Project 3 - FYS3150 Computational Physics

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Contents

1 Introduction

In this project, we will look at the Ising model and use it to study phase transistions in magnetic systems. We will implement the Metropolis algorithm to simulate the Ising model of a two-dimensional $L \times L$ spin lattice with periodic boundary conditions and compare our simulated values to analytic expressions for the theoretical values. We will also consider the specific temperatures $t = 1.0$ and $t = 2.4$ (the latter of which is very close to the critical temperature), and look at how the simulations behave at these temperatures and others near the critical temperature.

2 Methods

a) We want to find analytical solutions for the expected energy, expected absolute magnetization, specific heat capacity and susceptibility of the 2×2 lattice Ising model with periodic boundary conditions.

For convenience, we define the "dimensionless temperature" $t = \frac{kT}{J} = \frac{1}{\beta J}$ and $\beta = \frac{1}{kT} = \frac{1}{Jt}$.

In table 1, we see the possible states we can have. Looking at this, we can see that the partition function Z is

$$\begin{aligned} Z &= \sum_i g(i) e^{-\beta E_i} \\ &= 2e^{8\beta J} + 12e^{-0\cdot\beta J} + 2e^{-8\beta J} \\ &= 2e^{8\beta J} + 12 + 2e^{-8\beta J} \\ &= 4\cosh(8\beta J) + 12 \\ &= 4\cosh(8/t) + 12 \end{aligned}$$

Number of spins up	**Degeneracy**	**Energy**	**Magnetiation**
4	1	$-8J$	4
3	4	0	2
2	4	0	0
2	2	$8J$	0
1	4	0	-2
0	1	$-8J$	-4

Table 1: Energy and magnetization for the two-dimensional Ising model with $N = 2 \times 2$ spins with periodic boundary conditions. (Table 13.4 in lecture notes.)

The expected energy is then

$$
\begin{aligned}
\langle E\rangle &= \frac{1}{Z}\sum_i g(i)E_i e^{-\beta E_i} \\
&= -\frac{1}{Z}\frac{\mathrm{d}Z}{\mathrm{d}\beta} \\
&= -\frac{1}{Z}\cdot 32J\sinh(8\beta J) \\
&= -8J\cdot\frac{4\sinh(8\beta J)}{4\cosh(8\beta J)+12} \\
&= -8J\cdot\frac{\sinh(8\beta J)}{\cosh(8\beta J)+3} \\
&= -8J\cdot\frac{\sinh(8/t)}{\cosh(8/t)+3}
\end{aligned}
$$

The expected absolute magnetization is

$$
\begin{aligned}
\langle|\mathscr{M}|\rangle &= \frac{1}{Z}\sum_i g(i)|\mathscr{M}_i|e^{-\beta E_i} \\
&= \frac{1}{Z}\big(2\cdot 4e^{8\beta J}+8\cdot 2e^{-0\cdot\beta J}+4\cdot 0e^{-0\cdot\beta J}+2\cdot 0e^{-8\beta J}\big) \\
&= \frac{8e^{8\beta J}+16}{4\cosh(8\beta J)+12} \\
&= 2\left(1+\frac{\sinh(8\beta J)-1}{\cosh(8\beta J)+3}\right) \\
&= 2\left(1+\frac{\sinh(8/t)-1}{\cosh(8/t)+3}\right)
\end{aligned}
$$

The specific heat capacity is

$$
\begin{aligned}
C_V &= \frac{\partial\langle E\rangle}{\partial T} \\
&= -8J\cdot\frac{\partial}{\partial T}\left(\frac{\sinh(8\beta J)}{\cosh(8\beta J)+3}\right) \\
&= -8J\cdot\frac{\mathrm{d}\beta}{\mathrm{d}T}\frac{\partial}{\partial\beta}\left(\frac{\sinh(8\beta J)}{\cosh(8\beta J)+3}\right) \\
&= \frac{64J^2}{kT^2}\left(\frac{3\cosh(8\beta J)+1}{(\cosh(8\beta J)+3)^2}\right) \\
&= \frac{64k}{t^2}\left(\frac{3\cosh(8/t)+1}{(\cosh(8/t)+3)^2}\right)
\end{aligned}
$$

(This can also be expressed as $\big(\langle E^2\rangle-\langle E\rangle^2\big)/kT^2$.)

We can calculate the susceptibility with $\chi = \left(\langle \mathscr{M}^2 \rangle - \langle \mathscr{M} \rangle^2\right)/kT$.

$$
\begin{aligned}
\langle \mathscr{M} \rangle &= 0 \\
\left\langle \mathscr{M}^2 \right\rangle &= \sum_i g(i) \mathscr{M}_i^2 e^{-\beta E_i} \\
&= \frac{1}{Z}\left(2 \cdot 4^2 e^{8\beta J} + 8 \cdot 2^2 e^{-0 \cdot \beta J} + 4 \cdot 0^2 e^{-0 \cdot \beta J} + 2 \cdot 0^2 e^{-8\beta J}\right) \\
&= \frac{32 e^{8\beta J} + 32}{4\cosh(8\beta J) + 12} \\
&= \frac{8 e^{8\beta J} + 8}{\cosh(8\beta J) + 3} \\
&= 8 \cdot \left(1 + \frac{\sinh(8\beta J) - 2}{\cosh(8\beta J) + 3}\right) \\
&= 8 \cdot \left(1 + \frac{\sinh(8/t) - 2}{\cosh(8/t) + 3}\right)
\end{aligned}
$$

With this, we see that the susceptibility is

$$
\begin{aligned}
\chi &= \frac{1}{kT}\left(\left\langle \mathscr{M}^2 \right\rangle - \underbrace{\langle \mathscr{M} \rangle^2}_{=0}\right) = \frac{1}{Jt}\left\langle \mathscr{M}^2 \right\rangle \\
&= \frac{8}{Jt}\left(1 + \frac{\sinh(8/t) - 2}{\cosh(8/t) + 3}\right)
\end{aligned}
$$

3 Results

b) We want to compare our analytical results to results we get from a Monte Carlo simulation of the model. For this, we implement the following algorithm:

1. Start with a random state.
2. For each Monte Carlo cylce:
   (a) Flip a single spin at random.
   (b) Calculate the difference in energy ΔE from the flip.
   (c) If $\Delta E \leq 0$, accept state.
   (d) If $\Delta E \geq 0$, accept state with probability $w = e^{-\beta \Delta E}$.

We calculate the average energy, absolute magnetization, specific heat capacity and susceptibility at the end of each Monte Carlo cycle. We see these plotted as a function of temperature t, along with the analytic results we got earlier, in figure 1. When we adjust the total number of Monte Carlo cycles, we see that we need approximately 100 000 cycles to get results that are close to the analytic results.

c) After this, we study how $\langle E \rangle$, $\langle |\mathscr{M}| \rangle$ and the number of accepted states behave as a function of the number of Monte Carlo cycles n in a 20×20 Ising model, for ordered and random initial states, as we see in figures 2 and 3.

It's worth noting that at temperature $t = 1.0$, the equalibrium point lies almost at the ordered states already, so the model will use many orders of magnitude fewer cycles to achieve equalibrium than by starting at a random initial state. We can also note that the number of accepted state increases linearly with n, while the random states only approach the equalibrium and approximately linear number of accepted states after $n \approx 10^6$.

At temperature $t = 2.4$, the picture is a bit different, however: the equalibrium energy is about midway between the random inital state (at energy ≈ 0) and the ordered initial state (at energy $-800J$). This means that both the initial state use an approximately equal number of cycles to reach eqalibrium, after $n \approx 10^7$.

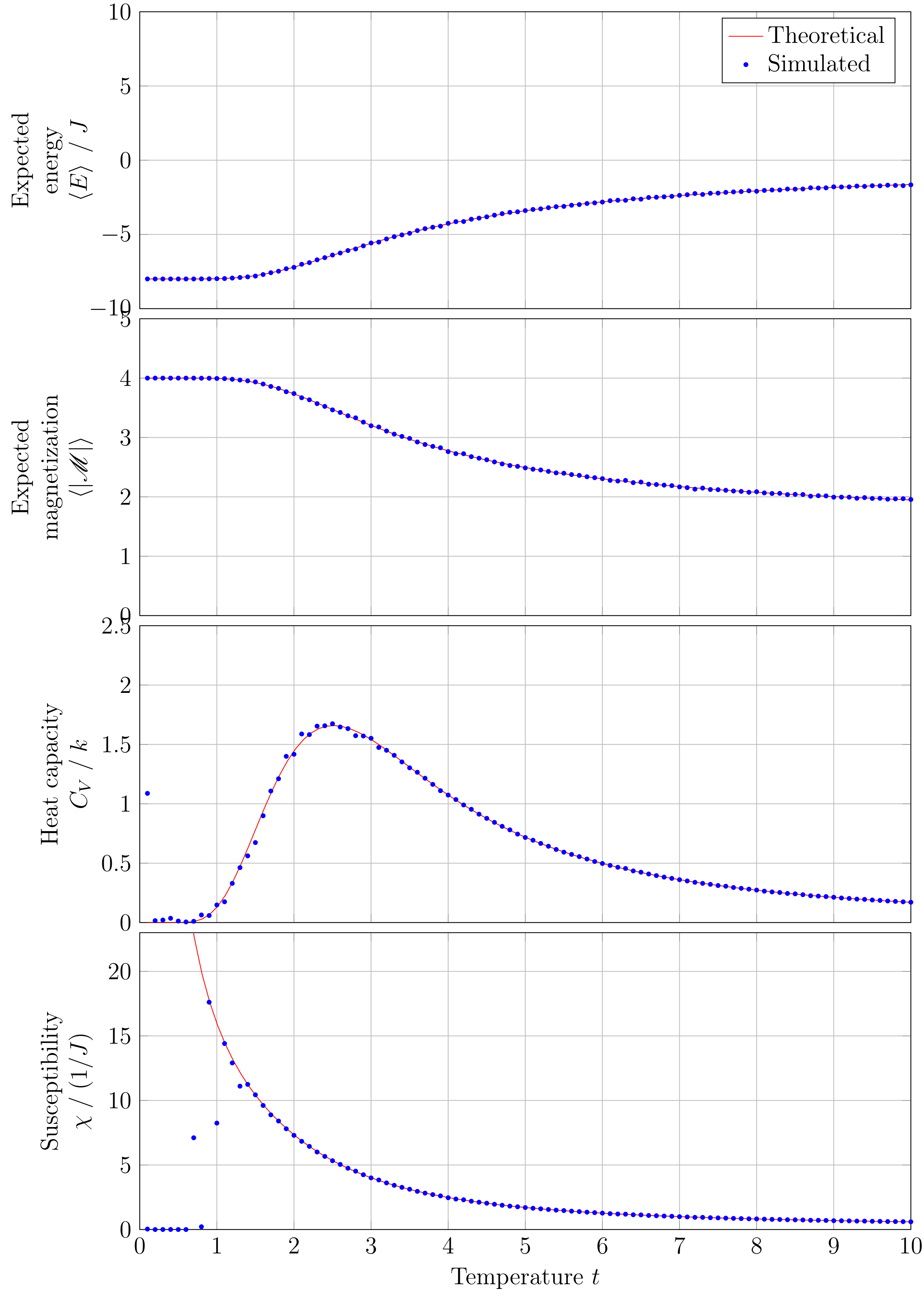


Figure 1: Plots that show theoretical and simulated values of $\langle E \rangle$, $\langle |\mathscr{M}| \rangle$, C_V and χ for the Ising model of a 2×2 square spin lattice, from **a)** and **b)**.

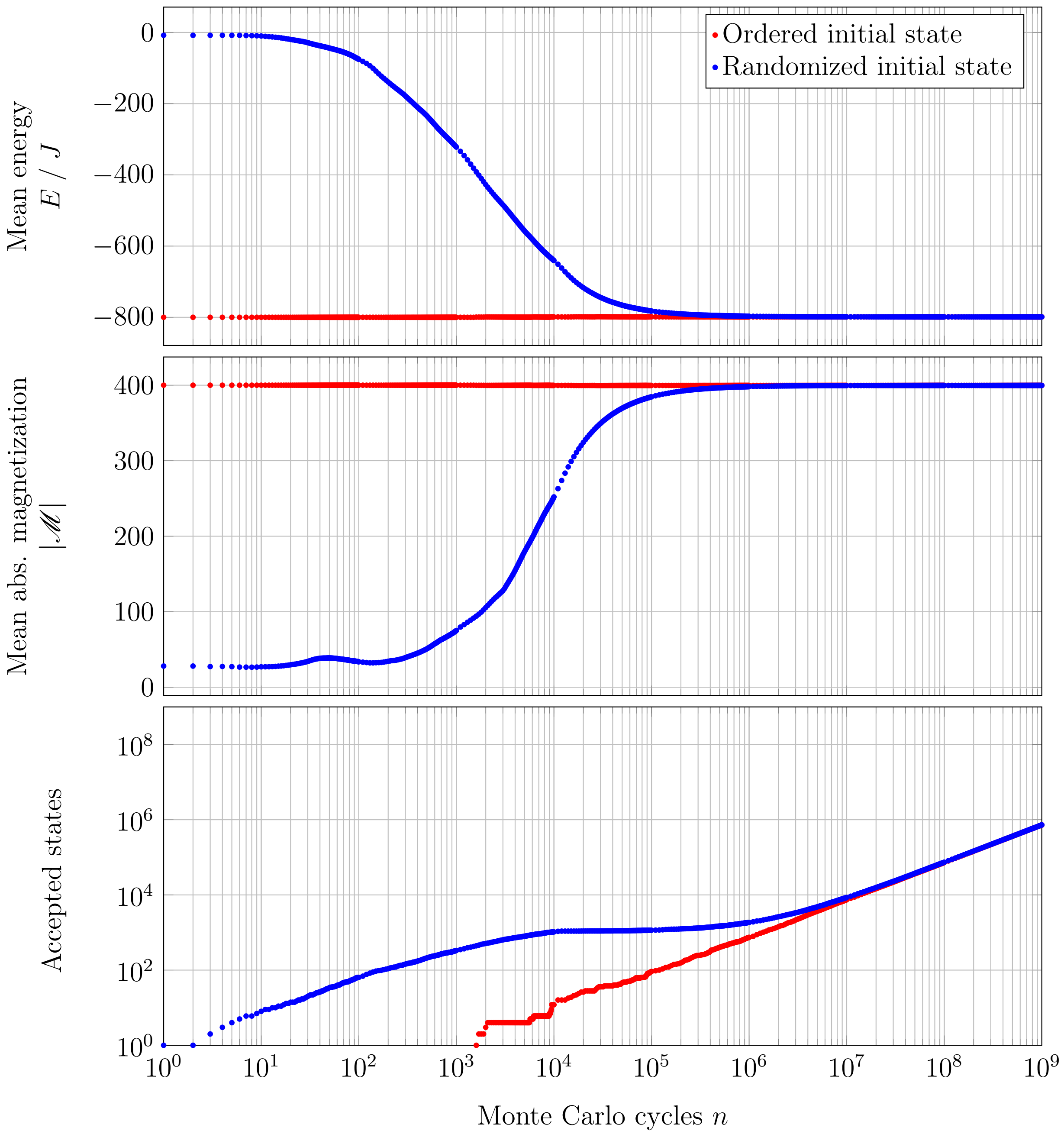


Figure 2: Mean energy, mean absolute magnetization and number of accepted states as a function of the number of Monte Carlo cycles for $t = 1.0$.

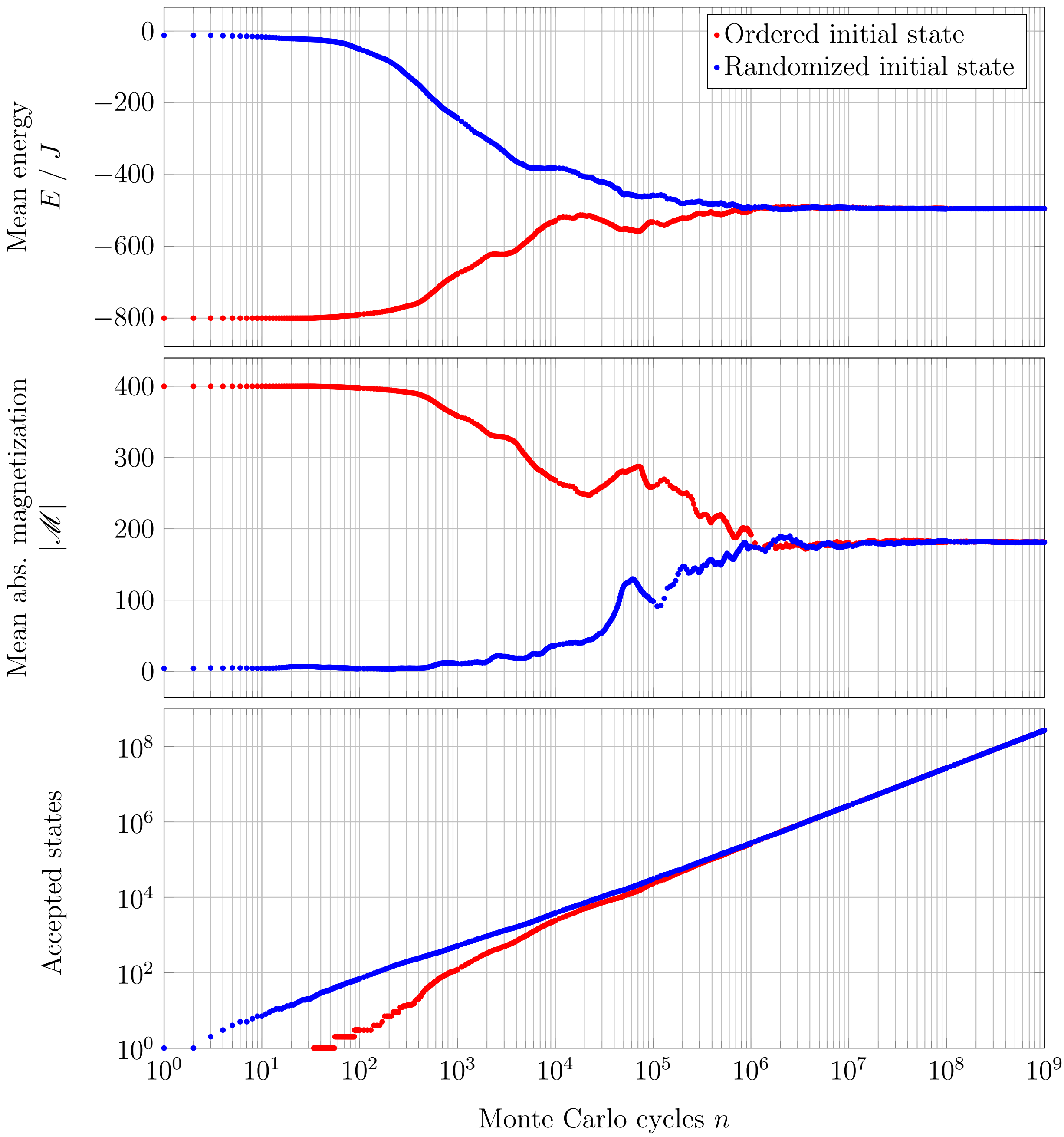


Figure 3: Mean energy, mean absolute magnetization and number of accepted states as a function of the number of Monte Carlo cycles for $t = 2.4$.

d) We can then look at how the probability distribution of the energy states for the same two temperatures ($t = 1.0$ and $t = 2.4$) for the same 20×20 Ising model. For this, we simply skip ahead until we get a steady state, and then count the number of times each energy level occur during the simulation.

First of all, we note that for $t = 1.0$, the most likely energy level is $-800J$, which is the same as the equalibrium energy level we got for this temperature earlier (see figure 2). For $t = 2.4$, the most likely energy level is about $-480J$, which is about the same as the equalibrium level we got for this temperature as well (see figure 3).

We can also tell that the probability distribution for $t = 2.4$ is much wider, with a standard deviation that we calculate to be $\sigma_E = 57.04$, while the probability distribution for $t = 1.0$ only has a standard deviation of $\sigma_E = 3.063$. A quick comparision with the plots in figure 2 and 3 confirm that these are reasonable numbers.

e) We run the Metropolis algorithm for the Ising model at temperatures in the range $t \in [2.0, 2.3]$ in temperature steps of $\Delta t = 0.005$, for lattices of sizes $L = 40, 60, 100, 140$. For each lattice, we run $100\,000 \cdot L^2$ Monte Carlo cycles. For the latter half of these cycles (after we assume we have reach a somewhat stable state) we calculate the mean energy $\langle E \rangle$ and mean absolute magnetization $\langle |\mathscr{M}| \rangle$, along with the specific heat capacity C_V and susceptibility χ, for each time step. (This took about 2-3 hours to run on 4 processor cores.)

From these results which are shown in figure 4, we can tell that as the temperature approaches the critical temperature, the number of cycles we used is no longer sufficient to get a stable state, and instead we get big fluctuations from one time step to another. For some reason I can't explain, the heat capacity C_V *decreases* in this interval, although we expect that it increase in this interval; this is unexpected since we know that

$$C_V = \frac{\partial \langle E \rangle}{\partial T}$$

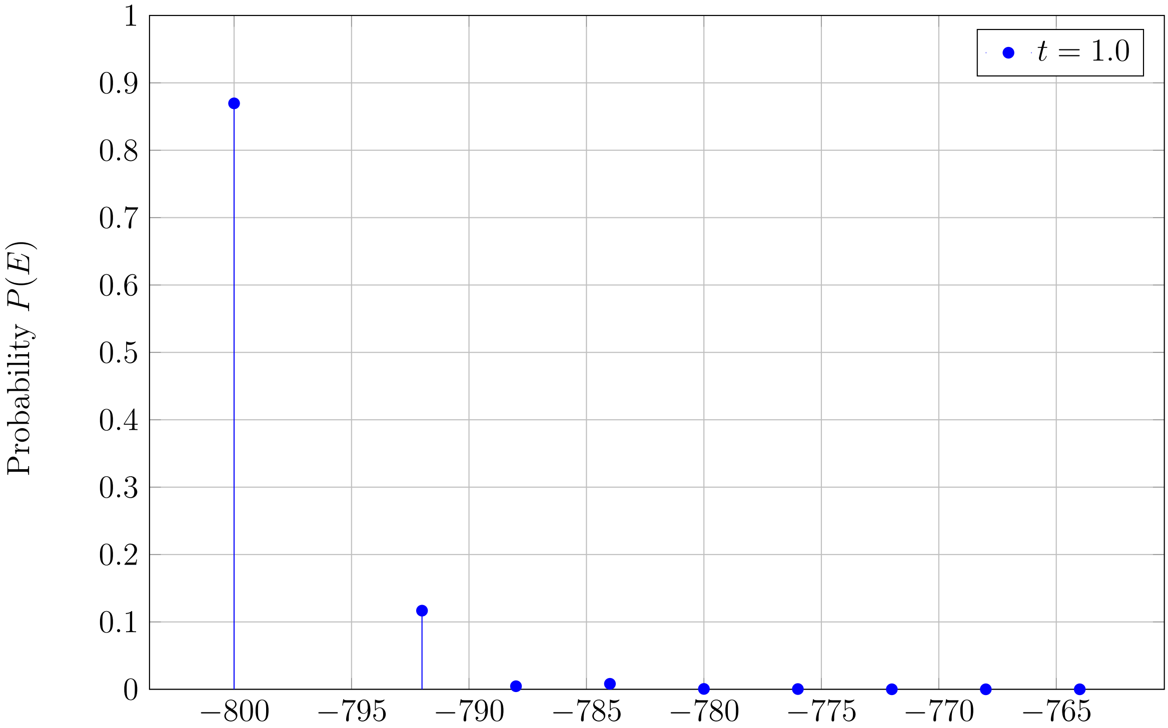
and $\langle E \rangle$ is definitely increasing more with higher temperature on this interval.

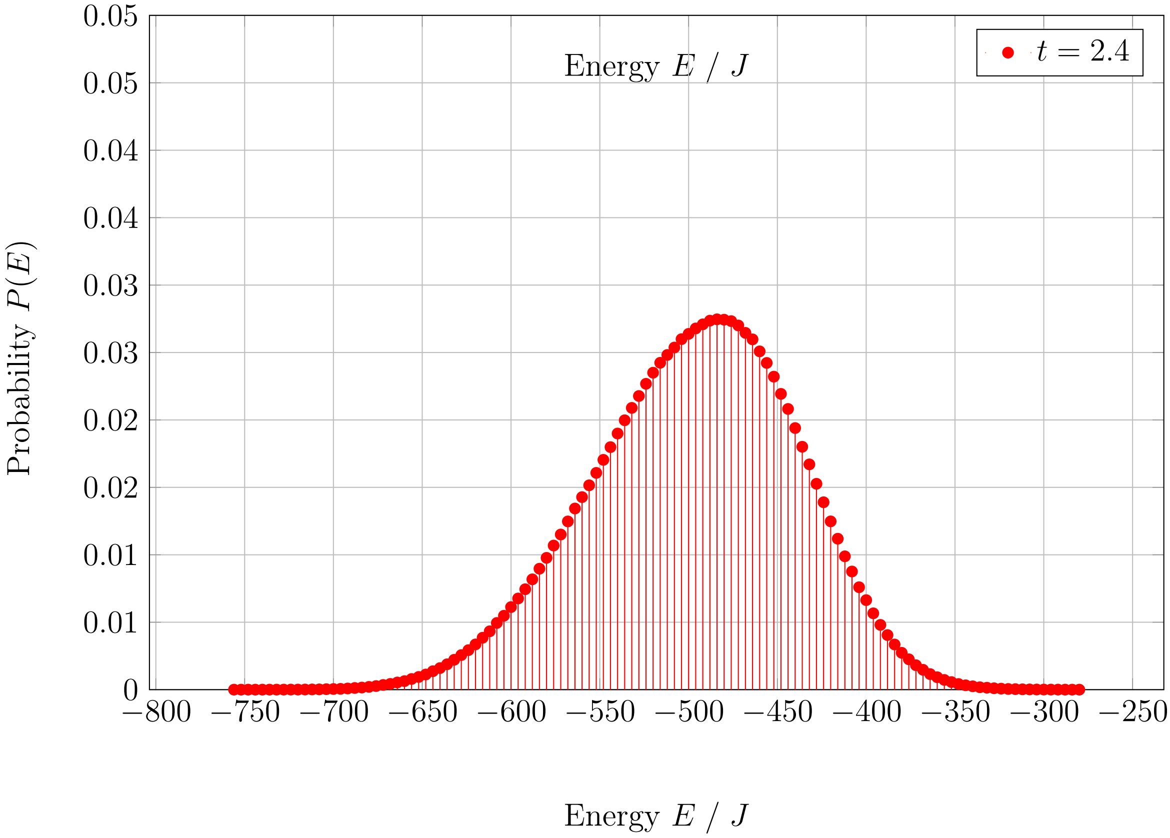
f) At this point, if we got the expected curves for C_V in figure 4, we should have seen spikes in the heat capacity around the critical temperature. We should then have been example to use the equation

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

and find a best-fit for the three parameters a, b, ν (or just a, b if we are assuming $\nu = 1$). The parameter b would then be the critical temperature in the thermodynamical limit $L \to \infty$.

4 Conclusion





Relative frequencies of the different energy levels after a steady state is reached, for temperatures $t = 1.0$ and $t = 2.4$ on a 20×20 Ising model.

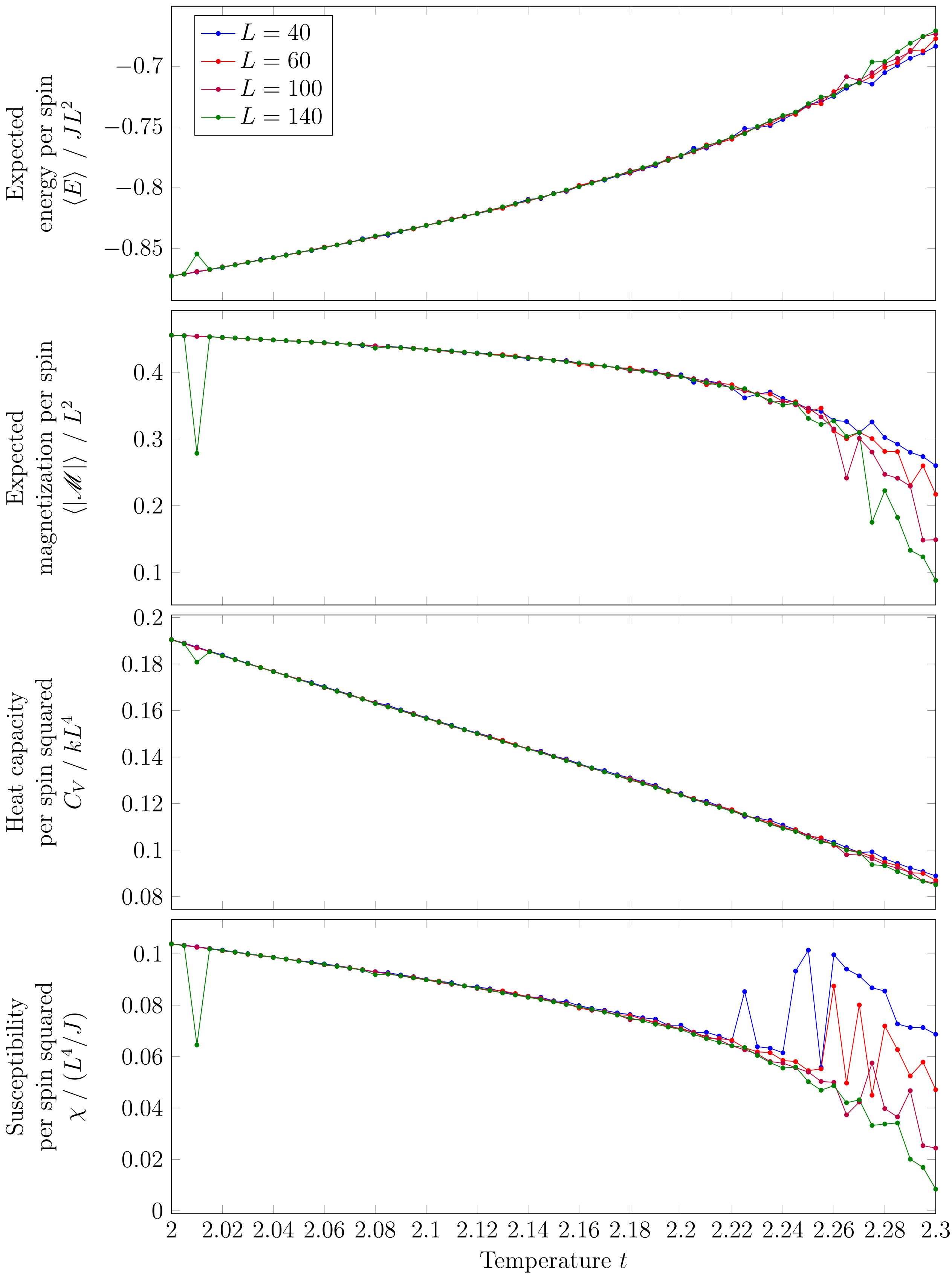


Figure 4: Plots that show the simulated values of $\langle E \rangle$, $\langle |\mathscr{M}| \rangle$, C_V and χ for the Ising model of a $L \times L$ square spin lattice, where $L = 40, 60, 100, 140$.

A Appendix