mathbb{E}(E) &= \sum_{i=1}^{M} E_i P_i = \frac{1}{Z} \sum_{i=1}^{M} E_i e^{-\beta E_i} \\ \mathbb{E}(\mathcal{M}) &= \sum_{i=1}^{M} E_i P_i = \frac{1}{Z} \sum_{i=1}^{M} \mathcal{M}_i e^{-\beta E_i} \end{aligned}, \tag{14}$$

respectively. Further, the heat capacity C_V and magnetic susceptibility χ are given by

$$\begin{aligned} C_V &= \frac{\sigma_E^2}{k_B T^2} \\ \chi &= \frac{\sigma_{\mathcal{M}}^2}{k_B T} \end{aligned}, \tag{15}$$

where the variances $\sigma_E^2, \sigma_{\mathcal{M}}^2$ again are given by

$$\begin{aligned} \sigma_E^2 &= \frac{1}{Z} \sum_{i=1}^{M} E_i^2 e^{-\beta E_i} - \mathbb{E}^2(E) \\ \sigma_{\mathcal{M}}^2 &= \frac{1}{Z} \sum_{i=1}^{M} \mathcal{M}_i^2 e^{-\beta E_i} - \mathbb{E}^2(\mathcal{M}) \end{aligned}. \tag{16}$$

We see that in addition to Z, summing over M reappears in these equations. Our strategy will therefore be to use Monte Carlo simulation and approximate the expectation values and variances by *sample means* and *sample variances*. We will simulate the evolving configurations $\mathcal{L}_i$ of the lattice by the stochastic Markov process described in Equations (5) through (8), then wait until the process reaches steady state (Equation (13)), and start sample the configuration energies and magnetic moments $E_i, \mathcal{M}_i$.

The general equations for sample mean $\bar{\mu}_X$ and variance $\bar{\sigma}_X^2$ by N samples are given by

$$\begin{aligned} \bar{\mu}_X &= \frac{1}{N} \sum_{i=1}^{N} X_i \\ \bar{\sigma}_X^2 &= \frac{1}{N} \sum_{i=1}^{N} X_i^2 - \bar{\mu}_X^2 \end{aligned}, \tag{17}$$

which have the limits $\bar{\mu}_X \to \mathbb{E}(X)$ when $N \to \infty$ [3].

We will now study how to best implement our Monte Carlo simulation of the Ising model in a computer program. To get good approximations for the expectation values, we will need to do hundreds of thousands or even millions of spin flip tests on our lattice. That we develop efficient code is therefore a high priority.

Our lattice $\mathcal{L}$ has limited extension with $L \times L$ spins, and the first thing we need do is to define the boundary conditions. Since we wish to simulate as large

lattices as possible, we will use so-called *periodic* boundary conditions, where the spins on the lattice edges are imagined to neighbor on each other. See [1].

Next we randomly pick a candidate to flip among the spins in the lattice, say s_k. We use the Metropolis algorithm in Equation (8) to decide whether the flip is accepted or not, based on the change $\Delta E_{i\to j}$ in the lattice's energy from state $\mathcal{L}_i$ to $\mathcal{L}_j$. The change in the lattice's energy is given by

$$\Delta E_{i\to j} = E_j - E_i = 2Js_k^{(i)} \sum_{\langle l \rangle} s_l, \tag{18}$$

where $\langle l \rangle$ denotes s_k's four neighbors and $s_k^{(i)}$ denotes its state in $\mathcal{L}_i$. We observe that the sum over s_l can take only five different values, such that

$$\Delta E_{i\to j} = \{-8J, -4J, 0, 4J, 8J\}. \tag{19}$$

Consequently, the Metropolis algorithm acceptance criteria $A_{i\to j}$ in Equation (8) can take only five corresponding values at a given temperature T;

$$A_{i\to j} = \{1, 1, 1, e^{-4J\beta}, e^{-8J\beta}\}, \quad \text{where} \quad \beta = \frac{1}{k_B T}. \tag{20}$$

Pre-calculating these values and keeping them in a lookup table before we start the Markov process thus saves the potentially expensive calculation of the exponential function during the Monte Carlo simulation.

Before we start the process we should also calculate the lattice's energy and magnetic moment in the initial condition, $E, \mathcal{M}$. Then, whenever a candidate is accepted, the change in energy and magnetic moment are accumulated. However, to avoid clogging the CPU pipeline with conditionals when we implement the Metropolis algorithm, we should use a facility that is available in many programming languages which is that boolean expressions return `integer`s when they are evaluated; `0` for a `FALSE` expression and `1` for a `TRUE`. If we let b denote the result of the Metropolis algorithm (accept/not accept), we get the update rules

$$\begin{aligned} s_k &\leftarrow s_k - 2bs_k \\ \mathcal{M} &\leftarrow \mathcal{M} + 2bs_k^{(j)} \\ E &\leftarrow E + 2bJs_k^{(i)} \sum_{\langle l \rangle} s_l \end{aligned}. \tag{21}$$

Listing 1 gives an outline of an algorithm for solving the Ising model in two dimensions. It is implemented as a Markov chain and runs a Monte Carlo simulation with the Metropolis algorithm as acceptance criteria.

Note that we accumulate the absolute value `Mabs` of the magnetic moment. The reason for this is that the model becomes unstable and may shift between positive and negative values close to the critical temperature. Note also that one Monte Carlo cycle is defined here as one sweep over the whole lattice, meaning that we do L^2 Metropolis spin flip tests per cycle.

Before we start sampling magnetic energy and moment with `Eacc`, `E2acc`, `Macc` and `M2acc`, we must let the model reach its steady state (equilibration). This is handled by running a number of cycles defined by the `equilibration_cycles` parameter. The number of cycles to run before equilibration depends on the size of the lattice, its initial and target temperatures, and also the sequence of numbers coming from the random number generator. It can only be determined by trial and error, but equilibration will generally be slower for a larger lattice, and for a larger difference in initial and target temperatures.

The equilibration process is a sequential process, but the sampling process can be parallelized without any influence on the results. It is important, however, that each process has its own random number generator to avoid oversamping.

Listing 1: Solving the Ising model in two dimensions with Monte Carlo simulation and the Metropolis algorithm to approximate the mean values and variances of the magnetic energy and moment. Note that we accumulate the absolute value of the magnetic moment.

```
// Declarations
Tinit : "initial temperature of the lattice"
T : "target temperature of the lattice"
lattice : "LxL 2D array containing the spins"
wij : "pre-calculated lookup table with Metropolis acceptance limits"
equilibration_cycles : "non-sampled thermalizing cycles"
monte_carlo_cycles : "sampled cycles"
E, Mabs : "Energy and absolute value of magnetic moment in the lattice"
Eacc, Macc : "Accumulated energy and magn. moment for mean calculation"
E2acc, M2acc : "Acc. energy and magn. moment squared for variance calc."

// Initializing
init_lattice(lattice, Tinit) // gives some initial state to spins
init_metropolis(wij, T) // Equation (20)

// Monte Carlo
// Thermalizing...
FOR i = 1...equilibration_cycles DO
  FOR j = 1...L*L DO
    sk : "randomly drawn spin from the lattice"
    dE : "delta-energy for sk acc. to Equation (18)"
    b : "1 or 0 based on metropolis algorithm with dE, wij (Equation (9))"
    sk ← sk - 2*b
  END FOR
END FOR

// Sampling energy and magnetic moment
"Initialize E, Mabs"
"Set Eacc, Macc, E2acc, M2acc to 0"
"Parallelize FOR loop with individual RNGs; reduce Eacc, E2acc, etc"
FOR i = 1...monte_carlo_cycles DO
```

```
  Eacc ← Eacc + E
  E2acc ← E2acc + E*E
  Macc ← Macc + M
  M2acc ← M2acc + M*M
  FOR j = 1...L*L DO
    sk : "randomly drawn spin from the lattice"
    dE : "delta-energy for sk acc. to Equation (18)"
    b : "1 or 0 based on metropolis algorithm with dE, wij (Equation (9))"
    sk ← sk - 2*b
    E ← E + b*dE
    M ← Mabs + 2*b*sk
  END FOR
END FOR

// Expectation values
Emean ← Eacc / monte_carlo_cycles
Mmean ← Macc / monte_carlo_cycles

// Variances
Evar ← E2acc / monte_carlo_cycles - Emean*Emean
Mvar ← M2acc / monte_carlo_cycles - Mmean*Mmean
```

3 Results

The 2x2 lattice is the most demanding model, since it has very few fundamental states and all spins are on the edge of the lattice, which puts our boundary conditions to the test.

3.1 Evaluation of the Model

The partition function $Z(\beta)$ is prohibitively expensive to calculate for any lattice of more than a few spins in each direction. But to evaluate our model, we can let $L = 2$, which leaves us with only $M = 2^4 = 16$ different configurations. As we see in Table 1, they can be aggregated to six fundamental states.

Table 1: Fundamental states of the 2×2 lattice.

# up spins	# configs	energy	moment
4	1	-8J	4
3	4	0	2
2	4	0	0
2	2	+8J	0
1	4	0	-2
0	1	-8J	-4

When we calculate the partition function for the 2×2 lattice, only three fundamental states exist. The function then becomes

$$Z_{2\times2}(\beta) = 12 + 2e^{8J\beta} + 2e^{-8J\beta} = 12 + 4\cosh 8J\beta. \tag{22}$$

For the magnetic energy the corresponding expectation value and variance become

$$\begin{aligned} \mathbb{E}(E_{2\times2}) &= -\frac{32J}{Z_{2\times2}} \sinh 8J\beta \\ C_{V,2\times2} &= \frac{1}{k_B T^2}\left(\frac{256J}{Z_{2\times2}} \cosh 8J\beta - \mathbb{E}^2(E_{2\times2})\right) \end{aligned}, \tag{23}$$

and likewise for the magnetic moment;

$$\begin{aligned} \mathbb{E}(|\mathcal{M}_{2\times2}|) &= \frac{8J}{Z_{2\times2}}(2 + e^{8J\beta}) \\ \chi_{2\times2} &= \frac{1}{k_B T}\left(\frac{32J}{Z_{2\times2}}(1 + e^{8J\beta}) - \mathbb{E}^2(|\mathcal{M}_{2\times2}|)\right) \end{aligned}. \tag{24}$$

Here, we state again that $\beta = \frac{1}{k_B T}$.

In Tables 2 and 3 we see the results of the simulations for temperature $T = 1.0\ J/k_B$ over the range 10^1 to 10^7 Monte Carlo cycles. We see that the

model produces the expected values, but that we need to run up to 10^5 cycles to get good estimates of the expectation values. For the variances, the energy variance error is only $8.3 \cdot 10^{-3}$ for 10^7 cycles, while the magnetic moment variance error never improves beyond about 10^{-2} to 10^{-3}, unless we run up to 10^5 cycles! Figure 1 shows the evolution for the first 10^7 cycles.

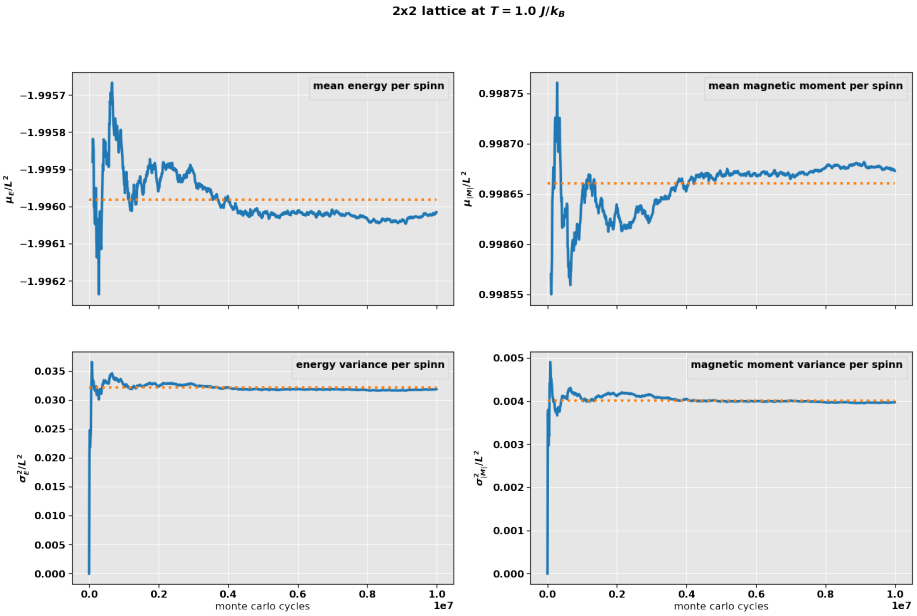

Figure 1: Evolution of the mean values and variances for the first 10^7 Monte Carlo cycles in a 2×2 lattice at $T = 1.0\ J/k_B$. Note the differing scales. The dotted line indicates analytical values. Good agreement is reached after about 10^6 cycles, but the relative error still remains in the 10^{-2} to 10^{-3} range for the variances. See Tables 2 and 3.

3.2 Reaching Equilibration

With the 2×2 lattice in the previous section, equilibration *to* any temperature *from* any temperature is a few cycles at most since the lattice will always be in one of the six possible fundamental configurations listed in Table 1. A larger model, like the 20×20 that we will study here, allows for more configurations, and we therefore need to allow the model to reach equilibration before we can start sampling the magnetic energy and moment. Figure 2 clearly shows this. We see that starting at different configurations may bring some benefit – especially for lower temperatures. At $T = 1.0\ J/k_B$ all spins are usually up, corresponding well to the initial conditions. We also see that for this lattice, equilibration is reached at around 6000 cycles at the latest (lower right pane), but in reality sooner than that since the calculation of the average has a memory

Table 2: Calculated energy for the 2×2 lattice at temperature $T = 1.0\ J/k_B$. We see that for the estimation of $\mathbb{E}(E)$, the error improves with a factor of about 10 up to $N = 10^5$, and a factor of 2 thereafter. For the estimation of σ_E^2, the error is about 100 times higher, and improvement is less for increasing N. True values are $\mathbb{E}(E) = -1.995982$ and $\sigma_E^2 = 3.208233 \cdot 10^{-2}$.

$\log_{10} N$	$\bar{\mu}_E$	ε	$\bar{\sigma}_E^2$	ε
1	-1.81818e+00	8.90791e-02	1.32231e+00	4.02163e+01
2	-1.98020e+00	7.90792e-03	1.56847e-01	3.88890e+00
3	-1.99201e+00	1.99105e-03	6.36806e-02	9.84911e-01
4	-1.99700e+00	5.10132e-04	2.39616e-02	2.53121e-01
5	-1.99586e+00	6.11451e-05	3.30511e-02	3.01967e-02
6	-1.99592e+00	3.01014e-05	3.25574e-02	1.48093e-02
7	-1.99602e+00	1.67910e-05	3.18149e-02	8.33595e-03
8	-1.99600e+00	7.17146e-06	3.19676e-02	3.57728e-03
9	-1.99598e+00	2.39515e-07	3.20777e-02	1.42978e-04

Table 3: Calculated magnetic moment values for the 2×2 lattice at temperature $T = 1.0\ J/k_B$. The same observations for the mean value can be done here as for the energy mean value in Table 2. For the variance, however, the error seem to hit a limit at around 10^4, and it seems to be unstable after that. True values are $\mathbb{E}(|\mathcal{M}|) = 0.9986607$ and $\sigma_{|\mathcal{M}|}^2 = 4.010740 \cdot 10^{-3}$.

$\log_{10} N$	$\bar{\mu}_{\lvert\mathcal{M}\rvert}$	ε	$\bar{\sigma}_{\lvert\mathcal{M}\rvert}^2$	ε
1	9.09091e-01	8.96899e-02	3.30579e-01	8.14233e+01
2	9.90099e-01	8.57320e-03	3.92118e-02	8.77671e+00
3	9.97003e-01	1.65996e-03	9.95408e-03	1.48186e+00
4	9.98800e-01	1.39574e-04	4.19382e-03	4.56479e-02
5	9.98560e-01	1.00853e-04	4.49166e-03	1.19908e-01
6	9.98648e-01	1.27485e-05	4.02668e-03	3.97554e-03
7	9.98673e-01	1.25342e-05	3.96926e-03	1.03425e-02
8	9.98666e-01	4.90383e-06	3.99568e-03	3.75535e-03
9	9.98661e-01	8.18624e-08	4.01068e-03	1.50076e-05

of the equilibration process.

Figure 3 shows the evolution of the lattice energy E_i in each configuration for the first 500 cycles. We see that the hot start energy confluences with the cold start energy as early as after 160-170 cycles for $T = 1.0\ J/k_B$, and not very much later for $T = 2.4\ J/k_B$. At this point the Markov process has converged. The probability distribution of the lattice has reached the Boltzmann distribution

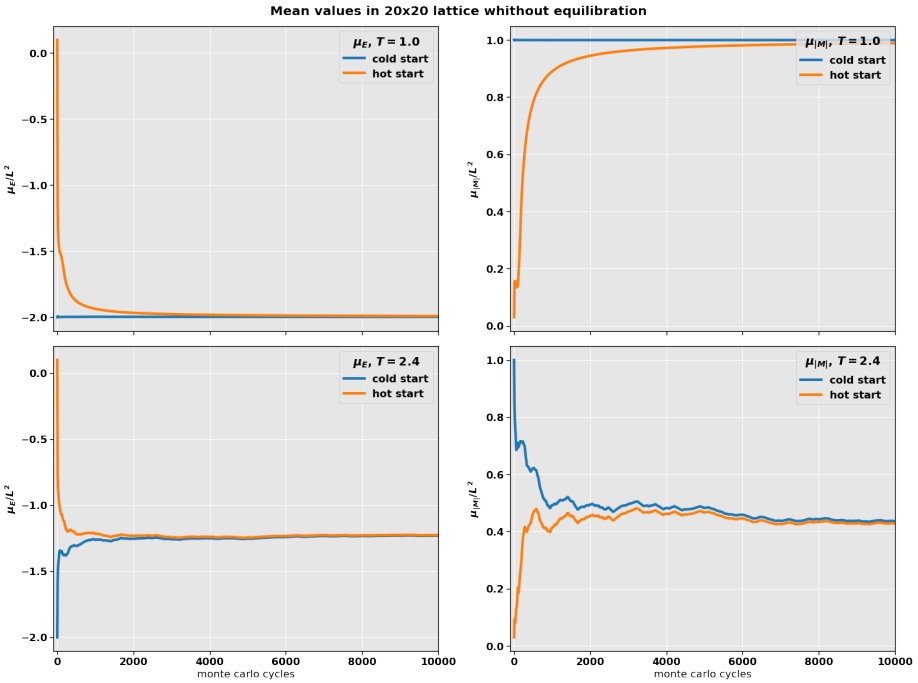

Figure 2: Evolution of the mean values for the first 10^4 Monte Carlo cycles in a 20×20 lattice at $T = 1.0\ J/k_B$ in the upper panes, and $T = 2.4\ J/k_B$ in the lower panes. We clearly see that we must allow some cycles for the model to reach equilibration, especially for higher temperatures. Cold start: all spins up; hot start; random spins.

for the lattice at T, as shown in Equations (10) to (13). That is; $\mathbf{w}_t \to \mathbf{v}_1$. This becomes visible also when we look at the evolution of the number of accepted flips per Monte Carlo cycle in Figure 4; the hot start and cold start curves follow each other perfectly. Snapshots to confirm this are shown in Figure 5, where we see in the middle and right pane that the lattices match *perfectly*.

We should note that this result depends on that each process draws the same sequence of semi-random numbers from our random number generator, and may also be subject to the numerical precision in a CPU.

3.3 Approximation of the Probability Distribution

As we saw in Equation (3) in Section 2, calculation of a lattice's probability distribution $P(\beta)$ involves evaluating the partition function $Z(\beta)$, which is prohibitively time consuming. Measuring it by simulation, on the other hand, involves only that we sample the configuration energies and sort them from lowest to highest.

Figure 6 shows the probability distributions at temperatures $T = 1.0\ J/k_B$

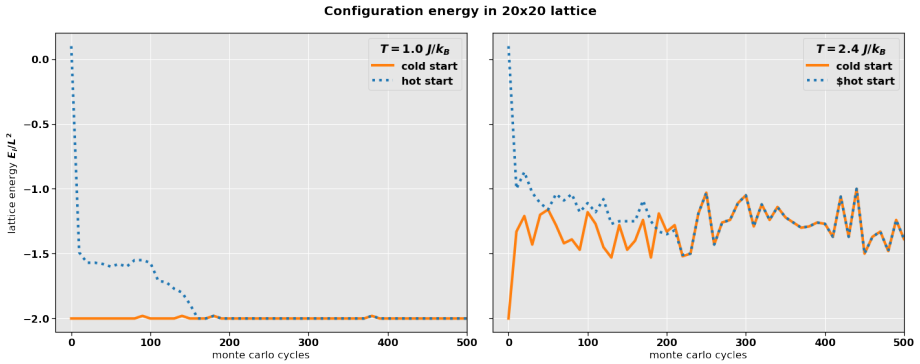

Figure 3: Evolution of the lattice energy E_i in each configuration during the first 500 Monte Carlo cycles for a 20×20 lattice. The hot and cold start confluence at around 160 cycles for $T = 1.0\ J/k_B$, and 200 for $T = 2.4\ J/k_B$.

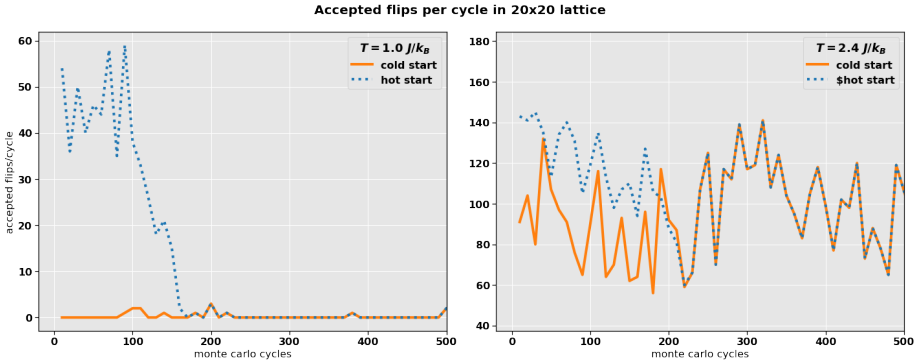

Figure 4: Accepted spin flips per Monte Carlo cycle during the first 500 Monte Carlo cycles for a 20×20 lattice. After confluence, the Markov process has converged and the evolution is independent of the lattice's initial configuration. Higher lattice temperature gives more accepted flips, as should be expected due to the higher kinetic energy of the spins.

and $T = 2.4\ J/k_B$ for our 20×20 lattice. We have sampled the energy after every Monte Carlo cycle for 10^4, 10^5 and 10^6 cycles. We have allowed 10^3 cycles for the equilibration of the model. Note the different scales on the x axes.

As expected from the discussion in the previous section, the distribution is concentrated to the left at lower temperatures, with only about one in one hundred cycles having a single down spin and one in one thousand having three. We see that increasing the temperature shifts the distribution to higher energies and also makes it broader. This is reflected in the higher variance of approximately 8.2, which is around 0.025 for the low temperature in the best estimate, and corresponds well to our Figures 3, 4 and 5.

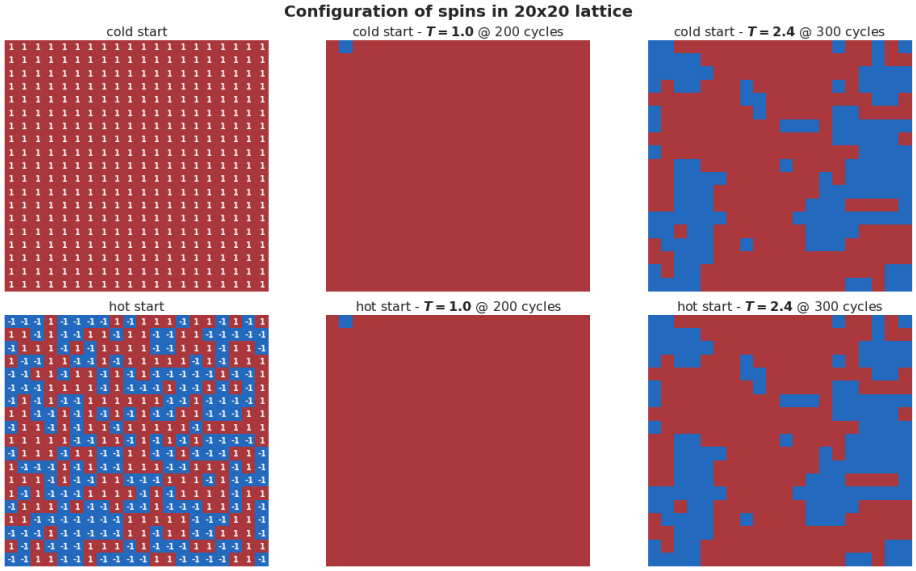

Figure 5: Configuration of spins in a 20×20 lattice at the start of the process to the left ($T = 0$ in the upper and $T \to \infty$ in the lower). In the middle and to the right we see that after the confluence of the hot and cold trajectories in Figure 4, the evolution is independent of the starting conditions.

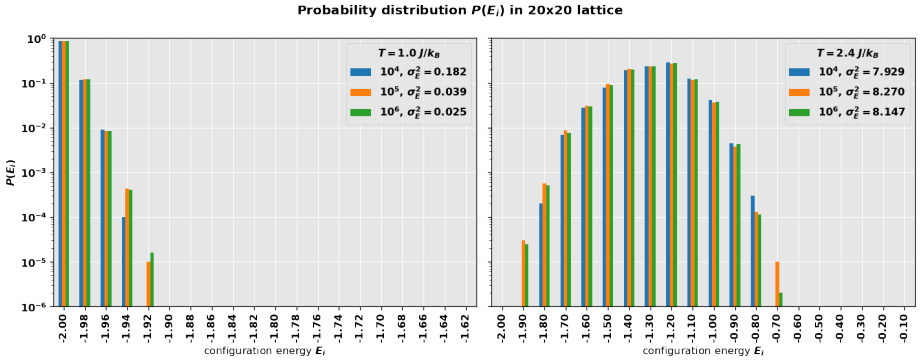

Figure 6: Probability densitiies for a 20×20 lattice at temperatures $T = 1.0$ J/k_B and $T = 2.4$ J/k_B. Note the logarithmic scale. At low temperature, the distribution is heavily concentrated at the lower energies. For higher temperatures, the distribution is shifted to higher energies and is much broader. This corresponds well to the change in variance.

3.4 Finding the Phase Transitions

We have seen that at low temperatures, all or almost all spins are aligned up, and as temperature in the lattice increases, scattered areas of downs appear. See Figure 5. In an infinite lattice, this process reaches a critical temperature T_C, where the $\mathbb{E}(\mathcal{M})$ abruptly goes to zero. Any increase beyond this temperature makes the scattered areas of up and down spins smaller until $T \to \infty$, where complete randomness prevails.

Our simulation model must have finite extension to be of any use to us, but we will not observe the same abrupt changes in mean magnetization. The critical temperature is still visible to us, especially in the heat capacity, but it is shifted to a higher temperature. See Figure 7, where we have plotted the analytical mean magnetic moment and heat capacity for a 2×2 lattice using Equations (23) and (3.1).

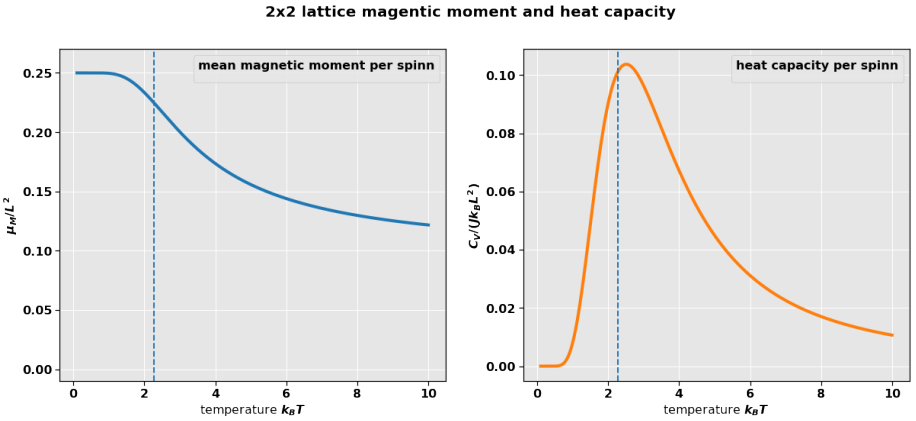

Figure 7: Plots of the analytical magnetic moment expectation value and heat capacity for a 2×2 lattice as a function of T. The critical temperature $T_C \approx 2.269\ J/k_B$ of the infinite lattice is indicated by the vertical dotted line. The critical temperature is shifted to a higher temperature for any finite lattice.

The critical temperature $T_C^{(\infty)}$ of the infinite lattice is indicated by the vertical line, while the critical temperature $T_C^{(2\times 2)}$ occurs at the maximum value of the heat capacity. The relation between the critical temperatures of the finite and the infinite lattices are given by

$$T_C^{(L\times L)} - T_C^{(\infty)} = \frac{\alpha}{L}, \tag{25}$$

where α is an unknown constant and L is the lattice size. See [4]. By running simulations with two lattice sizes L_1, L_2, we find the infinite lattice critical temperature as

$$T_C^{(\infty)} = \frac{L_1 T_C^{(L_1\times L_1)} - L_2 T_C^{(L_2\times L_2)}}{L_1 - L_2}. \tag{26}$$

Figure 8 shows plots of the approximated properties for lattice sizes $L = 40$, 60, 80 and 100. We have made two runs for each lattice size. First once over a wide range $T \in [2.0, 2.35]$ with step size $dT = 0.05$ and 1×10^5 samples at each step. Then in a narrower range $T \in [2.25, 2.35]$ steps $dT = 0.01$ and 2×10^5 samples to get a finer precision.

In the upper right pane we see that the mean magnetic moment drops off sharper for increased lattice size, corresponding well with what we would expect. We also see that the peak in the heat capacities and susceptibilities seem to move left towards $T_C^{(\infty)}$, which again is indicated by the vertical line. The expected tendency is that larger L should move the peak closer to $T_C^{(\infty)}$, but from these results, that is not clear.

For the 80×80 and 100×100 lattices. the peaks seem to lay in the [2.27, 2.29] range. We narrow our search further to only include these two lattices, and run simulations at each step $dT = 0.002$ with 1×10^6 samples.

The results are shown in Figure 9. Still, the curves do not show a smooth development, fluctuating up to 5-6 % for the 100×100 lattice. But picking the maximum values gives a fairly good estimate

$$T_C^{(\infty)} \approx \frac{100 \cdot 2.278 - 80 \cdot 2.282}{100 - 80} = 2.262, \tag{27}$$

which deviates about 0.31 % from the analytical value $T_C^{(\infty)} = 2/\ln(1+\sqrt{2}) \approx 2.269\ J/k_B$ [4].

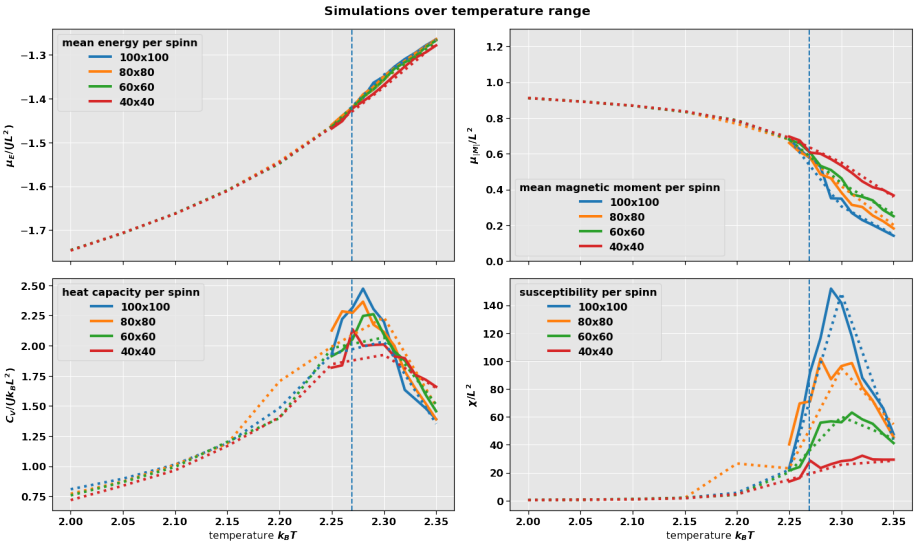

Figure 8: Simulations over temperature range with different lattice sizes. The dotted lines indicate the first run with lower sampling, and the full lines the second run with higher sampling. The critical temperature for each lattice $T_C^{(L\times L)}$ are best visible as the peaks in the heat capacities and susceptibilities (bottom panes).

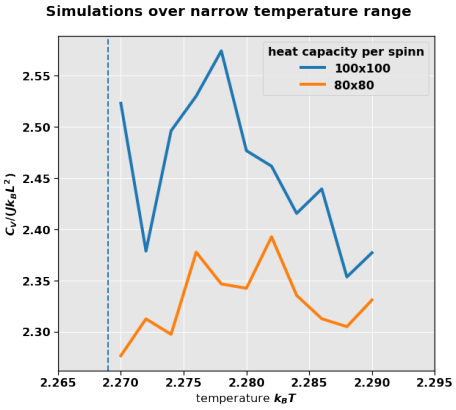

Figure 9: Narrowed search for the critical temperature with finer steps and higher sampling than in Figure 8. Still, the heat capacity estimates do not have a smooth development, but the approximation of $T_C^{(\infty)}$ deviates only 0.31 % from the analytical value.

4 Discussion and Conclusion

We have shown that the two-dimensional Ising model can be interpreted as a reversible Markov process. We have used Monte Carlo simulations with the Metropolis algorithm as acceptance criteria for evolving the process, and seen that it converges towards its most likely state, independently of the initial conditions. As such, the initial conditions can be selected freely, but the equilibration time will depend on our selection.

We have seen that the configuration of spins starts with almost all being in the up state at low temperatures, and that increasing temperature leads to higher number of downs. We have also seen that the ups and downs tend to form patches, corresponding well to the spins' preference of attaining the same state as their nearest neighbors.

Monte Carlo simulation can also be used to approximate the probability distribution of the spin configuration, expressed as the configuration energy E_i. The distribution is heavily weighted towards the lower energy limit $-2J$ per spin at lower temperatures, and moves to higher energies as temperature increases. We have seen that this corresponds to increased variance, meaning that the distribution broadens. This is a consequence of the increased kinetic energy which means that more energy states are likely to occur. The higher energy limit of the lattice is $+2J$ per spin, but the mean value of the distribution will never move 0, since that corresponds to $T \to \infty$.

For a small lattice of 2×2 spins, where analytical expressions are easily attained, we have shown that our model approximates the magnetic energy and moment expectation value and variance with high precision, but that this requires $> 10^6$ Monte Carlo cycles. Proofing our model on the 2×2 lattice has the added benefit of putting our model to the test with regards to the correct implementation of boundary values, since all spins are one the edge of the lattice.

Finally, we have shown that our model correctly reproduces the critical temperature, which in an infinite lattice leads to phase transition (the magnetic moment goes to zero). Based on our simulations, we estimated the analytical critical temperature with an error of 0.31 %.

As an extension of the study done in this report, it would be interesting to look at how the Ising model could be used in other settings. Many phenomena present themselves as scattered continuous areas of equal orientation. These may be the formation of ice on a pond or the electoral map of USA, and further insight into the Ising model, by tuning of the coupling J or extension into higher dimensions could help solve such problems.

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