Simulating phase transitions in the Ising model using the Metropolis algorithm

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Abstract

In this report we consider numerical and physical aspects of the ferromagnetic Ising model and Metropolis algorithm. We find that the Metropolis algorithm produces a probability distribution resembling the gamma distribution, but no further analysis is done. A correspondence is found when comparing the distribution with the expectation value and standard deviation. Correlation between the probability distributions and accepted states is also found. Furthermore, we find an increase in energy and decrease in absolute magnetisation with increasing temperature, as well as signs of a phase transition from a maxima in the heat capacity and susceptibility in the temperature domain $T \in [2.26, 2.30]$. Closer analysis employing a power law yields a critical temperature of $2.271 \pm 0.012\,[\frac{k_b K}{J}]$, which is within one standard deviation of the estimated analytical value. We therefore conclude that the Metropolis algorithm yields relatively accurate results in simulating the Ising model.

1 Introduction

Statistical mechanics aims to describe thermodynamics from a quantum mechanical point of view. By making a system large enough, we should approach the thermodynamic limit where classical behaviour emerges. A concept which relates quantities such as the total energy, heat capacity, entropy, and pressure, is the partition function

$$Z = \sum_s e^{-\frac{E_s}{kT}}, \tag{1}$$

where k is Boltzmann's constant, T is the temperature, and E_s is the energy for each microstate s. The partition function describes the statistical properties of a system in thermal equilibrium. While useful and interesting theoretically, analytical solutions are rare to come by. In particular, it is quite difficult to calculate the microstate energies.

The aim of this report is then to find some of these quantities (observables) numerically, using the Metropolis algorithm to see how the energy and magnetisation vary as functions of temperature. We begin by describing the Ising model and Metropolis algorithm in the Methods section, before moving on to results. Here we start by presenting a brief analysis of the Ising model and Metropolis algorithm, and end by giving describing the different observables as functions of temperature. Finally, in the discussion section, we consider the error in our results, discuss the probability distribution of our Metropolis algorithm, and place the data in a physical context looking for phase transitions.

2 Methods

2.1 Ising model

To study phase transitions emerging from statistical mechanics, we will use the Ising model. In the Ising model we consider a lattice of interacting spins which are influenced by each other and an magnetic field B. In general then, we can express the Ising model as an Hamiltonian:

$$H = -\sum_{\langle i\, j\rangle} J_{ij} s_i s_j - \mu \sum_j B_j s_j, \qquad (2)$$

where $\langle i\, j\rangle$ denotes a multiplication only over neighbours, J_{ij} is a coupling parameter, μ is the magnetic moment, and B_j is a component of a external magnetic field. As our interest primarily lay in identifying phase transitions, we will simplify the model. We assume that the coupling parameter J_{ij} is the same for all spins and is positive, i.e. the interaction is ferromagnetic, and that the lattice is not affected by an external magnetic field. Our model then becomes

$$E \equiv H = -J \sum_{\langle i\, j\rangle} s_i s_j. \qquad (3)$$

Furthermore, we will enforce periodic boundary conditions, i.e "wrap" the lattice around itself, and so the endpoints at each side of the lattice will neighbour each other (like a torus). From eq. 3 we can get the mean energy of the system, of which we can use to calculate the specific heat capacity:

$$\langle c_V\rangle = \frac{\beta}{T}\frac{\partial \langle E\rangle}{\partial \beta} = \frac{\beta}{T}\Big(\langle E^2\rangle - \langle E\rangle^2\Big). \qquad (4)$$

Here $\beta = \frac{1}{kT}$ (see eq. 1) is the Boltzmann factor relating the energy of the system with the temperature. Furthermore, we can obtain the mean magnetisation of the system

$$\langle M\rangle = \sum_i s_i, \qquad (5)$$

and use this to construct the susceptibility function:

$$\chi = \beta\frac{\partial M}{\partial \beta} = \beta\Big(\langle M^2\rangle - \langle M\rangle^2\Big). \qquad (6)$$

These then are the observables we are interested in, and to obtain a measure of the relative error, we also solve these analytically for the case of a 2x2 lattice ($L = 2$). The energies, as well as degeneracy and spin orientation, are shown in Table 1.

# ↑	g	E [J]	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

Table 1: Microstates for the 2x2 Ising lattice.

Solving the partition function, we get the following relations:

$$Z = 12 + 4\cosh 8\beta J \qquad (7)$$

$$\langle E\rangle = -\frac{8J\sinh 8\beta J}{3+\cosh 8\beta J} \qquad (8)$$

$$c_V = \frac{64\beta J^2}{T}\frac{1+3\cosh 8\beta J}{(\cosh 8\beta J+3)^2} \qquad (9)$$

$$M = \frac{2e^{-8\beta J}+4}{3+\cosh 8\beta J} \qquad (10)$$

$$\chi = \beta\left[8\frac{e^{8\beta J}+1}{3+\cosh 8\beta J} - \left(2\frac{e^{8\beta J}+2}{3+\cosh 8\beta J}\right)^2\right] \qquad (11)$$

Throughout the article, we will use dimensionless units where $[T] = \frac{k_b K}{J}$.

2.2 Second-order phase transitions and the critical temperature

A second-order phase transition is characterised by divergent susceptibility and heat capacity. Such a discontinuity occurs at the critical temperature, T_C, i.e. a "boiling" or "melting" point. In the Ising model then, we would expect divergent susceptibility to occur for an infinite lattice, $L \leftarrow \infty$. In the case where L is finite however, this will not happen, and thus in our simulations we looked for a maxima in the heat capacity. We denote the temperature at this point as $T_C(L)$. Using the following power law (see [1] for a more in-depth discussion)

$$T_C(L) - T_C(L \leftarrow \infty) = aL^{-\frac{1}{\nu}}, \tag{12}$$

we can, by setting $\nu = 1$, obtain the following relation

$$T_C(L \leftarrow \infty) = \frac{T_C(L_I)L_I - T_C(L_i)L_i}{L_I - L_i}, \tag{13}$$

where $L_I > L_i$, so $T_C > 0$. Eq. 13 lets us estimate the critical temperature in the thermodynamic limit. An analytical value to this expression is given by Onsager [2] as

$$\frac{kT_C}{J} = \frac{2}{\ln\left(1+\sqrt{2}\right)} \approx 2.269. \tag{14}$$

2.3 Metropolis algorithm

A natural choice of algorithm for studying our system is the Metropolis method, a Markov-chain based algorithm which simulates random behaviour. It does this by comparing the possible change in energy due to flipping a random spin, with a random number from a $[0, 1]$ uniform distribution. The Metropolis algorithm accepts a change if it causes the new state to be more likely. This is the fact that lets us neglect calculating the partition function (see eq. 1), and only the ratio of probability between two states:

$$w = e^{-\beta \Delta E}. \tag{15}$$

From quantum mechanics we have that the most likely state is the ground state, i.e. the state of lowest energy, and so our implementation of the algorithm will check if the energy decreases or not. Of course, the ground state energy is a particular value, and so we will have to keep the possibility of the energy increasing to prevent too large a decrease. The complete algorithm is then shown in Algorithm **??**

```
initialise energy of system E;
for i = 1, ..., MC Cycles do
    for s = 1, ..., L · L do
        calculate ΔE due to spin flip;
        if ΔE ≤ 0 then
            accept new state;
            flip spin
        else
            calculate transition
             probability w;
            generate random number
             r ∈ [0, 1];
            if r ≤ w then
                accept new state;
                flip spin
            else
                keep old state;
    update expectation values;
calculate mean expectation values;
```

Algorithm 1: Metropolis algorithm specialised for the Ising lattice.

Additionally, we will only sample after the system has reached thermal equilibrium, i.e. after the thermalisation time.

2.4 Implementation

We implement the Ising model and Metropolis algorithm in C++ using the armadillo library

to handle matrices and vectors. In analysing the algorithm and model itself, it was sufficient with lattice sizes $L = 2, 20$. When studying the different parameters however, it was necessary to study larger lattices ($L = 40, 60, 80, 100$), resulting in a long run-time. This prompted us to parallelise the program using MPI. Employing 4 nodes, this yielded an increase in speed of about 1.5, and was necessary to produce our data in time. All the figures were produced in python 3.6 using the matplotlib, pandas and seaborn packages. In most of them, we use a rolling mean to capture an overall picture of the function. This felt natural as we in most cases had very few points. We also implement the analytical values for the 2x2 lattice as unit tests. Another possible unit tests that could have been implemented, was to check if the probability distribution remained normalised. All our code and data can be found at a github repository by janadr. [1]

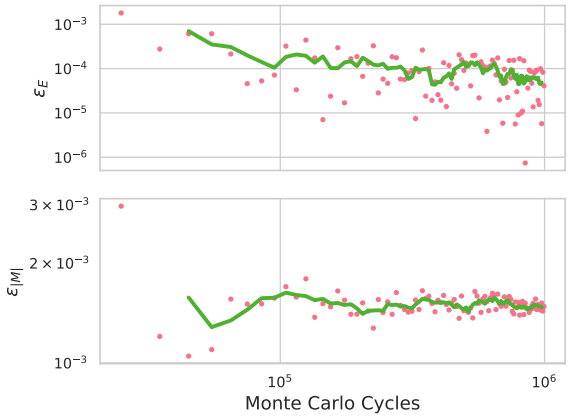

Figure 1: Here we show the relative error of the mean energy and magnetisation as a function of Monte Carlo cycles in the case of a 2x2 lattice. We use the same random seed for each Monte Carlo cycle.

3 Results

Beginning with the relative error in Figure 1, we see that the error in the mean energy has a decreasing trend all the way, while the error in absolute magnetisation seem to stabilise around a fixed value.

In Figure 2 we present the mean energy, and absolute magnetisation as functions of Monte Carlo cycles with both ordered and unordered initial states (see the Methods section for distinction). We see that both parameters converge rather rapidly for increasing Monte Carlo cycles, and in the $T = 1.0$ case it happens almost immediately for the ordered lattice.

Taking a closer look at the most likely state, we see the probability distribution of our Metropolis algorithm in Figure 3. For $T = 1.0$ there looks to be few likely states, while for $T = 2.4$ the distribution has a well defined

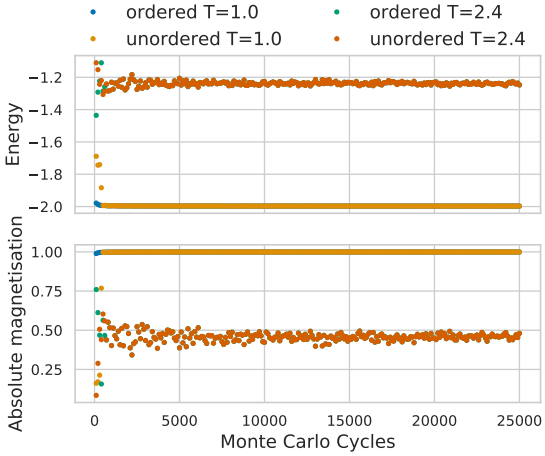

Figure 2: We compare between unordered and ordered initial lattices, i.e. a random lattice and a lattice where all elements are set to 1.

[1] https://github.com/janadr/FYS3150/tree/master/prosjekt4

defined interval of likely states between approximately $\langle E \rangle \in [-1.6, -0.8)$ with a peak at around $\langle E \rangle = -1.3$.

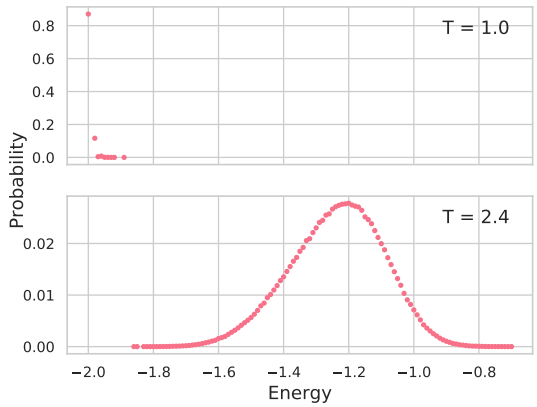

Figure 3: Shown here is the probability distribution obtained from the Metropolis algorithm for a $L = 20$ lattice over 10^6 Monte Carlo cycles.

Furthermore, we present the expectation value and standard deviation (sd) of the energy in Table 2. We see that when $T = 1.0$ the sd is relatively low, while for $T = 2.4$ it is over double the absolute magnitude of the expected energy.

T	$\langle E \rangle$	$\sigma_{\langle E \rangle}$
1.0	-1.997	0.15246889
2.4	-1.237	2.849

Table 2: Expected energy for $T = 1.0$ and $T = 2.4$ with standard deviation.

As for the amount of accepted states as a function of Monte Carlo cycles we see (Figure 4) that there generally is a lot more accepted states in the case of higher temperature. There also seem to be very little difference between the unordered and ordered lattices besides some small fluctuations.

Shown in Figure 5 is the mean energy of the

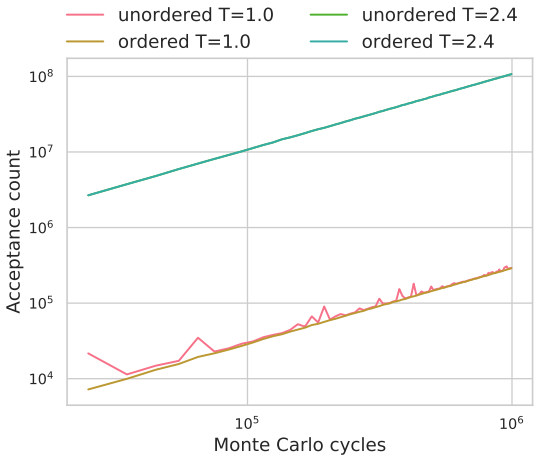

Figure 4: Number of accepted states as a function of Monte Carlo cycles.

system. We see that there is a steady increase with little difference between lattice sizes.

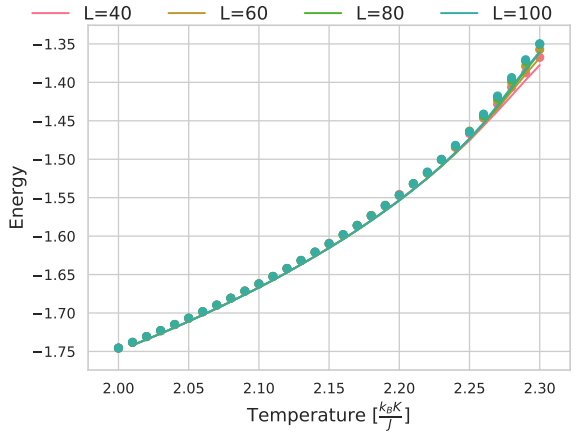

Figure 5: Mean energy as a function of $T \in [2.0, 2.3]$ for selected lattice sizes $L = 40, 60, 80, 100$.

Considering now the absolute magnetisation (see Figure 6), we observe a steady decline with little distinction between lattices until around $T = 2.25$, where the graphs slightly diverge with a lower minima for larger lattices.

Looking now at the heat capacity in Figure 7, we see a steady increase for all lat-

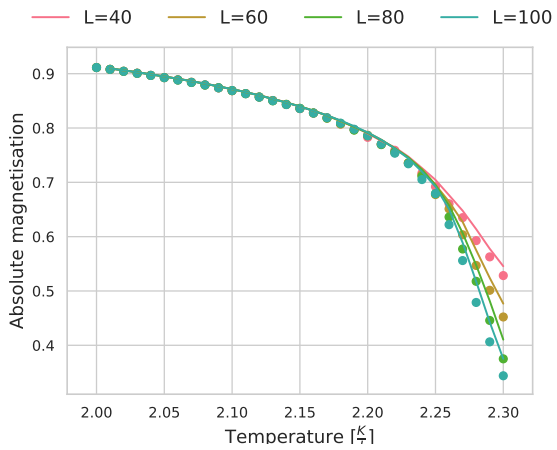

Figure 6: Absolute magnetisation as a function of $T \in [2.0, 2.3]$, for selected lattice sizes $L = 40, 60, 80, 100$.

tices, akin to the mean energy, until around $T = 2.2$. After $T = 2.25$ we can clearly distinguish between lattices. We also observe higher maxima for larger lattices, and in the case of $L = 60, 80, 100$, we observe a decrease after around $T = 2.26$.

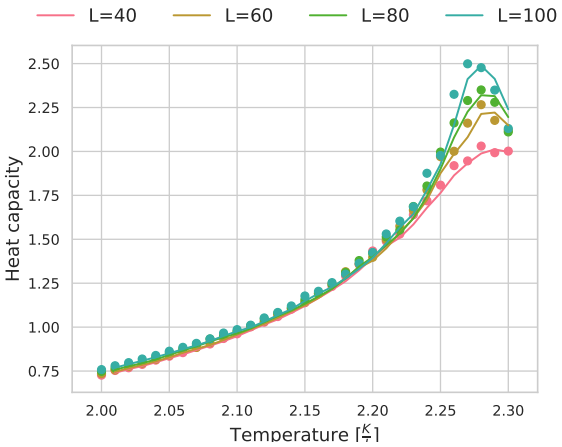

Figure 7: Specific heat capacity as a function of $T \in [2.0, 2.3]$, for selected lattice sizes $L = 40, 60, 80, 100$.

The susceptibility as a function of temperature is shown in Figure 8. There is little change until around $T = 2.1$ when the susceptibility starts slowly increasing until around 2.25 where it increases quicker for $L = 40, 60$ and rapidly for $L = 80, 100$, attaining higher maxima for larger lattices.

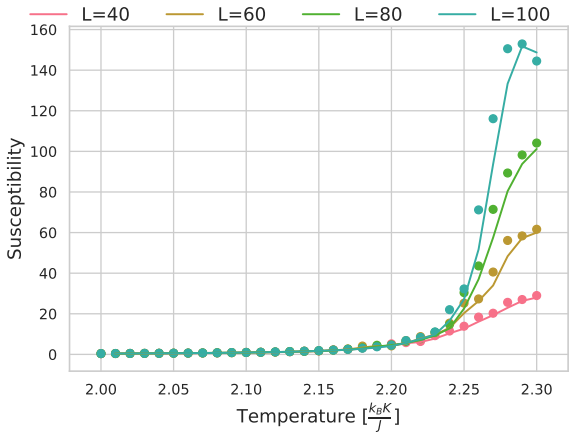

Figure 8: Susceptibility as a function of $T \in [2.0, 2.3]$, for selected lattice sizes $L = 40, 60, 80, 100$.

Zooming in on the heat capacity in the interval $T \in [2.26, 2.30]$ we get a closer look at the maximum's (see Figure 9). We find the temperature at the respective maxima numerically, which using eq. 13 yielded the critical temperature, shown in Table 3.

$\boldsymbol{dT}$	0.01	0.01 (RM)	0.001	0.001 (RM)
$\boldsymbol{T_C}$	2.265	2.271	2.262	2.265
STD	0.018	0.012	0.016	0.018

Table 3: Critical temperature for low and high resolution with and without rolling mean (RM), window size 2 and 5 respectively.

We produced more figures, which can be found in the appendix.

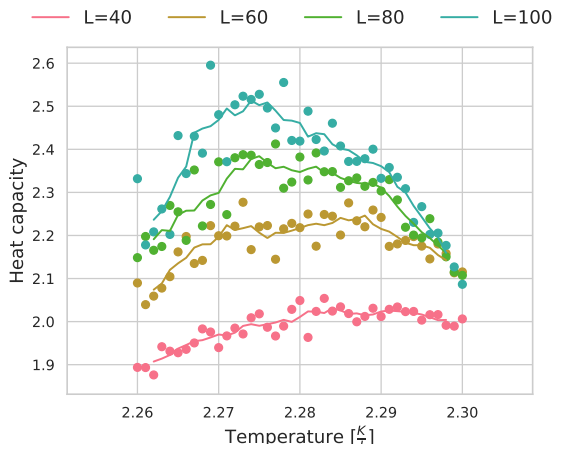

Figure 9: Restricting the temperature domain to $[2.26, 2.30]$ *we take a closer look at the heat capacity as a function of temperature for lattice sizes* $L = 40, 60, 80, 100$. *Here the graph is obtained from a rolling mean with window 4*

4 Discussion

The relative error in our algorithm, as shown in Figure 1, behave as expected in case of the mean energy. As for the absolute magnetisation, the relative error remaining approximately constant might be due to a systematic error.

Determining the amount of Monte Carlo cycles required to reach a equilibrium state (see Figure 2) was important to get a good sample, as we are only interested in the equilibrium state. Including the cycles before this point would increase variance in our results and make them more inaccurate as a consequence. From the figures we determined that equilibrium was obtained after around 5000 Monte Carlo Cycles for both ordered and unordered lattices in the case of the mean energy. For the absolute magnetisation, the thermalisation time seem to be longer, and we determine equilibrium to be at around 15000 cycles. In our program we set this to be 25000 cycles. This is to make certain that equilibrium is reached for all cases, and because it does not alter our results by much as the magnitude of Monte Carlo cycles is of order $\mathcal{O}(6) - \mathcal{O}(7)$. As for the probability distribution function (pdf) of our Metropolis algorithm, we see from Figure 3 for $T = 2.4$, a pdf that resembles the gamma distribution, due to the tail left in the figure. When $T = 1.0$ there seems to be no apparent pdf behind the algorithm. This implies that there are less available microstates for lower temperatures. Comparing this with the obtained values of the expected energy and standard deviation (see Table 2), we see agreement in the standard deviation being quite low for $T = 1.0$ and high for $T = 2.4$, fitting the shape of their distributions. This behaviour also fits well with the observed amount of accepted states (see Figure 4) as there are more available states in the $T = 2.4$ case.

We determine the phase transition to be at the maxima observed in the heat capacity (see Figure 9), as there are many indications of transitioning. The susceptibility function increases quite rapidly for increasing L in the temperature region (see Figure 8), implying divergence. Looking back at Table 3 we see that all obtained critical temperatures using this point is within a standard deviation of the estimated analytical value of 2.269 (see eq. 14). An issue is that the standard deviation is relatively large. Comparing with similar analyses, we are led to believe that this might be caused by an error in implementation when producing the $L = 40, 60, 80, 100$ data, as we neglected initialising the Ising lattice for each temperature step. Nevertheless, we conclude that the Metropolis algorithm yields good result when used to simulate the Ising model.

References

[1] Jacques Kotze. Introduction to monte carlo methods for an ising model of a ferromag-

net. *arXiv preprint arXiv:0803.0217*, 2008.

[2] Lars Onsager. Crystal statistics. i. a two-dimensional model with an order-disorder transition. *Phys. Rev.*, 65:117–149, Feb 1944.

A

Here are figures of data we gathered, but didn't end up using. Most of them are zoomed in cases, but we also include the mean magnetisation.

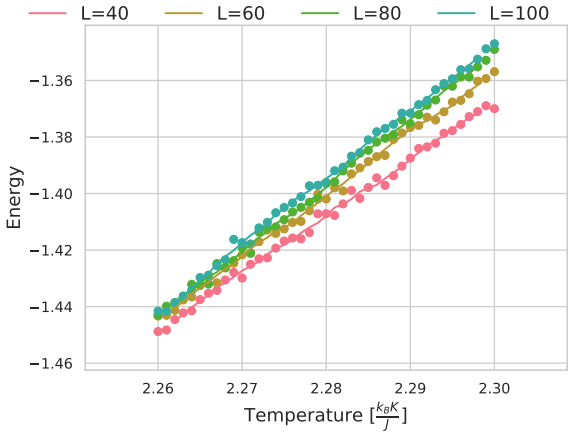

Figure 10: Mean energy as a function of temperature $T \in [2.26, 2.3]$ for lattice sizes $L = 40, 60, 80, 100$, with a rolling mean, window size 5.

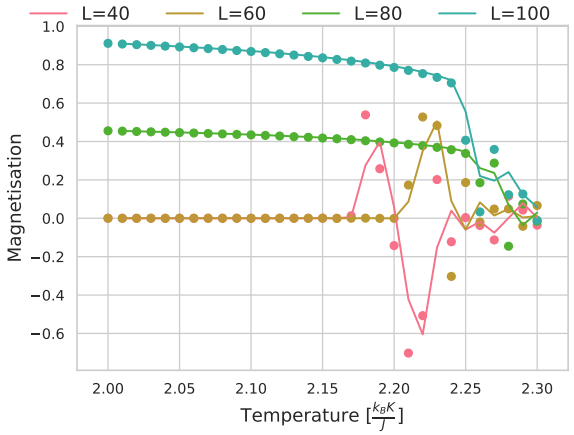

Figure 11: Mean magnetisation as a function of temperature $T \in [2.0, 2.3]$ for lattice sizes $L = 40, 60, 80, 100$, with a rolling mean, window size 2.

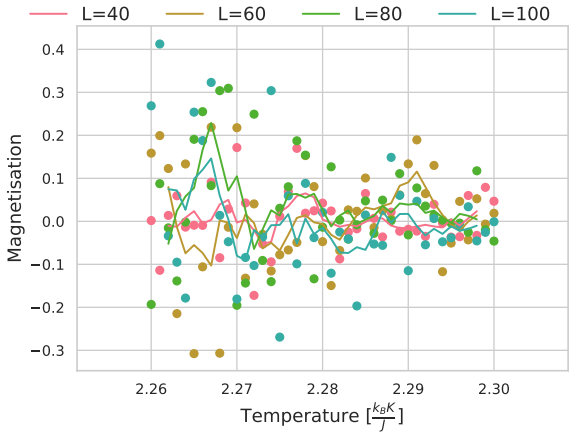

Figure 12: Mean magnetisation as a function of temperature $T \in [2.26, 2.3]$ for lattice sizes $L = 40, 60, 80, 100$, with a rolling mean, window size 5.

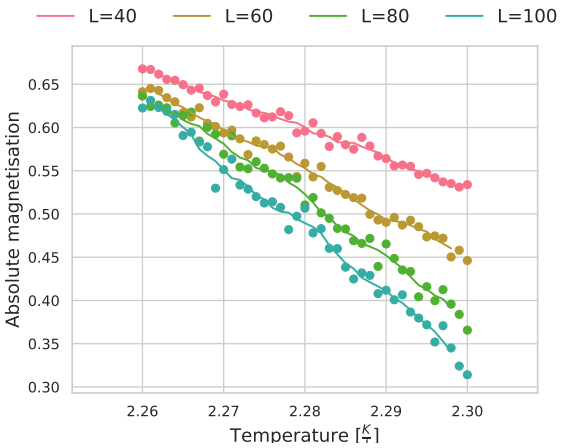

Figure 13: Absolute magnetisation as a function of temperature $T \in [2.26, 2.30]$ for lattice sizes $L = 40, 60, 80, 100$, with a rolling mean, window size 5.

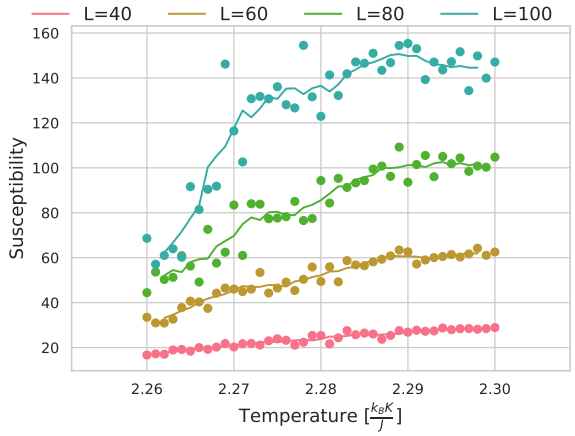

Figure 14: Susceptibility as a function of temperature $T \in [2.26, 2.30]$ for lattice sizes $L = 40, 60, 80, 100$, with a rolling mean, window size 5.