FYS3150 Project 4

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3.1 Example: Analytical expression for the 2×2 case

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

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

To summarise, we have

Number of $\uparrow$	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):

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

$$= \frac{8\left(e^{8J\beta}+2\right)}{2e^{8J\beta}+2e^{-8J\beta}+12} = \frac{4\left(e^{8J\beta}+2\right)}{e^{8J\beta}+e^{-8J\beta}+6}$$

Magnetic susceptibility:

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

3.2 Comparison with numerical results

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

$$\langle E\rangle = -7.9839 \qquad C_V = 0.128\,329$$
$$\langle |M|\rangle = 3.994\,64 \qquad \chi = 15.9732$$

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

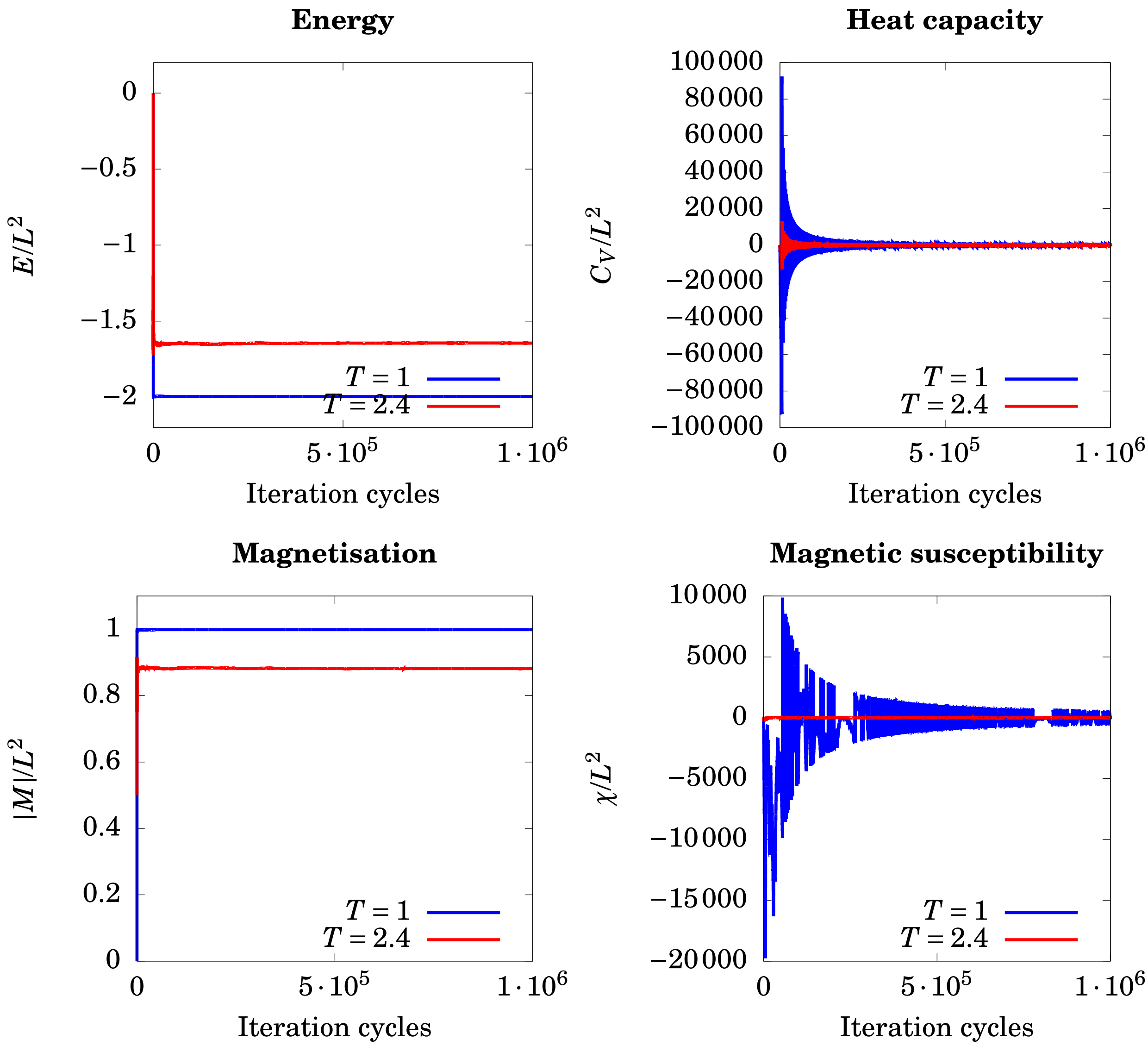

Figure 1: Numerical results from 100 000 Monte Carlo cycles. Generated by 2by2.cpp.

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 -1.99606 0.0163514 0.998683 9.49919 46.6804
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where the numbers are i, T, $\langle E\rangle$, $\langle E^2\rangle$, $\langle M\rangle$, $\langle M^2\rangle$, $\langle |M|\rangle$, C_V and χ. The results fit very well with the analytical results.

3.3 Analysis

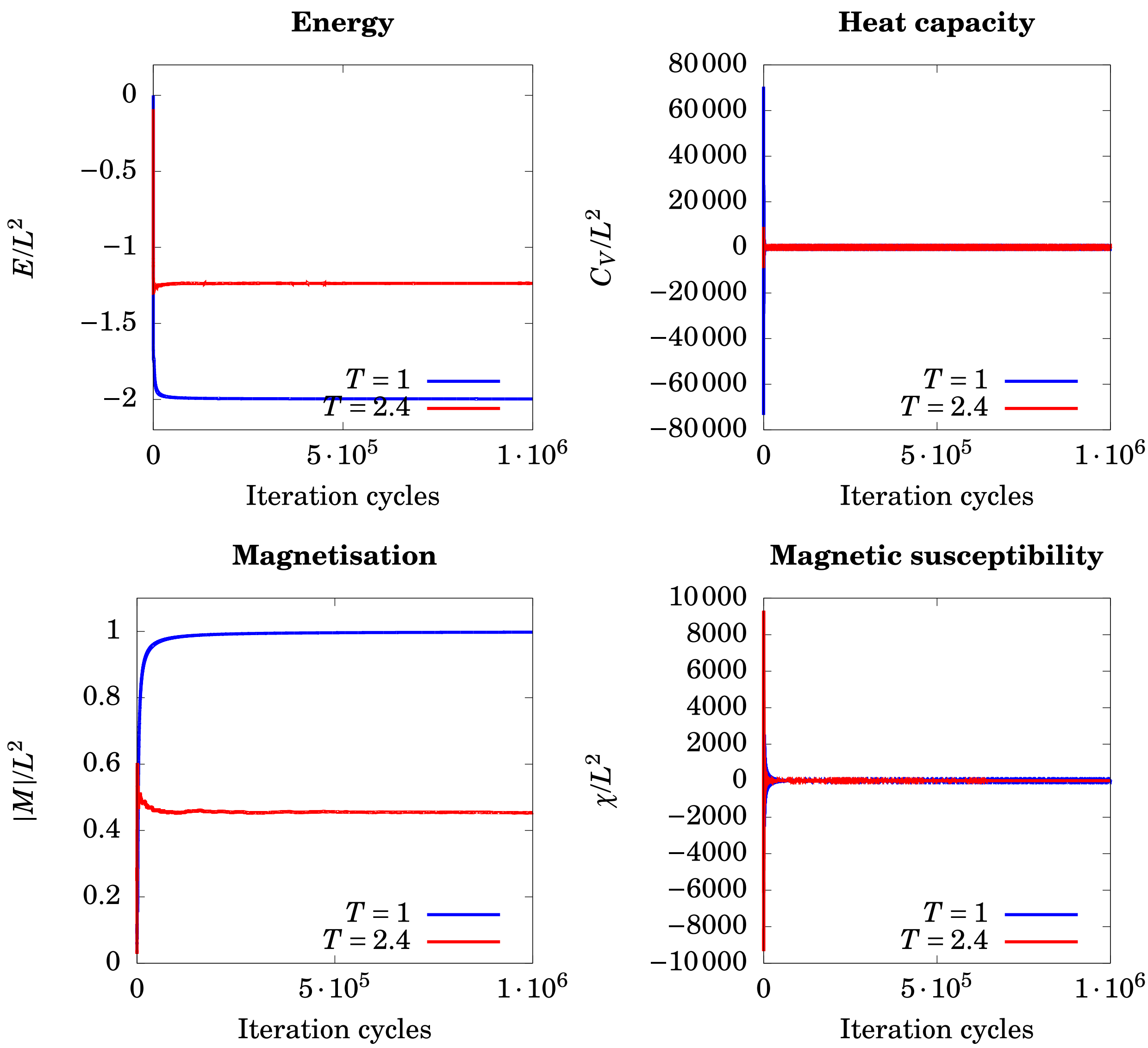

Figure 2: Simulation for 10^6 Monte Carlo cycles with two different temperatures and random initial states. Generated by analysis.cpp.

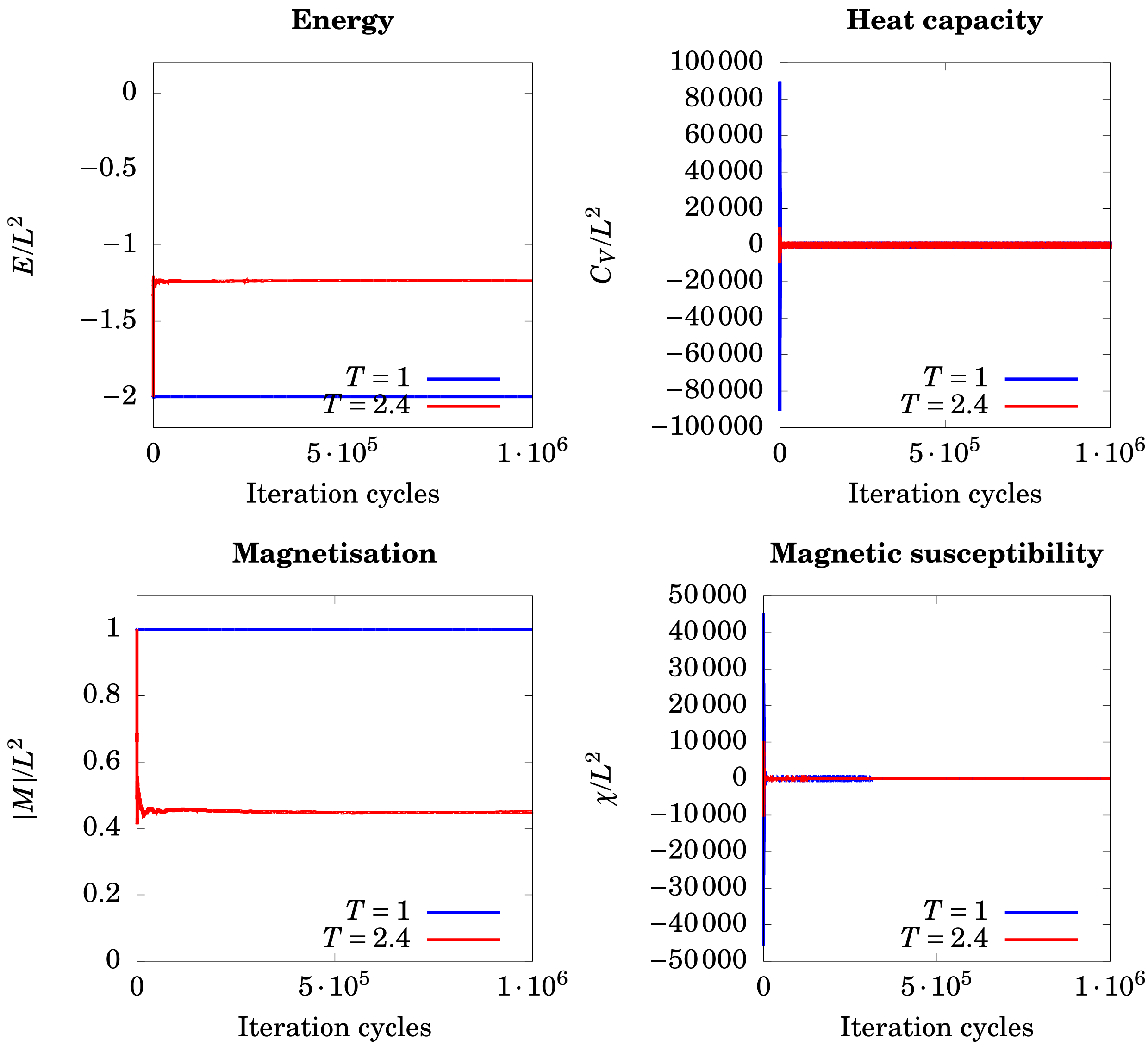

Figure 3: Simulation for 10^6 Monte Carlo cycles with two different temperatures and all spins initially pointed upwards. Generated by analysis.cpp.

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.