A numerical study of a phase transition of a ferromagnetic material using the Ising model

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Abstract

A numerical simulation of a ferromagnetic material in the canonical ensemble is performed using the two-dimensional Ising model and Markov chain Monte Carlo methods. We study a phase transition of the ferromagnetic material and use the power law behavior of the heat capacity and the magnetic moment as well as linear regression to obtain an estimate of the critical temperature of an infinite system in order to confirm the analytical value obtained by Kramers and Wannier. We observe what appears to be a phase transition near the critical temperature for a 100×100 spin lattice. We find $T_C = 2.263$ with a statistical uncertainty of $\sigma_{T_C} = 0.0005$, although our method for finding the uncertainty is highly biased.

Introduction

In this report we aim to confirm the analytical value obtained by Kramers and Wannier of the critical temperature for an infinite sized spin lattice. We do this by simulating the system numerically using the Ising model and we consider the system to be in the canonical ensemble. The numerical simulation will be performed using Markov chain Monte Carlo methods, more specifically the Metropolis-Hastings algorithm, to randomly generate a proposal state with some likelihood associated with it provided that it is in thermal equilibrium with the reservoir, i.e we use the Boltzmann distribution. The proposed state will differ from the current state by a single spin flipped. To extract the critical temperature we will exploit the power law behavior of certain physical quantities of the system and perform a linear regression.

Theory

The canonical ensemble

The canonical ensemble is an ensemble of systems each of which are in thermal equilibrium with a much larger system commonly called "the reservoir" or "a heat bath". For one of the smaller systems, the probability that it is in some particular microstate s is given by the Boltzmann distribution

$$P(s) = \frac{1}{Z} e^{-\beta E(s)} \tag{1}$$

where $E(s)$ is the energy of the microstate s and

$$Z = \sum_{s} e^{-\beta E(s)} \tag{2}$$

is the partition function which is a sum over all the Boltzmann factors $e^{-\beta E(s)}$ for each microstate. $\beta \equiv 1 \,/\, kT$ where k is Boltzmann's constant and T is the temperature of the system. The expectation value of any quantity X of the system is given by

$$\langle X \rangle = \frac{1}{Z} \sum X(s) e^{-\beta E(s)} \tag{3}$$

From this it can be shown that

$$\langle E \rangle = -\frac{1}{Z} \frac{\partial Z}{\partial \beta} \tag{4}$$

and

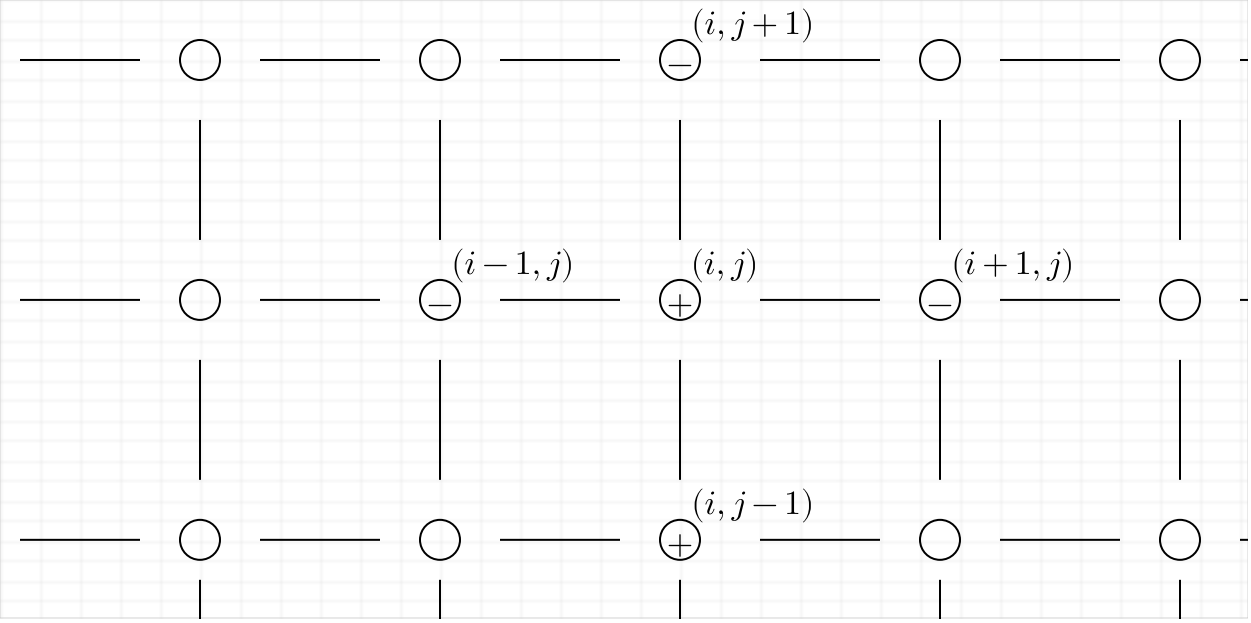
$$\langle E^2 \rangle = \frac{1}{Z} \frac{\partial^2 Z}{\partial \beta^2} \tag{5}$$

The heat capacity at constant volume is given by $C_V = \partial_T \langle E \rangle$. Using Eq. (4) it can be shown that

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

The Ising model

Consider a system consisting of spins arranged in a quadratic crystal structure.



Each spin can have "spin up" or "spin down" and interacts with their nearest neighbors. For example, spin (i, j) interacts with spins $(\pm i, j)$ and $(i, \pm j)$. This is called the Ising model which is used to model the behavior of ferromagnetic materials. To reflect the fact that alignment of spins is energetically favorable the energy of one particular spin configuration is given by

$$E = -J\sum_{\langle kl \rangle}^{N} s_k s_l \tag{7}$$

where N denotes that the lattice is $N \times N$ and $s = \pm 1$, representing "spin up" or "spin down". $J > 0$ is a coupling constant which expresses the strength of the interaction between the spins. In the Ising model the spins are taken to be dimensionless, meaning that J has dimension energy. $\langle kl \rangle$ means that the sum is to be taken over nearest neighbors only. For example, the energy contribution from the interactions of spin (i, j) and its neighbors is

$$E_{(i,j)\ \&\ \text{co}} = -J\Big[\overbrace{1\cdot(-1)}^{(i,j)\text{ and }(i-1,j)} + \overbrace{1\cdot(-1)}^{(i,j)\text{ and }(i+1,j)} + \overbrace{1\cdot 1}^{(i,j)\text{ and }(i,j-1)} + \overbrace{1\cdot(-1)}^{(i,j)\text{ and }(i,j+1)}\Big]$$

No interaction between a pair of spins is to be counted twice. In addition, we're using periodic boundary conditions, meaning that $(i,\ 1)$ interacts with $(i,\ N)$ and $(1,\ j)$interacts with $(N,\ j)$ for each i and j. The magnetization of one particular spin configuration is given by

$$\mathscr{M} = \sum_{i=1}^{N}\sum_{j=1}^{N} s_{i,j} \tag{8}$$

which is simply a sum of all the spins in the lattice. Assuming the lattice of spins is in thermal equilibrium with a "reservoir" at temperature T the probability that the system is in one particular spin configuration with energy E is given by Eq. (1). The expectation value of the energy $\langle E \rangle$ and the heat capacity C_V are given by Eq. (4) and (6) respectively. The magnetic susceptibility is given by

$$\chi = \frac{1}{kT}\left(\langle \mathscr{M}^2 \rangle - \langle \mathscr{M} \rangle^2\right) \tag{9}$$

The partition function of this system is hideously complicated, but was in fact derived by Lars Onsager in a 1944 article, thus obtaining an exact solution to this system for which he was nominated to a Nobel prize in physics [1].

Power law behavior

It can be shown that at temperatures near the critical temperature $T = T_C$ that a few physical quantities of a ferromagnetic material has a power law behavior. The mean magnetization behaves like

$$\langle M \rangle \propto (T - T_C)^{\beta} \tag{10}$$

where $\beta \approx 5\,/\,16$. The heat capacity at constant volume and the magnetic susceptibility behave like

$$C_V \propto |T_C - T|^{-\alpha(13)} \tag{11}$$

$$\chi \propto |T_C - T|^{-\gamma} \tag{12}$$

respectively, where $\alpha \approx 1\,/\,8$ and $\gamma \approx 5\,/\,4$ [2]. What Eq. (10) is saying is that the critical temperature occurs at $\langle M \rangle = 0$. Meanwhile Eq. (11) and Eq. (12) are saying that the critical temperature occurs at the maximum of C_V and χ (take the first derivative of these equations and set them to zero to see this).

One can also show that the critical temperature as a function of the lattice size N behaves like

$$T_C(N) = aN^{-1} + T_C(N = \infty) \tag{13}$$

where a is a constant and $T_C(N = \infty)$ is the critical temperature of the infinite lattice. The exact value of the critical temperature of the infinite lattice was found in 1941 by Kramers and Wannier [3]

$$\frac{kT_C(N = \infty)}{J} = \frac{2}{\ln\left(1 + \sqrt{2}\right)} \approx 2.269$$

Methods

Markov chain Monte Carlo

To study the behavior of the spin lattice as a function of the temperature, we want to randomly generate spin configurations according to the Boltzmann distribution in Eq. (1). The energy and magnetization is calculated for each generated spin configuration.
The expectation value of the energy is approximated by

$$\langle E \rangle \approx \frac{1}{M} \sum_{i=1}^{M} E_i \tag{14}$$

where E_i is the energy of spin configuration i and M is the total number of randomly generated spin configurations. $\langle E^2 \rangle$, $\langle \mathscr{M} \rangle$ and $\langle \mathscr{M}^2 \rangle$ are approximated accordingly.

To avoid having to deal with the partition function we'll use the concept of Markov chains to generate the spin configurations. Recall that a discrete Markov chain involves a transition probability matrix P and a state vector w_i such that $w_{i+1} = Pw_i$.

As an easy example, consider a group of undergraduate physics students one particular year. The next year some will become graduate students, some have decided to take another year as undergraduates and others will have dropped out. The next year some of the undergraduates become graduate students while some of the graduate students become undergraduates. Some of the dropouts have decided to try again as undergraduates, and so it goes year after year. In this process there are three possible states: undergraduate (U), graduate (G) or dropout (D). The probability transition matrix might look something like this:

$$P = \begin{bmatrix} \overbrace{1/3}^{U\to U} & \overbrace{1/5}^{G\to U} & \overbrace{1/3}^{D\to U} \\ \overbrace{1/3}^{U\to G} & \overbrace{3/5}^{G\to G} & \overbrace{0}^{D\to G} \\ \overbrace{1/3}^{U\to D} & \overbrace{1/5}^{G\to D} & \overbrace{2/3}^{D\to D} \end{bmatrix}$$

The initial state vector is $w_0^T = \left(\overbrace{1}^{U}, \overbrace{0}^{G}, \overbrace{0}^{D}\right)$. The state vectors may be thought of as probability distributions, i.e they give the probabilities that some student chosen at random are in any of the three states. In general $0 \leq P_{ij} \leq 1$ gives the probability of transitioning to state i given current state j and the sum of the elements along a column has to add up to 1. Such a matrix is called a stochastic matrix and you may recall that the largest eigenvalue of a stochastic matrix is equal to one, with the corresponding eigenvector being the steady-state vector.

What we're going to do now is to *construct a transition probability matrix such that the steady state vector is the Boltzmann distribution in Eq.* (1). That may sound utterly impossible, but it's actually quite easy to understand the process which is referred to as the Metropolis-Hastings algorithm. One assumption is needed though. Let w be the steady state vector and P be the transition probability matrix. The assumption is that once we have reached the steady state, the probability of being in state i and then going to state j is equal to the probability of being in state j and then going to state i, i.e

$$P_{ij}w_j = P_{ji}w_i \tag{15}$$

This is called detailed balance. It can be shown that any vector w that satisfies Eq. (15) is a steady state vector by summing over j on both sides and using that the sum over the elements of P along any column is one:

$$\sum_j P_{ij}w_j = \sum_j P_{ji}w_i = w_i \sum_j P_{ji} = w_i$$

which is index notation for $w = Pw$. Rearranging Eq. (15) we obtain

$$\frac{P_{ij}}{P_{ji}} = \frac{w_i}{w_j}$$

and if w is the Boltzmann distribution we have

$$\frac{P_{ij}}{P_{ji}} = e^{-\beta(E_i - E_j)} \tag{16}$$

and we have happily gotten rid of the partition function. We can use whatever transition probabilities we like as long as they satisfy Eq. (16), so what are we going to use? Say $E_i > E_j$. Then $P_{ji} > P_{ij}$ so let's just fix $P_{ji} = 1$. Then

$$P_{ij} = e^{-\beta(E_i - E_j)} \tag{17}$$

and that's it! Say that the system is in some state j with energy E_j. We then *propose* a new state i with energy E_i. If $E_i \leq E_j$ the transition probability is one so we set the state to i. If $E_i > E_j$ we calculate the transition probability P_{ij} as in Eq. (17) and compare it to some random number $r \in [0,\ 1]$ generated from the uniform distribution. If $r \leq P_{ij}$ we set the state to i. Else we keep state j.

Implementation

First and foremost we're setting $J = k = 1$ meaning that all quantities are hereby dimensionless.

We can represent the lattice of spins by an $N \times N$ matrix S with its elements being ± 1. The initial spin configuration can be randomly generated or something more ordered, e.g. having all the spins aligned. We could randomly generate the following spin configurations as well. An algorithm for calculating the energy and magnetization of a spin configuration according to Eq. (7) and Eq. (8) goes as follows:

```
E = M = 0
im = jm = N
```

```
for i = 1 : N
  for j = 1 : N
    E -= S(i, j)*(S(im, j) + S(i, jm))
    M += S(i, j)
```

And then we could compare the energy of the proposed new spin configuration with the current spin configuration using the Metropolis-Hastings algorithm.

However this is an inefficient approach. Instead of proposing a randomly generated spin configuration we're instead going to be proposing a new configuration where only a single spin is flipped. That way we don't have to calculate the energy of the proposed spin configuration by brute force because there are only five possible energy differences when flipping a single spin. These energy differences are $\Delta E = -8,\ -4,\ 0,\ 4,\ 8$ so we can precalculate the transition probabilities for each of them as in Eq. (17). Notice that if we compare these transition probabilities with a random number $r \in [0,\ 1]$ that a transition to lower energy will always get accepted.

We still need to calculate the energy difference of a transition to know which transition probability to use. Say that we're proposing to flip spin $(i,\ j)$ with $S^2_{i,j} = \pm 1$ and $S^1_{i,j} = \mp 1$. The energy difference can be calculated efficiently in the following way:

$$\Delta E = -\left(S^2_{i,j} - S^1_{i,j}\right)\left(S_{i-1,j} + S_{i+1,j} + S_{i,j-1} + S_{i,j+1}\right)$$

Using that $S^2_{i,j} = -S^1_{i,j}$ we obtain

$$\Delta E = 2S^1_{i,j}(S_{i-1,j} + S_{i+1,j} + S_{i,j-1} + S_{i,j+1}) \tag{18}$$

Similarly the magnetization difference can be calculated as

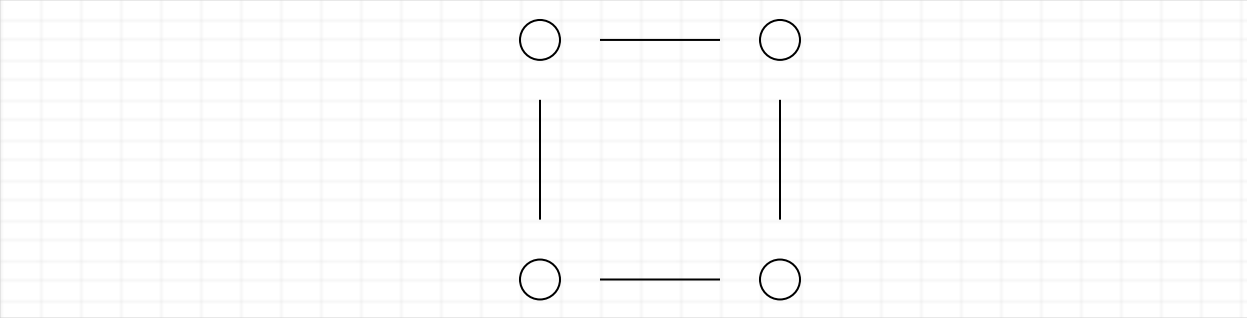
$$\Delta \mathscr{M} = S^2_{i,j} - S^1_{i,j} = 2S^2_{i,j}$$

To account for the periodic boundary condition we can substitute i in Eq. (18) by

$$i \to (i + N)\mathrm{Mod}(N)$$

and we can substitute j similarly. This is how we implement Eq. (18) in the program where indices run from 0 to $N-1$. The spin that we propose to flip will be chosen at random. The expectation values are updated as in Eq. (14) after $N \times N$ *proposed* spin flips. We will hereby refer to $N \times N$ proposed spin flips as a Monte Carlo sweep.

Verification - The 2×2 lattice



We'll test our implementation on the simple case of a 2×2 lattice of spins. There are $2^4 = 16$ possible configurations so calculating the partition function for this system isn't so bad. A macrostate of this system may be denoted by the number of positive spins. The following table shows the multiplicity Ω, energy E and magnetization $\mathscr{M}$ for each of these macrostates.

# of $+1$ spins	Ω	E	$\mathscr{M}$
4	1	-8	$+4$
3	4	0	$+2$
2	4	0	0
2	2	$+8$	0
1	4	0	-2

0	1	-8	-4

Using Eq. (2) the partition function of this system is given by

$$Z = 4\cosh 8\beta + 12$$

The energy expectation values $\langle E \rangle$ and $\langle E^2 \rangle$ are given by Eq. (4) and Eq. (5) respectively.

$$\langle E \rangle = -\frac{8\sinh 8\beta}{\cosh 8\beta + 3} \tag{19}$$

$$\langle E^2 \rangle = \frac{64\cosh 8\beta}{\cosh 8\beta + 3}$$

From Eq. (6) the heat capacity is

$$C_V = \frac{1}{T^2}\left[\frac{64\cosh 8\beta}{\cosh 8\beta + 3} - \left(\frac{8\sinh 8\beta}{\cosh 8\beta + 3}\right)^2\right] \tag{20}$$

The magnetization expectation values $\langle \mathscr{M} \rangle$, $\langle \mathscr{M}^2 \rangle$ and $\langle |\mathscr{M}| \rangle$ are calculated according to Eq. (3). We may see rather quickly that $\langle \mathscr{M} \rangle = 0$. The others are given by

$$\langle \mathscr{M}^2 \rangle = \frac{8e^{8\beta} + 8}{\cosh 8\beta + 3}$$

$$\langle |\mathscr{M}| \rangle = \frac{2e^{8\beta} + 4}{\cosh 8\beta + 3} \tag{21}$$

Thus from Eq. (9) the magnetic susceptibility is

$$\chi = \frac{1}{T} \frac{8e^{8\beta} + 8}{\cosh 8\beta + 3} \tag{22}$$

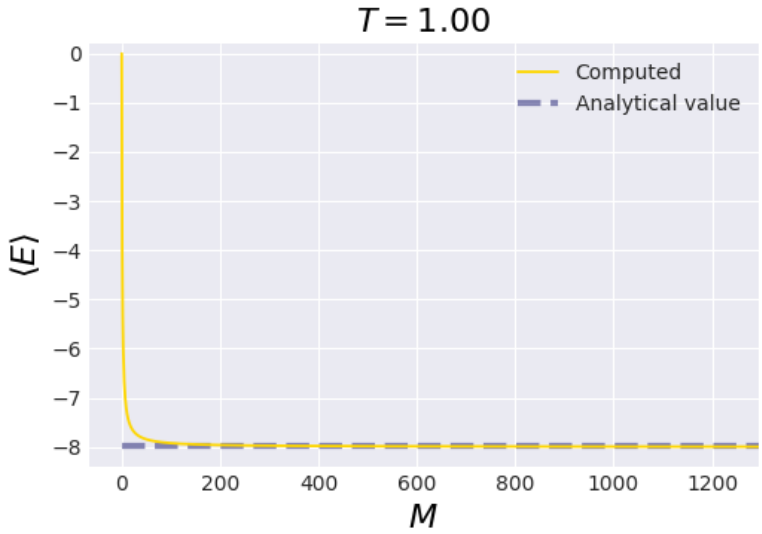


Figure 1: The expectation value of the energy $\langle E \rangle$ at temperature $T = 1.00$ as a function of the number of Monte Carlo sweeps M for the 2×2 lattice. The purple horizontal dashed line represents the analytical value obtained from Eq. 19.

Figure 1 shows the expectation value of the energy $\langle E \rangle$ at temperature $T = 1.00$ as a function of the number of Monte Carlo sweeps M for the 2×2 lattice. It is computed as in Eq. (14). The starting spin configuration of the lattice was randomly generated. One million Monte Carlo sweeps was used, but plotting only the first 1200 is sufficient. We see that the computed expectation value converges to the analytical value obtained from Eq. (19).

Figure 2 and Figure 3 similarly shows that the computed mean absolute magnetization $\langle |\mathscr{M}| \rangle$ and the computed heat capacity C_V converge to the analytical values obtained from Eq. (21) and Eq. (20) respectively. Again only plotting the first 1200 Monte Carlo sweeps is sufficient. The magnetic susceptibility χ looks somewhat more troublesome, and converges far more slowly as we see in Figure 4. Here plotting the first 500 thousand Monte Carlo sweeps was necessary to show that the magnetic susceptibility properly converges. Looking at Figure 2 this would seem like a surprising result, but Figure 5 reveals what's actually going on. It shows that the computed expectation value of the magnetization $\langle \mathscr{M} \rangle$

doesn't properly converge to the analytical value before at least a million Monte Carlo sweeps. It seems to have a particularly troublesome behavior early on in accordance with χ in Figure 4. The magnetization behaves more nicely after 200 thousand or so Monte Carlo sweeps, but the dataset is sort of bedeviled by its troubled past making it more difficult to converge to the analytical value.

This suggests that we should wait until the system is in it's most likely state (most of the time) before we start sampling the energies and magnetization of the accepted spin configurations. We'll run the program with a much larger system and try to estimate a relaxation time in terms of the number of Monte Carlo cycles in the next section.

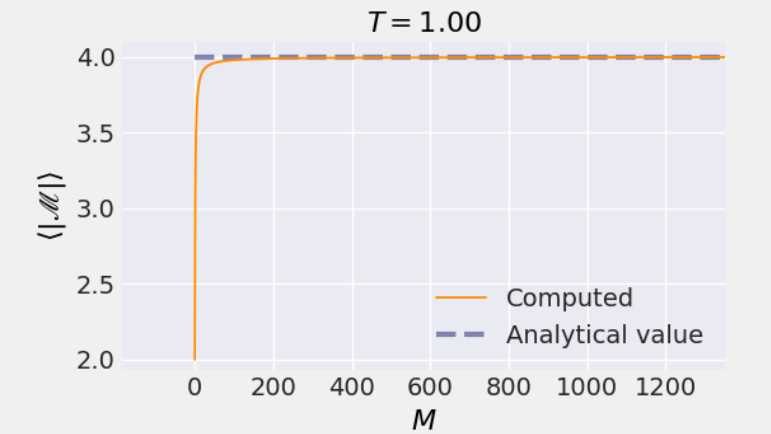


Figure 2: The mean absolute magnetization $\langle|\mathscr{M}|\rangle$ as a function of the number of Monte Carlo sweeps M.

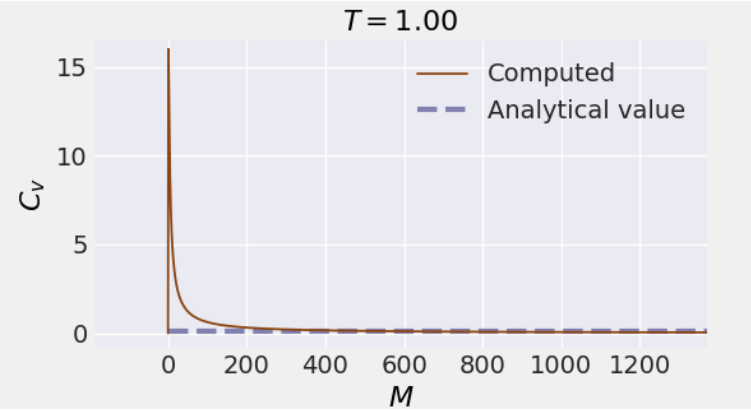


Figure 3: The computed heat capacity C_V according to Eq. 20 as a function of the number of Monte Carlo sweeps M.

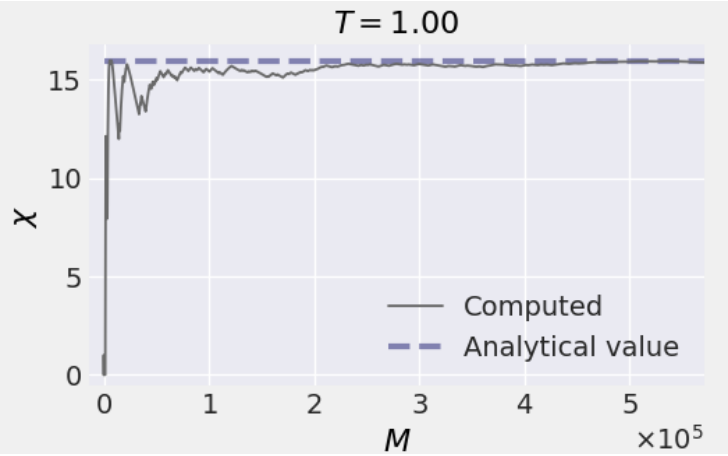


Figure 4: The computed magnetic susceptibility χ according to Eq. 22 as a function of the number of Monte Carlo sweeps M.

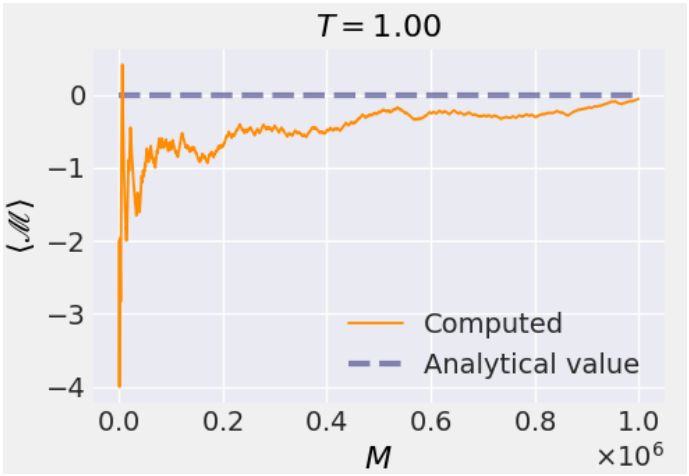


Figure 5: The expectation value of the magnetization $\langle \mathscr{M} \rangle$ as a function of the number of Monte Carlo sweeps M.

The computed expectation value of the energy and the absolute magnetization, the heat capacity and the magnetic susceptibility are plotted as functions of the temperature together with their respective analytical expressions in figures Figure 6 through Figure 9. This is to properly substantiate that our methods and implementation indeed are correct. Every data point was computed using a million Monte Carlo sweeps. We see in these figures that every data point sits reasonably close to the curve of the analytical expression, which is promising for further analysis of much larger systems.

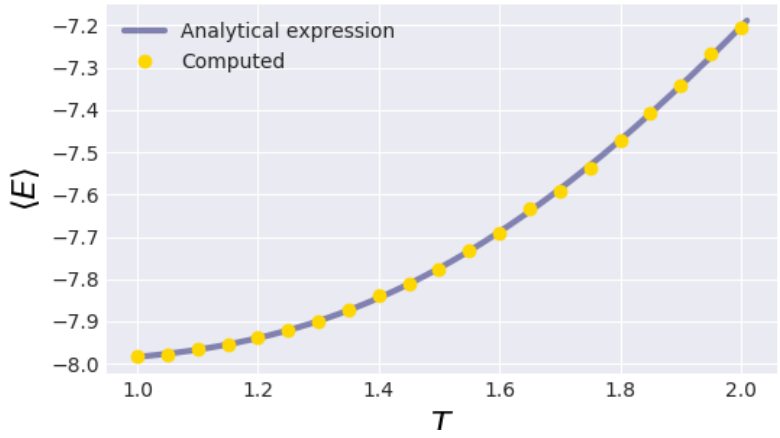


Figure 6: The computed mean energy $\langle E \rangle$ as a function of the temperature T together with the analytical expression in Eq. 19.

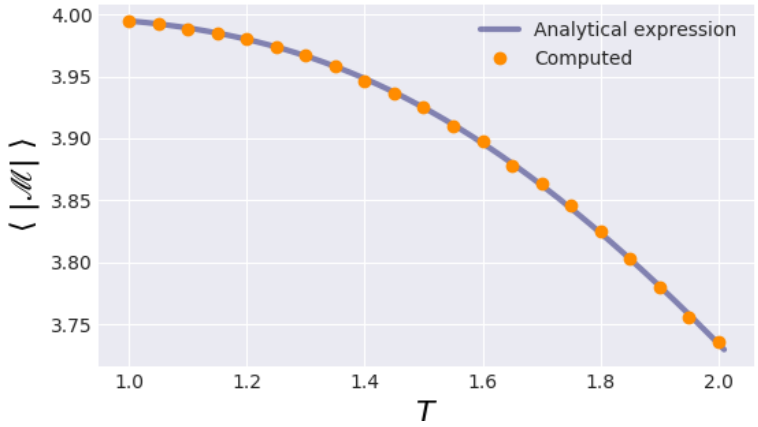


Figure 7: The computed mean absolute magnetization $\langle |\mathscr{M}| \rangle$ as a function of the temperature T together with the analytical expression in Eq. 21.

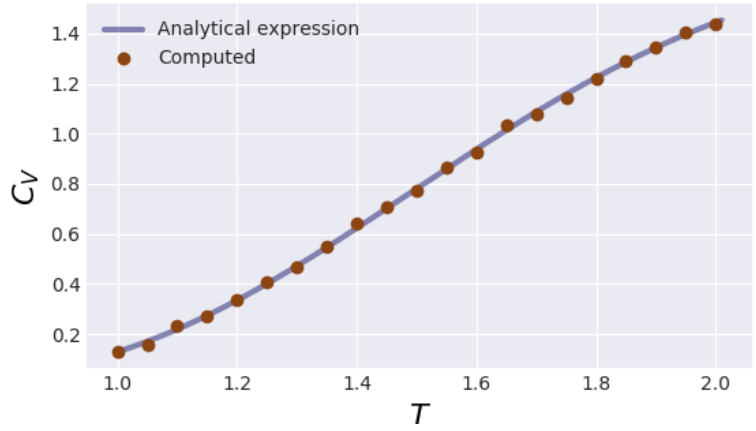


Figure 8: The computed heat capacity C_V as a function of the temperature T together with the analytical expression in Eq. 20.

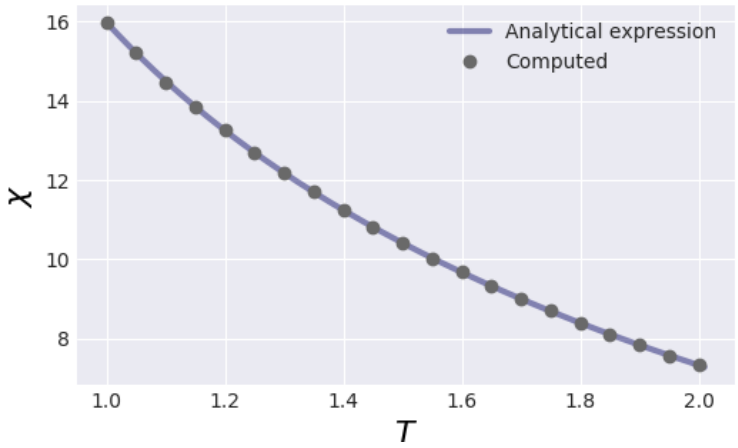


Figure 9: The computed magnetic susceptibility χ as a function of the temperature T together with the analytical expression in Eq. 22.

Convergence

We saw in the last section that we should wait a few Monte Carlo cycles before we start sampling the energies and the magnetization of the accepted spin configurations. In this section we'll discuss just how many Monte Carlo cycles we should wait before the sampling starts using a 20×20 spin lattice. Since the computed value of $\langle \mathscr{M} \rangle$ was by far the most troublesome of the plotted quantities in the previous section it is the only quantity that will be plotted for the 20×20 lattice.

We'll also check that the sampled energies indeed approaches the Boltzmann distribution $P(E) \propto \Omega(E) e^{-\beta E}$. We cannot plot a histogram of the energies together with an analytical expression for the corresponding Boltzmann distribution because we do not know the multiplicity function $\Omega(E)$. We do know that lower energies are always more likely than larger energies regardless of temperature, so the height of the columns in the histogram should decrease with larger energies. But we also need to keep in mind the possibility that higher energies may have a larger multiplicity than lower energies, which is indeed the case for the 2×2 lattice as we have seen. The larger multiplicity of higher energies may outweigh the larger probabilities of lower energies.

Figure 10 shows the mean magnetization per spin $\langle \mathscr{M} \rangle$ in the 20×20 lattice as

function of the number of Monte Carlo cycles M. It suggests along with Figure 5 that the mean magnetization behaves more nicely as the size of the system increases. From Figure 10 alone one would've thought that running less than 100 thousand Monte Carlo sweeps before sampling starts is sufficient for systems larger than 20×20. But figure Figure 11 suggests that $\langle \mathscr{M} \rangle$ becomes more troublesome at higher temperatures. Still we see that the mean magnetization has pretty much converged at $M = 0.6 \cdot 10^6$ Monte Carlo sweeps. As we will not go to temperatures as high as $T = 2.40$ it should be more than sufficient to start sampling the energy and magnetization after this many Monte Carlo sweeps.

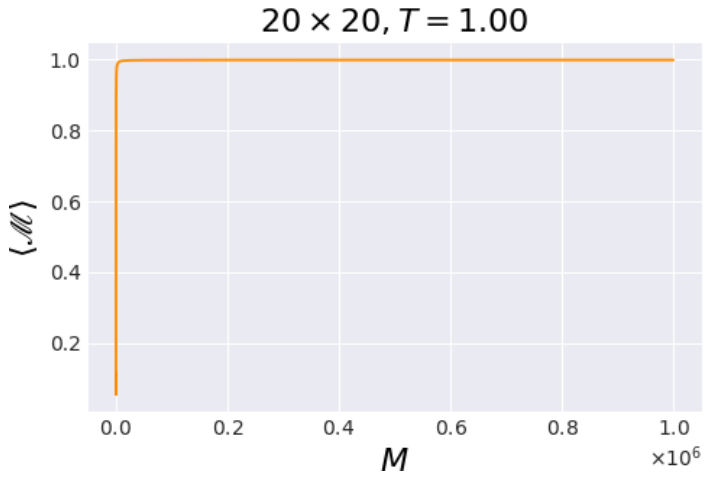


Figure 10: The computed mean magnetization $\langle \mathscr{M} \rangle$ per spin as a function of the number of Monte Carlo cycles M at temperature $T = 1.00$ for a 20×20 lattice.

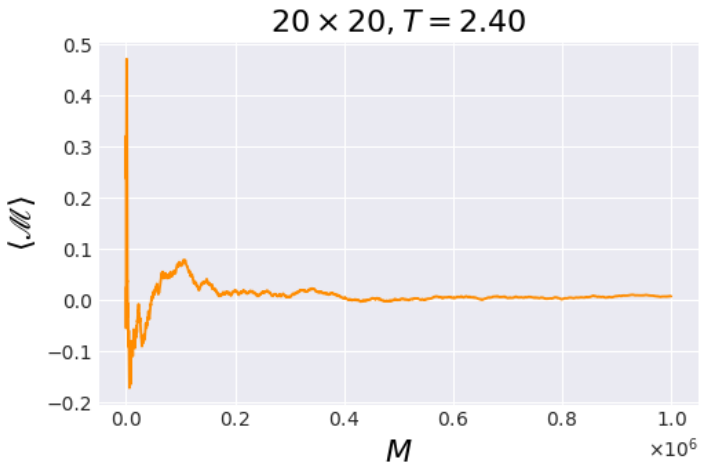


Figure 11: The computed mean magnetization $\langle \mathscr{M} \rangle$ per spin as a function of the number of Monte Carlo cycles M at temperature $T = 2.40$ for a 20×20 lattice.

Figures Figure 12 and Figure 13 shows a histogram of the sampled energies for the 20×20 lattice at temperatures $T = 1.00$ and $T = 2.40$. We see in Figure 12 that the vast majority of the sampled energies are in the low energy spectrum, as expected. The standard deviation of the energy samples $\sigma = 3.28$ is extremely small compared to the energy spectrum.

Figure Figure 13 tells a different tale. At $T = 2.40$ most of the energy samples have energy over $E = -500$ as compared to only three out of a million energy samples in figure Figure 12. The standard deviation of the energy samples $\sigma = 56.90$ has increased significantly. Although a single microstate with lower energy is always more likely than a higher energy microstate, figure Figure 13 suggests that at higher temperatures the multiplicity of a particular energy becomes the dominant factor.

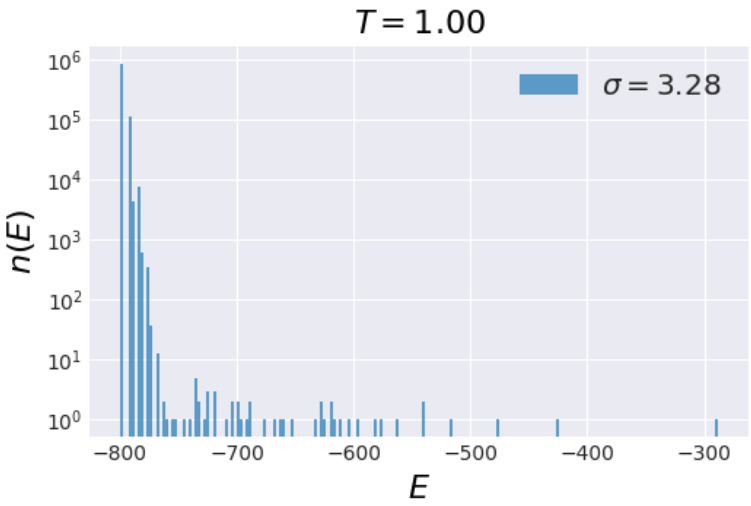


Figure 12: Histogram of the sampled energies of for the 20×20 lattice at temperature $T = 1.00$. Notice the logarithmic scaling of the y-axis.

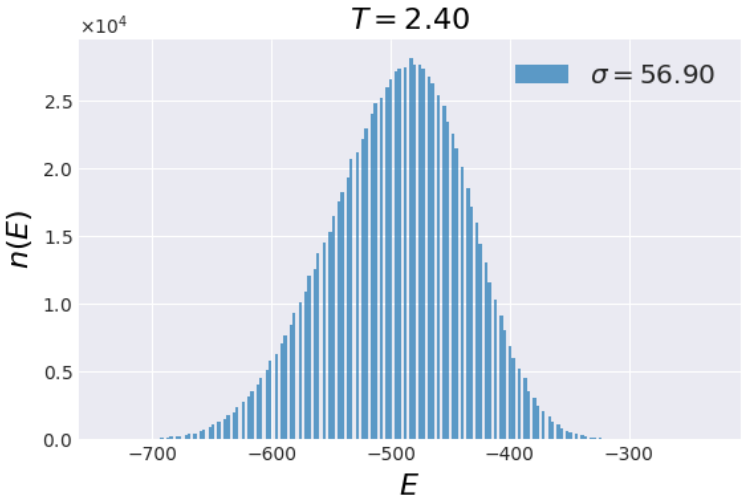


Figure 13: Histogram of the sampled energies for the 20×20 lattice at temperature $T = 2.40$.

Results

Figure 14 shows the mean energy $\langle E \rangle$ of the energy samples per spin as a function of the temperature T for the 100×100 lattice. It shows that the mean energy increases with temperature as expected. What's far more interesting are the Figure 15, Figure 16 and Figure 17. Figure 15 shows a sudden decrease in the mean absolute magnetization at temperatures $2.25 \leq T \leq 2.30$. It suggests that we indeed see a phase transition in the 100×100 lattice where it ceases to be ferromagnetic.

Figure 16 shows the heat capacity C_V per spin as a function of the temperature. As predicted by Eq. (11) we get a maximum heat capacity near the temperature where the mean absolute magnetization drops abruptly in Figure 15. Figure 17 similarly shows that we get a maximum magnetization near the same temperature, which further supports that we do indeed see a phase transition at this temperature.

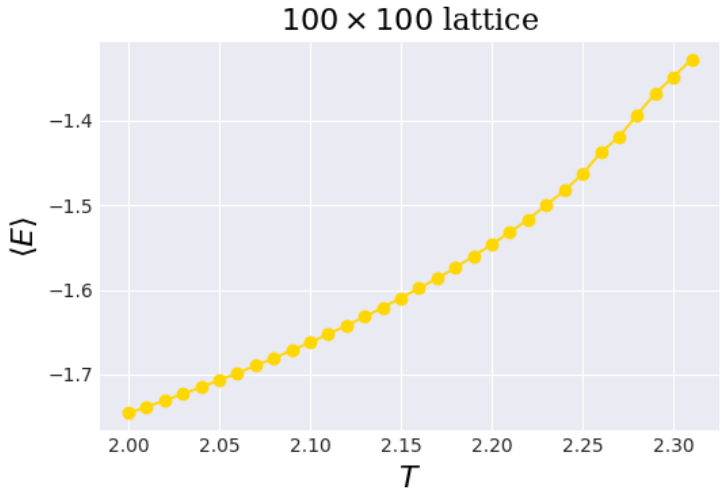


Figure 14: The mean energy $\langle E \rangle$ per spin as a function of the temperature T for the 100×100 lattice.

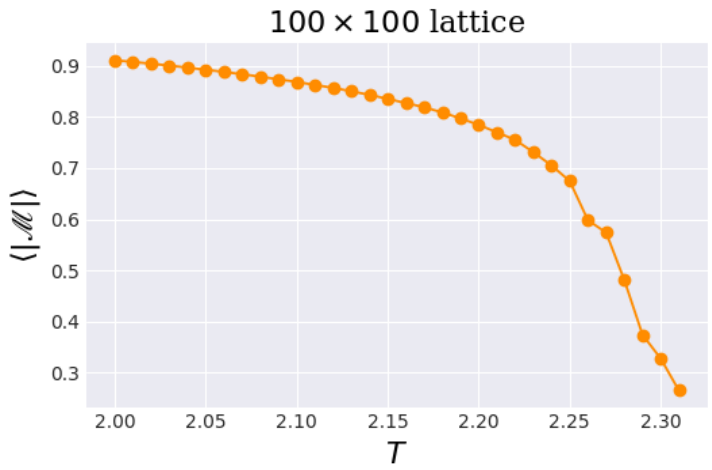


Figure 15: The mean absolute magnetization $\langle|\mathscr{M}|\rangle$ per spin as a function of the temperature T for the 100×100 lattice.

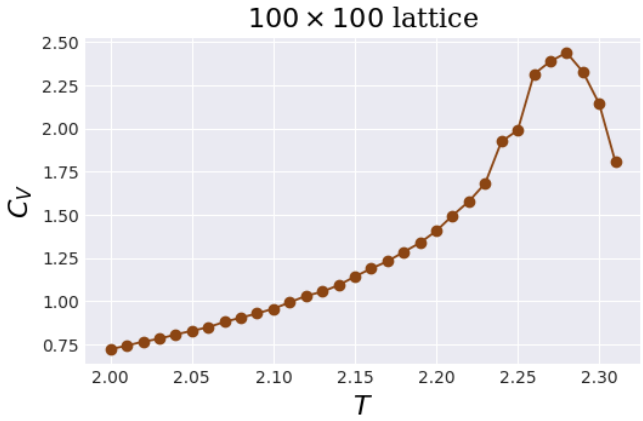


Figure 16: The heat capacity C_V per spin as a function of the temperature T for the 100×100 lattice.

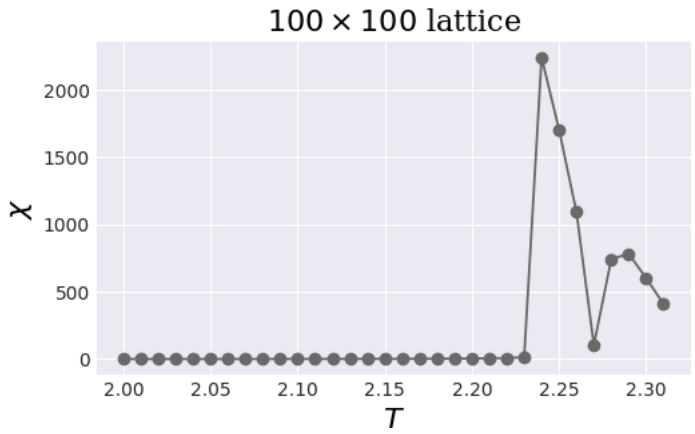


Figure 17: The magnetic susceptibility χ per spin as a function of the temperature T for the 100×100 lattice.

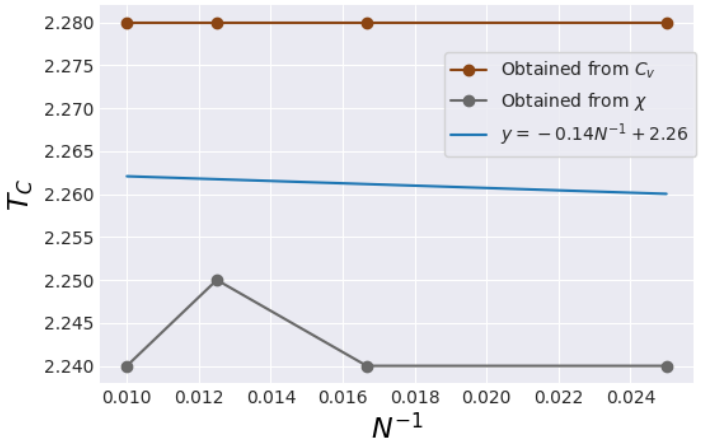


Figure 18: The temperature where the heat capacity C_V and the magnetic susceptibility χ are at a maximum for four lattices of sizes 40×40, 60×60, 80×80 and 100×100. Linear regression was performed using the dataset obtained from both C_V and χ.

Figure 18 shows an attempt to extract the temperature where the phase transition takes place. The heat capacity and the magnetic susceptibility has been calculating for lattices of sizes 40×40, 60×60, 80×80 and 100×100. Although a step size of $\Delta T = 0.01$ were used for the 100×100 lattice, we do not have the same resolution for the other lattices as time became a factor. The plot was

generated using the temperatures $T = 2.23,\ 2.24,\ 2.25,\ 2.26,\ 2.28,\ 2.30$ only. The figure shows at which of these temperatures the heat capacity and the magnetic susceptibility where at a maximum as a function of the inverse lattice size N^{-1}. A linear regression using the dataset obtained from both C_V and χ was performed according to Eq. (13) in order to extract the temperature at an infinite lattice size $T_C(N = \infty)$. Zero points of the mean magnetization $\langle \mathscr{M} \rangle$ was not used due to its troubled behavior.

The critical temperature was calculated to be $T_C(N = \infty) = 2.263$ with a statistical uncertainty of $\sigma_{T_C} = 0.0005$. This uncertainty is the $(2,\ 2)$ element of the covariance matrix obtained from performing the linear regression. There is reason to be skeptical of this uncertainty, considering the low resolution of the temperatures which makes it more likely that the data points will lay on the same horizontal line. Nevertheless, we came surprisingly close to the analytical value found by Kramers and Wannier.

Conclusion

We have performed numerical simulations of a ferromagnetic material of various sizes using the Ising model and Markov chain Monte Carlo methods. We have seen what appears to be a phase transition near the exact value of the critical temperature obtained by Kramers and Wannier at $T_C(N = \infty) = 2.263$. Although the statistical uncertainty of this value was very low at $\sigma_{T_C} = 0.0005$, it must be taken with a grain of salt considering the low resolution in the temperatures used to obtain the critical temperature. For further analysis in the future one should use a higher resolution in the temperatures. To ease the total computation time only the temperature interval $T \in [2.23,\ 3.32]$ should be explored. As the critical temperature of a finite lattice size is a linear function of the inverse lattice size N^{-1} it is not necessary to use overly large lattice sizes.

References

[1] L. Onsager, *Crystal Statistics. I. A Two-Dimensional Model with an Order-Disorder Transition*, Phys. Rev. 65, 117

[2] M. Plischke, B. Bergersen, *Equilibrium Statistical Physics*, 2nd ed.

[3] H. A. Kramers, G. H. Wannier, *Statistics of the Two-Dimensional Ferromagnet. Part I,* Phys. Rev. 60, 252

Appendix - Example program for simulating an $N \times N$ spin lattice

```
#include "ising_montecarlo.h"

void ising(int N, vec Temps, int mcs)
{

  vec mcsrange = regspace(1, mcs);

  #pragma omp parallel for
  for (int i = 0; i < Temps.n_elem; ++i) {

    double E = 0, M = 0;

    char filename [16];

    imat spins(N, N); vec w(17);

    mat data(mcs, 7);

    double T = Temps[i];

    initialize(N, E, M, T, spins, w);

    for (int mc = 0; mc < mcs; ++mc) {

      metropolis(N, E, M, spins, w);

      data(mc, 0) = E; data(mc, 2) = M;
```

```
    }

    // Calculate <E>
    data(span::all, 1) = cumsum(       data(span::all, 0))
/mcsrange;

    // Calculate <M> and <|M|>
    data(span::all, 3) = cumsum(       data(span::all, 2))
/mcsrange;
    data(span::all, 4) = cumsum(   abs(data(span::all,
2)))/mcsrange;

    // Calculate Cv and X
    data(span::all, 5) = (cumsum(square(data(span::all,
0)))/mcsrange
                               - square(data(span::all,
1)))/(T*T);

    data(span::all, 6) = (cumsum(square(data(span::all,
2)))/mcsrange
                               - square(data(span::all, 3)))/T;

    // Scale by # of spins
    data /= (N*N);

    sprintf  (filename, "data-N=%d-T=%.2f.dat", N, T);
    data.save(filename, raw_ascii);

  }

  return;
}

void initialize(int N, double &E, double &M, double T, imat
&spins, vec &w)
{

  E = M = 0;
```

```
  random_device rd;
  mt19937_64 gen(rd());
  uniform_real_distribution<double>
RandomNumberGenerator(0.0,1.0);

  for (int i = 0; i < N; ++i) {
  for (int j = 0; j < N; ++j) {

      if (RandomNumberGenerator(gen) > 0.5) {spins(i, j) =  1;}
      else                                  {spins(i, j) = -1;}

    }}

  int im1 = N - 1;
  int jm1 = N - 1;

  for (int i = 0; i < N; ++i) {
  for (int j = 0; j < N; ++j) {

    E -= spins(i, j)*(spins(im1, j) + spins(i, jm1));

    M += spins(i, j);

    jm1 = j; }
    im1 = i; }

  for (int dE = -8; dE <= 8; dE += 4) w(dE + 8) = exp(-dE/T);

  return;

}

void metropolis(int N, double &E, double &M, imat &spins, vec w)
{

  random_device rd;
  mt19937_64 gen(rd());
  uniform_real_distribution<double>
RandomNumberGenerator(0.0,1.0);
```

```
  int l, k;

  int dE;

  for (int i = 0; i < (int) N*N; ++i) {

    l = (int) (RandomNumberGenerator(gen) * (double) N);
    k = (int) (RandomNumberGenerator(gen) * (double) N);

    dE = 2*spins(l, k) * (   spins(periodic(l - 1, N), k)
                           + spins(periodic(l + 1, N), k)
                           + spins(l, periodic(k - 1, N))
                           + spins(l, periodic(k + 1, N))
                         ) ;

    if (RandomNumberGenerator(gen) <= w(dE + 8)) {
      spins(l, k) *= -1;
      E += (double) dE;
      M += (double) 2*spins(l, k);

    }
  }

 return;

}

inline int periodic(int index, int limit){
  // Thanks to Daniel Heinesen!!
  return (index + limit)%(limit);
}
```