FYS3150 Project 4

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Contents

Abstract

In this project, the Ising model for a two-dimensional ferromagnetic i studied numerically using Monte Carlo simulations with the Metropolis algorithm. A 2×2 system is also solved analytically for comparison, and the numerical results fit well. A phase transition is confirmed at the same temperature as analytically predicted by Lars Onsager.

1 Introduction

The Ising model was developed by the famous physicist Wilhelm Lenz and given to Ernst Ising as a problem for his thesis, in which he found the analytical solution for the one-dimensional situation. Ising's model is based describes a coupled system in which there is only an interaction between the nearest neighbours. Aside from describing ferro- and antiferromagnetic materials as in this project, the model has also been used successfully to describe other coupled systems, for instance the development of birdsong dialects[1].

In this project, the Ising model is used to describe a two-dimensional ferromagnetic, chrystalline material, modelled as a grid of spins where each spin can have the values ± 1. For an infinite grid, the analytical solution was found by Lars Onsager, while a 2×2 grid is solved analytically in this project.

The problem with analytical solutions for other sizes is finding the partition function, which is the "holy grail" of statistical mechanics. From this quantity, all the other thermodynamic quantities like energy can be calculated. The difficulty arises from the formula for the partition function, which includes summing over all possible microstates. With each spin having two possible values, a simple 10×10 grid will have $2^{10 \cdot 10} \approx 10^{30}$ possible microstates. For comparison, only approximately 10^{17} seconds have passed since the creation of the universe.

As a consequence, calculating the partition function analytically for a grid of reasonable size is not a viable option, and numerical approximations must once again be applied. Fortunately, the Metropolis algorithm, declared one of the top 10 algorithms of the 20th century[2], fits the problem very well.

This report starts off with a lenghty introduction, before giving an overview of both the mathematical and the physical theory of the problem at hand. The above mentioned Metropolis algorithm is implemented and tested on the 2×2 grid, for which an analytical solution is also developed. The convergence of the Metropolis algorithm is then tested for a 20×20 grid, and the numerically approximated probability distribution is analysed. Finally, the phase transition is thoroughly studied for varying grid sizes, and the critical temperature is found.

2 Physical theory

2.1 The Ising model

As stated in the introduction, the Ising model describes a coupled system where nearest neighbours affect each other. In this project, the Ising model is applied to a two-dimensional magnetic material modelled as a grid or lattice of spins, where each spin s_i can have the values $+1$ or -1, denoted by $\uparrow$ and $\downarrow$ respectively. Assuming that all couplings are of equal magnitude, the coupling in the Ising model leads to the energy

$$E = -J \sum_{\langle ij \rangle} s_i s_j \tag{1}$$

where the sum is over the nearest neighbours. From this expression, we see that if J is positive, the energy is minimised when all spins are aligned in parallel, which is the behaviour of a ferromagnetic material. If, on the other hand, J is negative, a state where all spins are antiparallel to each other has the lowest energy, corresponding to an antiferromagnetic material.

2.2 Statistical physics

The basis for the statistical physics of this problem is the probability distribution used for the macrostates, which is the Boltzmann distribution. This distribution states that the probability of a system being in a state with energy E_i is proportional to $\mathrm{e}^{-\beta E_i}$, where $\beta = 1/kT$. This probability distribution needs to be normalised, and with the normalisation factor denoted $1/Z$, we get the equation

$$1 = \sum_i P(E_i) = \sum_i \frac{1}{Z}\mathrm{e}^{-\beta E_i} = \frac{1}{Z}\sum_i \mathrm{e}^{-\beta E_i} \implies Z = \sum_i \mathrm{e}^{-\beta E_i}$$

Z is called the partition function, and is perhaps the most important quantity in statistical physics, as it makes it possible to calculate most other thermodynamic quantities. The energy can be calculated directly as

$$E = -\frac{\partial \ln(Z)}{\partial \beta}$$

In general, the expectation value of any thermodynamic quantity A can be calculated through

$$\langle A \rangle = \sum_i A_i P(E_i)$$

For the two-dimensional Ising model, we are primarily interested in the expectation values of the energy E and magnetization $|M|$, as well as the heat capacity C_V and magnetic susceptibility χ. The latter quantities can be calculated from the formulas[3]

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

3 Mathematical theory

4 Results

4.1 Numerical and analytical results for a 2×2 lattice

4.1.1 Analytical result

For a 2×2 lattice, the thermodynamic quantities can be found analytically without too much work. To find the partition function, we need to write out all possible microstates and calculate their energies. Using the periodic boundary conditions, we get

Microstate	Energy	Magnetization
$\begin{array}{cccc} & \downarrow & \downarrow & \\ \downarrow & \downarrow & \downarrow & \downarrow \\ \downarrow & \downarrow & \downarrow & \downarrow \\ & \downarrow & \downarrow & \end{array}$	$E = -8J$	$M = -4$
$\begin{array}{cccc} & \downarrow & \uparrow & \\ \downarrow & \downarrow & \downarrow & \downarrow \\ \uparrow & \downarrow & \uparrow & \downarrow \\ & \downarrow & \downarrow & \end{array}$	$E = 0$	$M = -2$
$\begin{array}{cccc} & \uparrow & \downarrow & \\ \downarrow & \downarrow & \downarrow & \downarrow \\ \downarrow & \uparrow & \downarrow & \uparrow \\ & \downarrow & \downarrow & \end{array}$	$E = 0$	$M = -2$
$\begin{array}{cccc} & \uparrow & \uparrow & \\ \downarrow & \downarrow & \downarrow & \downarrow \\ \uparrow & \uparrow & \uparrow & \uparrow \\ & \downarrow & \downarrow & \end{array}$	$E = 0$	$M = 0$
$\begin{array}{cccc} & \downarrow & \downarrow & \\ \uparrow & \downarrow & \uparrow & \downarrow \\ \downarrow & \downarrow & \downarrow & \downarrow \\ & \downarrow & \uparrow & \end{array}$	$E = 0$	$M = -2$
$\begin{array}{cccc} & \downarrow & \uparrow & \\ \uparrow & \downarrow & \uparrow & \downarrow \\ \uparrow & \downarrow & \uparrow & \downarrow \\ & \downarrow & \uparrow & \end{array}$	$E = 0$	$M = 0$
$\begin{array}{cccc} & \uparrow & \downarrow & \\ \uparrow & \downarrow & \uparrow & \downarrow \\ \downarrow & \uparrow & \downarrow & \uparrow \\ & \downarrow & \uparrow & \end{array}$	$E = 8J$	$M = 0$

Microstate	Energy	Magnetization
$\begin{array}{cccc} & \uparrow & \uparrow & \\ \uparrow & \downarrow & \uparrow & \downarrow \\ \uparrow & \uparrow & \uparrow & \uparrow \\ & \downarrow & \uparrow & \end{array}$	$E = 0$	$M = 2$
$\begin{array}{cccc} & \downarrow & \downarrow & \\ \downarrow & \uparrow & \downarrow & \uparrow \\ \downarrow & \downarrow & \downarrow & \downarrow \\ & \uparrow & \downarrow & \end{array}$	$E = 0$	$M = -2$
$\begin{array}{cccc} & \downarrow & \uparrow & \\ \downarrow & \uparrow & \downarrow & \uparrow \\ \uparrow & \downarrow & \uparrow & \downarrow \\ & \uparrow & \downarrow & \end{array}$	$E = 8J$	$M = 0$
$\begin{array}{cccc} & \uparrow & \downarrow & \\ \downarrow & \uparrow & \downarrow & \uparrow \\ \downarrow & \uparrow & \downarrow & \uparrow \\ & \uparrow & \downarrow & \end{array}$	$E = 0$	$M = 0$
$\begin{array}{cccc} & \uparrow & \uparrow & \\ \downarrow & \uparrow & \downarrow & \uparrow \\ \uparrow & \uparrow & \uparrow & \uparrow \\ & \uparrow & \downarrow & \end{array}$	$E = 0$	$M = 2$
$\begin{array}{cccc} & \downarrow & \downarrow & \\ \uparrow & \uparrow & \uparrow & \uparrow \\ \downarrow & \downarrow & \downarrow & \downarrow \\ & \uparrow & \uparrow & \end{array}$	$E = 0$	$M = 0$
$\begin{array}{cccc} & \downarrow & \uparrow & \\ \uparrow & \uparrow & \uparrow & \uparrow \\ \uparrow & \downarrow & \uparrow & \downarrow \\ & \uparrow & \uparrow & \end{array}$	$E = 0$	$M = 2$
$\begin{array}{cccc} & \uparrow & \downarrow & \\ \uparrow & \uparrow & \uparrow & \uparrow \\ \downarrow & \uparrow & \downarrow & \uparrow \\ & \uparrow & \uparrow & \end{array}$	$E = 0$	$M = 2$
$\begin{array}{cccc} & \uparrow & \uparrow & \\ \uparrow & \uparrow & \uparrow & \uparrow \\ \uparrow & \uparrow & \uparrow & \uparrow \\ & \uparrow & \uparrow & \end{array}$	$E = -8J$	$M = 4$

To summarise, we have

Number of ↑	Multiplicity	Energy	Magnetisation
4	1	$-8J$	4
3	4	0	2
2	2	$8J$	0
2	4	0	0
1	4	0	-2
0	1	$-8J$	-4

Summing over all microstates, we get the partition function

$$Z = \sum_{\substack{\text{all}\\\text{micro-}\\\text{states}}} \mathrm{e}^{-\beta E_i} = 2\mathrm{e}^{8J\beta} + 2\mathrm{e}^{-8J\beta} + 12$$

The expectation value of the energy can then be found from

$$\begin{aligned}
\langle E\rangle &= -\frac{\partial \ln(Z)}{\partial\beta} = -\frac{\partial}{\partial\beta}\left(\ln\left(2\mathrm{e}^{8J\beta} + 2\mathrm{e}^{-8J\beta} + 12\right)\right) \\
&= -\frac{1}{2\mathrm{e}^{8J\beta} + 2\mathrm{e}^{-8J\beta} + 12}\left(16J\mathrm{e}^{8J\beta} - 16J\mathrm{e}^{-8J\beta}\right) \\
&= -\frac{8J\left(\mathrm{e}^{8J\beta} - \mathrm{e}^{-8J\beta}\right)}{\mathrm{e}^{8J\beta} + \mathrm{e}^{-8J\beta} + 6}
\end{aligned}$$

yielding the heat capacity

$$\begin{aligned}
C_V &= \frac{\partial}{\partial T}(\langle E\rangle) = \frac{\partial\beta}{\partial T}\frac{\partial}{\partial\beta}(\langle E\rangle) = -\frac{1}{kT^2}\frac{\partial}{\partial\beta}(\langle E\rangle) \\
&= -\frac{1}{kT^2}\frac{\partial}{\partial\beta}\left(-\frac{8J\left(\mathrm{e}^{8J\beta} - \mathrm{e}^{-8J\beta}\right)}{\mathrm{e}^{8J\beta} + \mathrm{e}^{-8J\beta} + 6}\right) \\
&= \frac{8J}{kT^2}\frac{8J\left(\mathrm{e}^{8J\beta} + \mathrm{e}^{-8J\beta}\right)(\mathrm{e}^{8J\beta} + \mathrm{e}^{-8J\beta} + 6) - \left(\mathrm{e}^{8J\beta} - \mathrm{e}^{-8J\beta}\right)8J\left(\mathrm{e}^{8J\beta} - \mathrm{e}^{-8J\beta}\right)}{\left(\mathrm{e}^{8J\beta} + \mathrm{e}^{-8J\beta} + 6\right)^2} \\
&= \frac{64J^2}{kT^2}\frac{6\left(\mathrm{e}^{8J\beta} + \mathrm{e}^{-8J\beta}\right) + \left(\mathrm{e}^{8J\beta} + \mathrm{e}^{-8J\beta}\right)^2 - \left(\mathrm{e}^{8J\beta} - \mathrm{e}^{-8J\beta}\right)^2}{\left(\mathrm{e}^{8J\beta} + \mathrm{e}^{-8J\beta} + 6\right)^2} \\
&= \frac{64J^2}{kT^2}\frac{6\left(\mathrm{e}^{8J\beta} + \mathrm{e}^{-8J\beta}\right) + \mathrm{e}^{16J\beta} + 2 + \mathrm{e}^{-16J\beta} - \left(\mathrm{e}^{16J\beta} - 2 + \mathrm{e}^{-16\beta}\right)}{\left(\mathrm{e}^{8J\beta} + \mathrm{e}^{-8J\beta} + 6\right)^2} \\
&= \frac{64J^2}{kT^2}\frac{6\left(\mathrm{e}^{8J\beta} + \mathrm{e}^{-8J\beta}\right) + 4}{\left(\mathrm{e}^{8J\beta} + \mathrm{e}^{-8J\beta} + 6\right)^2}
\end{aligned}$$

To find the various quantities connected to magnetization, we use the general formula

$$\langle A\rangle = \frac{1}{Z}\sum_{\substack{\text{all}\\\text{micro-}\\\text{states}}} A_i\mathrm{e}^{-\beta E_i}$$

Mean magnetic moment(s):

$$
\begin{aligned}
\langle M \rangle &= \frac{1}{2e^{8J\beta} + 2e^{-8J\beta} + 12}\left(-4e^{8J\beta} + 4\cdot(-2) + 0 + 0 + 4\cdot 2 + 4e^{8J\beta}\right) = 0 \\
\langle M^2 \rangle &= \frac{1}{2e^{8J\beta} + 2e^{-8J\beta} + 12}\left((-4)^2 e^{8J\beta} + 4\cdot(-2)^2 + 0 + 0 + 4\cdot 2^2 + 4^2 e^{8J\beta}\right) \\
&= \frac{32\left(e^{8J\beta} + 1\right)}{2e^{8J\beta} + 2e^{-8J\beta} + 12} = \frac{16\left(e^{8J\beta} + 1\right)}{e^{8J\beta} + e^{-8J\beta} + 6} \\
\langle |M| \rangle &= \frac{1}{2e^{8J\beta} + 2e^{-8J\beta} + 12}\left(|-4| e^{8J\beta} + 4\cdot|-2| + 0 + 0 + 4\cdot 2 + 4e^{8J\beta}\right) \\
&= \frac{8\left(e^{8J\beta} + 2\right)}{2e^{8J\beta} + 2e^{-8J\beta} + 12} = \frac{4\left(e^{8J\beta} + 2\right)}{e^{8J\beta} + e^{-8J\beta} + 6}
\end{aligned}
$$

Magnetic susceptibility:

$$
\chi = \beta\left(\langle M^2 \rangle - \cancel{\langle M \rangle^2}\right) = \frac{16\beta\left(e^{8J\beta} + 1\right)}{e^{8J\beta} + e^{-8J\beta} + 6}
$$

4.1.2 Numerical results

With $J = 1$ and $\beta = 1$, the above expressions give

$$
\begin{aligned}
\langle E \rangle / L^2 &= -1.99598 & \qquad C_V / L^2 &= 0.03208 \\
\langle |M| \rangle / L^2 &= 0.99866 & \qquad \chi / L^2 &= 3.9933
\end{aligned}
$$

Running 100 000 Monte Carlo cycles with the same parameters gives figure 1 on the following page.

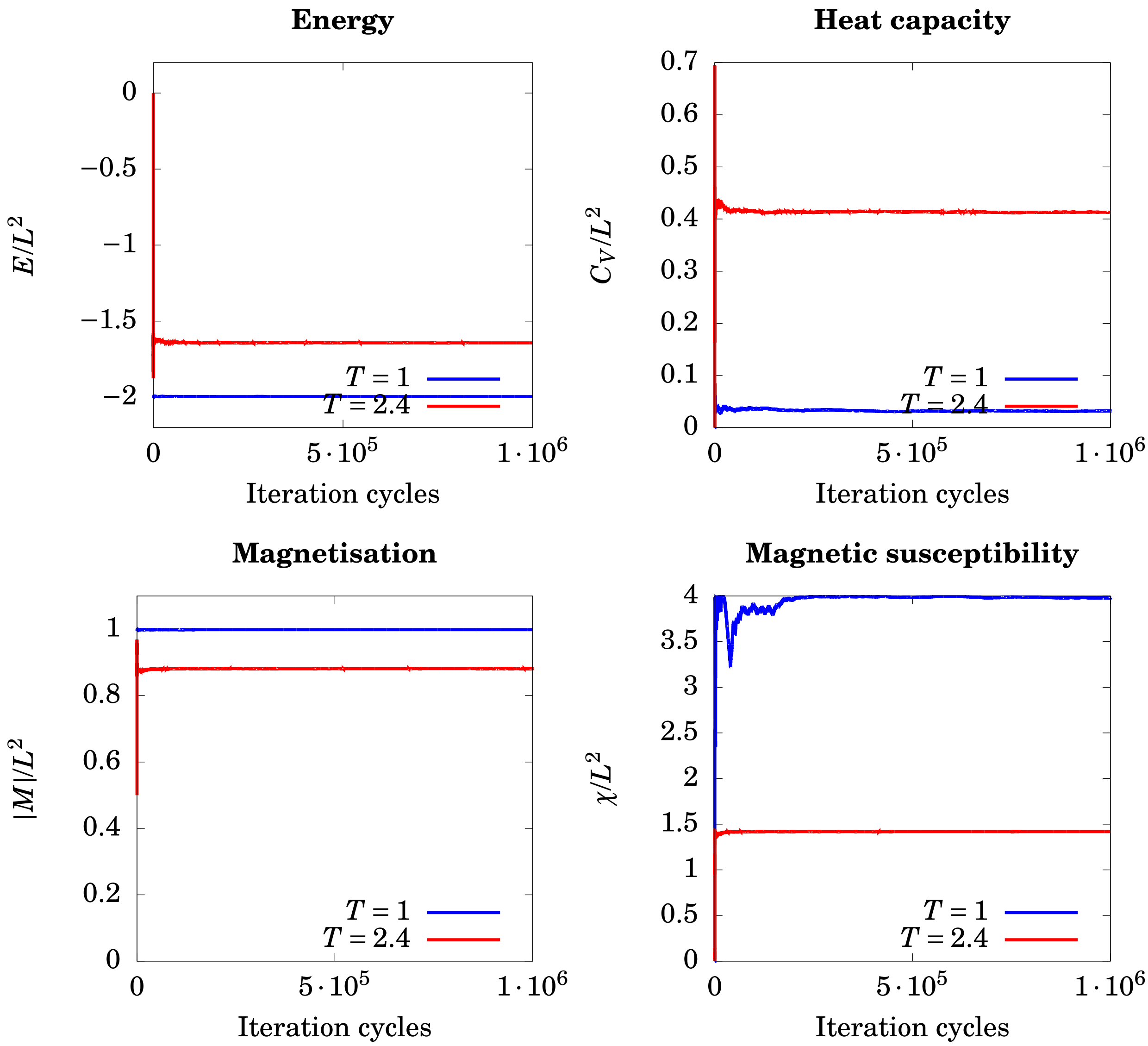

Figure 1: Numerical results from 100 000 Monte Carlo cycles. Generated by 2by2.cpp.

These results fit fairly well with the numbers calculated above, but we see from the graphs that the values for the heat capacity and magnetic susceptibility have yet to settle down completely. Running with 10 000 000 Monte Carlo cycles yields

```
10000000 -1.99592 -0.0146971 0.998631 0.0326149 3.99231
```

where the numbers are i, $\langle E\rangle/L^2$, $\langle M\rangle/L^2$, $\langle|M|\rangle/L^2$, C_V/L^2 and χ/L^2. The results fit very well with the analytical results.

4.2 Analysis

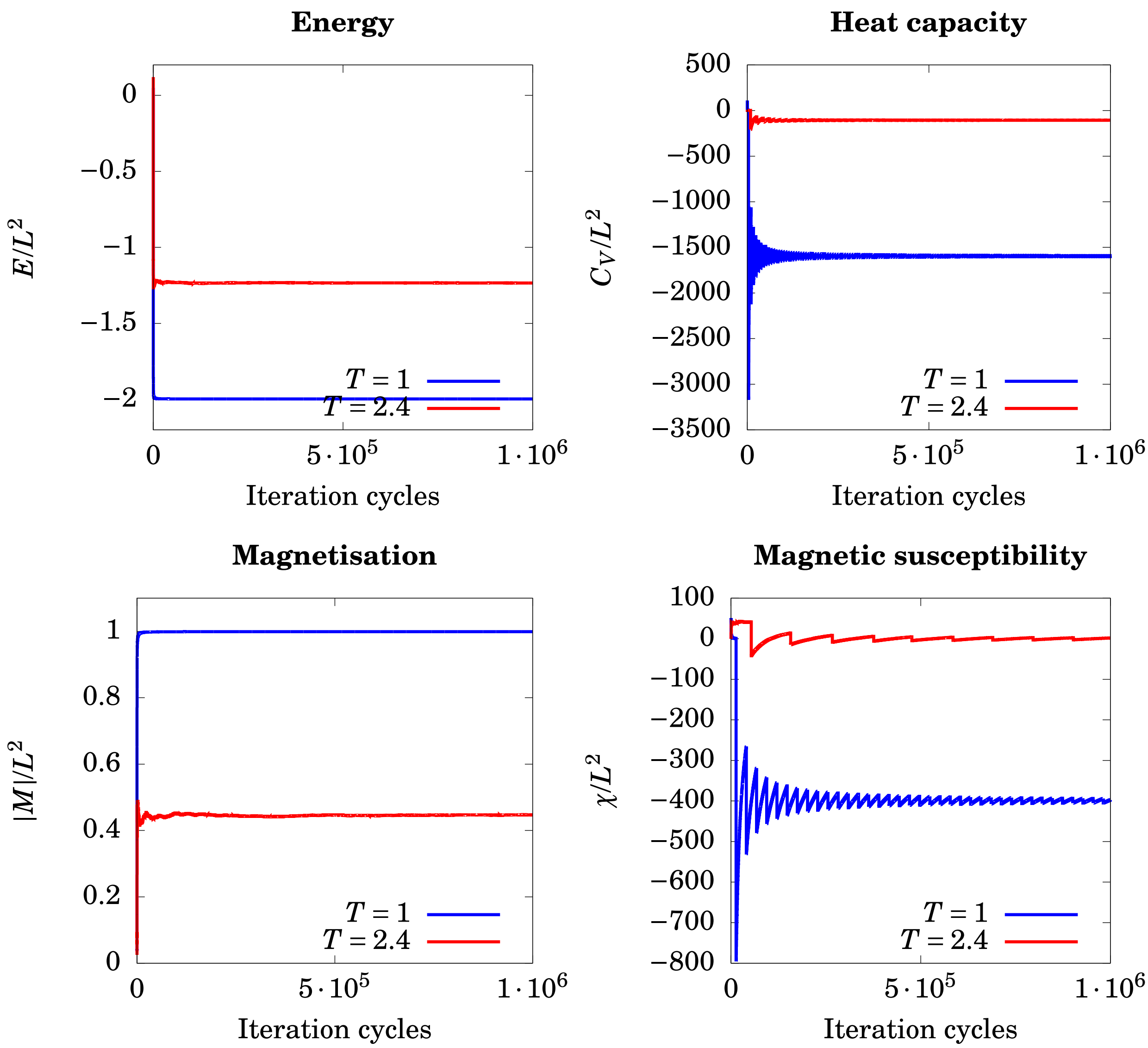

Figure 2: Simulation for 10^6 Monte Carlo cycles with two different temperatures and random initial states. Generated by analysis.cpp.

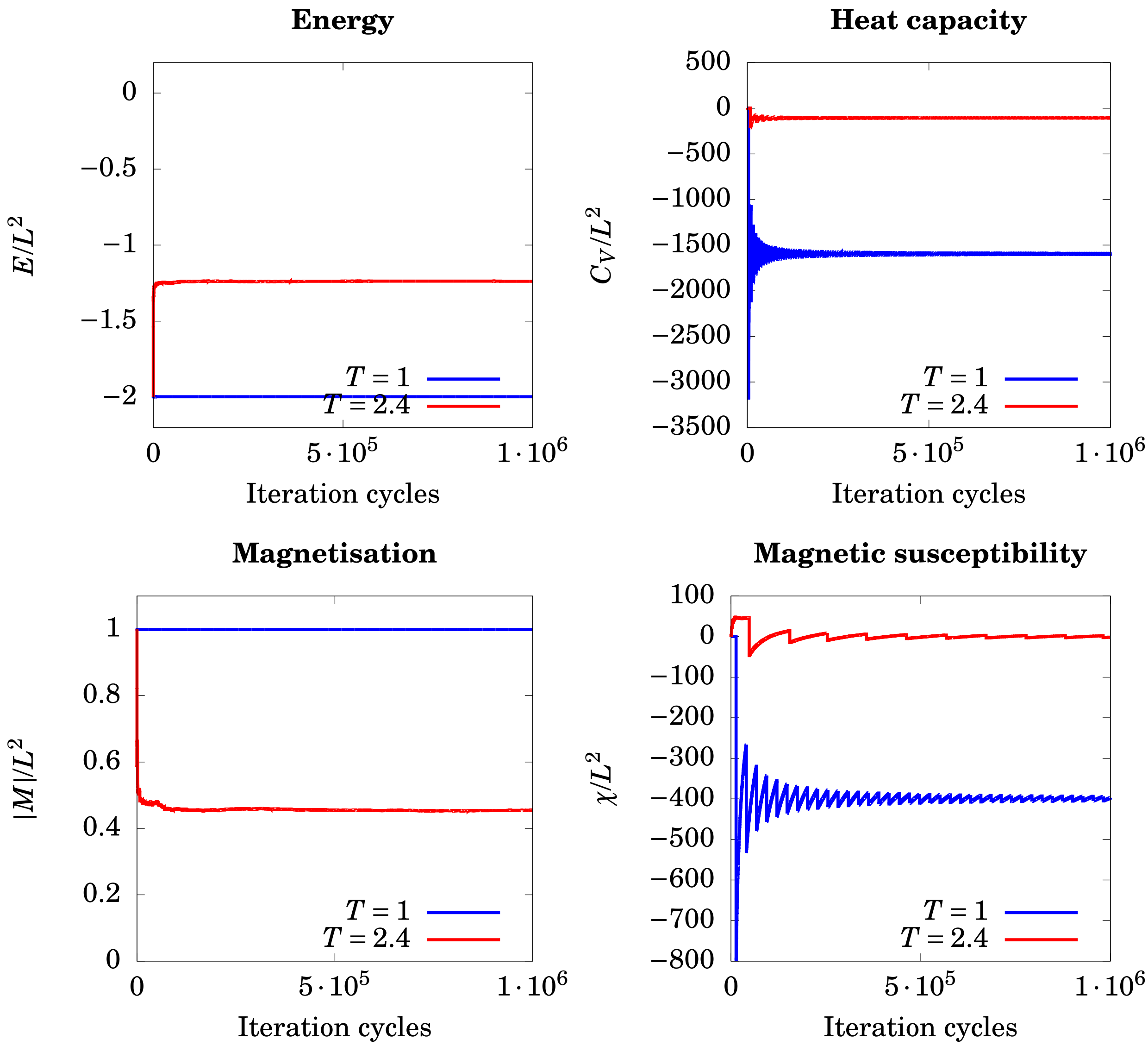

Figure 3: Simulation for 10^6 Monte Carlo cycles with two different temperatures and all spins initially pointed upwards. Generated by analysis.cpp.

Comparing figure 2 and figure 3, we see that the initial state has very little to say for the final values, as well as the time it takes to reach a steady state.

References

[1] James Burridge and Steven Kenney. "Birdsong dialect patterns explained using magnetic domains". In: *Physical Review E* 93.6 (2016), p. 062402.

[2] Barry A Cipra. "The best of the 20th century: editors name top 10 algorithms". In: *SIAM news* 33.4 (2000), pp. 1–2.

[3] Morten Hjorth-Jensen. *Computational Physics*. Lecture notes. 2015. URL: https://github.com/CompPhysics/ComputationalPhysics/blob/master/doc/Lectures/lectures2015.pdf.