FYS4150 Project 4:
The Ising model in two dimensions

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Abstract

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Github: *https://github.com/mariahammerstrom/Project4*

1 Introduction

In this project we look a the Ising model in two dimensions. The Ising model is a model to study phase transitions at finite temperature for magnetic systems. The model was invented in 1920[1] and the analytical solution to the two-dimensional case was found in 1944[2]. This project deals with the Ising model in two dimensions without an external magnetic field.

1.1 Theory

In the two-dimensional Ising model, the simplest form of the **energy** for a specific microstate i is expressed as

$$E_i = -J \sum_{\langle kl \rangle}^{N} s_k s_l, \tag{1}$$

with $s_k = \pm 1$ where $+1$ denotes spin up and -1 denotes spin down, N is the total number of spins and J is a coupling constant expressing the strength of the interaction between neighboring spins. The symbol $\langle kl \rangle$ indicates that the sum is over nearest neighbors only. We assume ferromagnetic ordering, meaning $J > 0$ and will make use of periodic boundary conditions.

The probability of finding the system in a given microstate i is expressed by the **Boltzmann probability distribution**

$$P_i(\beta) = \frac{e^{-\beta E_i}}{Z}, \tag{2}$$

where $\beta = 1/kT$ with k the Boltzmann constant and T the temperature, and with Z as the **partition function** for the canonical ensemble defined as

$$Z = \sum_{i=1}^{\infty} e^{-\beta E_i}, \tag{3}$$

summing over all micro states i.

The **magnetic moment** of a given microstate is

$$\mathcal{M}_i = \sum_j s_j. \tag{4}$$

Some quantities of interest are the **expection values** for the energy $\langle E \rangle$ and magnetic moment $\langle \mathcal{M} \rangle$:

$$\begin{aligned} \langle E \rangle &= \frac{1}{Z} \sum_i E_i e^{-\beta E_i} = kT^2 \frac{\partial \ln Z}{\partial T} = -\frac{\partial \ln Z}{\partial \beta} \\ \langle \mathcal{M} \rangle &= \frac{1}{Z} \sum_i \mathcal{M}_i e^{-\beta E_i}, \end{aligned} \tag{5}$$

as well as the **variances** for the energy σ_E^2 and for the magnetic moment σ_M^2, describing how the calculated values of E and M deviates from the expectation values:

$$\begin{aligned} \sigma_E^2 &= \langle E^2 \rangle - \langle E \rangle^2 \\ \sigma_{\mathcal{M}}^2 &= \langle \mathcal{M}^2 \rangle - \langle \mathcal{M} \rangle^2, \end{aligned} \tag{6}$$

These values can be used to calculate the **heat capacity** of a fixed volume given by

[1] Lenz, W. (1920). "Beitrge zum Verstndnis der magnetischen Eigenschaften in festen Krpern". *Physikalische Zeitschrift* 21: 613-615.

[2] Onsager, Lars (1944). "Crystal statistics. I. A two-dimensional model with an order-disorder transition". *Physical Review*, Series II 65 (3-4): 117-149.

$$C_V = \frac{\sigma_E^2}{kT^2} = \frac{\partial \langle E \rangle}{\partial T}, \tag{7}$$

and the **susceptibility**, which describes whether a material is attracted into or repelled out of a magnetic field, given by

$$\chi = \frac{\sigma_{\mathcal{M}}^2}{kT} = \frac{\langle \mathcal{M}^2 \rangle - \langle \mathcal{M} \rangle^2}{kT}. \tag{8}$$

We want to compute these quantities after the system has **thermalized**, which is when the system has reached its most likely state. The most likely state depends on the temperature T.

The model we are considering here undergoes a **phase transition**. Below a critical temperature T_C there is spontaneous magnetization $\langle \mathcal{M} \rangle \neq 0$ (magnetic phase), while above this temperature the average magnetization is zero (paramagnetic phase). Near T_C we can characterize the behavior of many physical quantities by a power law behavior.

An important quantity is the **correlation length**, which is expected to be of the order of the lattice spacing for $T \gg T_C$. Because the spins become more and more correlated as T approaches T_C, the correlation length increases as we get closer to the critical temperature. The divergent behavior of ξ near T_C is

$$\xi(T) \sim |T_C - T|^{-\nu}. \tag{9}$$

A second-order phase transition is characterized by a correlation length which spans the whole system. Since we are always limited to a finite lattice, ξ will be proportional with the size of the lattice. Through so-called finite size scaling relations it is possible to relate the behavior at finite lattices with the results for an infinitely large lattice. The critical temperature then scales as

$$T_C(L) - T_C(L = \infty) = aL^{-1/\nu}, \tag{10}$$

with a a constant and ν defined in Eq. (9). Here we will use $\nu = 1$.

1.2 Analytical solution

First we will assume that we only have two spins in each dimension, that is $L = 2$, where L is the lattice length. The situation looks like this:

$$\uparrow_{(1)} \quad \uparrow_{(2)}$$
$$\uparrow_{(3)} \quad \uparrow_{(4)}$$

where an upward arrow denotes spin up. We will make use of **periodic boundary conditions**, which means that the neighbor to the right of a given spin s_N takes the value of s_1. Similarly, the neighbor to the left of s_1 takes the value of s_N. This way of treating the boundaries are often used when approximating an infinite system that has a repeating structure. In our case, this mean we will treat our system as though it looked like this (where the original system is highlighted in magenta):

$$\begin{array}{cccc} \uparrow_{(4)} & \uparrow_{(3)} & \uparrow_{(4)} & \uparrow_{(3)} \\ \uparrow_{(2)} & \uparrow_{(1)} & \uparrow_{(2)} & \uparrow_{(1)} \\ \uparrow_{(4)} & \uparrow_{(3)} & \uparrow_{(4)} & \uparrow_{(3)} \\ \uparrow_{(2)} & \uparrow_{(1)} & \uparrow_{(2)} & \uparrow_{(1)} \end{array}$$

Closed form expression can be found for the partition function in Eq. (3) and the corresponding expectation values for E, $|\mathcal{M}|$, the specific heat C_V and the susceptibility χ as functions of T using periodic boundary conditions. In the case $L = 2$ we can write Eq. (1) for the different components as, making use of the periodic boundary conditions, giving

$$\begin{aligned} E_1 &= -J(s_1 s_2 + s_1 s_3) = -2J, \\ E_2 &= -J(s_1 s_2 + s_2 s_4) = -2J, \\ E_3 &= -J(s_1 s_3 + s_3 s_4) = -2J, \\ E_4 &= -J(s_3 s_4 + s_2 s_4) = -2J. \end{aligned}$$

Thus the total energy for the system is

$$E = E_1 + E_2 + E_3 + E_4 = -8J.$$

If going through this exercise for different configurations of spin up and spin down, we find values for energies, degeneracies and magnetization for different configurations as shown in Table 1, where magnetization is calculated from Eq. (4).

These calculations can be used to find the closed-form expressions, starting with the partition function, which can be expressed as

$$\begin{aligned} Z(\beta) &= \sum_E \Omega(E) e^{-\beta E} = 2e^{8J\beta} + 2e^{-8J\beta} + 12 \\ &= 4\cosh(8J\beta) + 12. \end{aligned} \tag{11}$$

Then the expectation value can be written, using the expression in Eq. (6), as

$$\langle E \rangle = -\frac{8J \sinh(8J\beta)}{\cosh(8J\beta) + 3} \approx -8J \tanh(8J\beta), \tag{12}$$

where we have used that $\cosh(8J\beta) \gg 3$ in the approximation. Using this approximation gives

$$C_V(\beta) = k\left(\frac{8J\beta}{\cosh(8J\beta)}\right)^2. \tag{13}$$

Similarly, using the values for magnetization in Table 1 and Eq. (4), gives

$$\begin{aligned} \langle |\mathcal{M}| \rangle &= \frac{1}{Z}\left(4e^{8J\beta} + 4 \cdot 2 + 4 \cdot |-2| + |-4| e^{8J\beta}\right) \\ &= \frac{8}{Z}(e^{8J\beta} + 2), \end{aligned} \tag{14}$$

and

$$\begin{aligned} \langle \mathcal{M} \rangle &= \frac{1}{Z}\left(4e^{8J\beta} + 4 \cdot 2 - 4 \cdot 2 - 4e^{8J\beta}\right) = 0, \\ \langle \mathcal{M}^2 \rangle &= \frac{1}{Z}\left(4^2 e^{8J\beta} + 4 \cdot 2^2 + 4 \cdot (-2)^2 + (-4)^2 e^{8J\beta}\right) \\ &= \frac{32}{Z}\left(e^{8J\beta} + 1\right). \end{aligned} \tag{15}$$

Thus

$$\chi(\beta) = \frac{\langle \mathcal{M}^2 \rangle - \langle \mathcal{M} \rangle^2}{kT} = \frac{32\beta}{Z}[e^{8J\beta} + 1] - \frac{\beta}{Z^2}[8e^{8J\beta} + 4]^2 \tag{16}$$

Number of spins up	Energy E	Degeneracy Ω	Magnetization $\mathcal{M}$
4	$-8J$	1	4
3	0	4	2
2	0	4	0
2	$8J$	2	0
1	0	4	-2
0	$-8J$	1	-4

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

2 Methods

We wrote a code for the Ising model which computes the mean energy E, mean magnetization $|\mathcal{M}|$, the specific heat C_V and the susceptibility χ as functions of T using periodic boundary conditions for in the x and y directions. Using the Ising model in two dimensions, the number of configurations is given by 2^N with $N = L \times L$ number of spins for a lattice of length L.

2.1 Algorithm

We will use the **Metropolis algorithm**. The algorithm goes as follows:

1. Generate a random configuration in the lattice to create an initial state with energy E_b.
2. Change the initial configuration by flipping for example one spin only. Compute the energy of this state E_t.
3. Calculate $\Delta E = E_t - E_b$ (t = trial state, b = beginning state).
4. *The Metropolis test:* If $\Delta E \leq 0$ the new configuration is accepted, meaning the energy is lowered and we are moving towards the energy minimum at a given temperature. If $\Delta E > 0$, calculate $w = e^{-\beta \Delta E}$. If $w < r$ where r is a random number, accept the new configuration. If else, keep the old configuration.
5. Compute the new energy $E' = E_t + \Delta E$. Calculate various expectation values using this energy.
6. Repeat steps $2 - 5$ for the chosen number of Monte Carlo (MC) cycles, meaning the number of times we should sweep through the lattice and summed over all spins.
7. Compute the various expectation values by dividing by the total number of cycles (and possibly the number of spins).

During the computation we want to check how many MC cycles we need before the system has reached its most likely state. This is done by comparing the new value of $\langle E \rangle$ with the previous value of $\langle E \rangle$. If the difference is smaller than 5%, we can say that the most likely state has been reached.

After the most likely state has been reached, we want to

2.2 Parallelization

We have parallelized our code using the Open MPI library. ADD DETAILS.

2.3 Calculating T_C

The critical temperature T_C is described by Eq. (10), where $T_C(L)$ is calculated for different lattice sizes L through our algorithm described above. $T_C(L = \infty)$ is described by the exact value of 2.269 kT/J. But we do not know what the constant a should be.

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3 Results

3.1 Checking the 2×2 case

Computing the mean energy E, mean magnetization $|\mathcal{M}|$, the specific heat C_V and the susceptibility χ with periodic boundary conditions numerically using the expressions from Sec. 1.1 can be compared with the results using the analytical closed form expressions given in Sec. 1.2. For temperature $T = 1.0$ (in units of kT/J), this gives the following results for a 2×2 spin system where the initial state has all spins pointing upwards:

Quantity	Closed form	Numerical
Mean energy E	-8.00	-8
Mean magnetization $\lvert\mathcal{M}\rvert$	3.99	4
Specific heat C_V	2.88×10^{-5}	0
Susceptibility χ	8.02×10^{-3}	0

The numerical results follow that of Table 1. The result from the closed form expressions are not as good. However, since we have done some approximations in order to derive these closed form expressions, some deviation is expected. The minimum number of MC cycles needed to achieve good agreement for the expectation value for energy is calculated to be 22-24 cycles, which will vary slightly for each run.

3.2 The 20×20 case

Next we looked at the case of $L = 20$ spins in the x and y directions. In this case we wanted to perform a study of the time (or number of MC cycles) we need before reaching an equilibrium situation and can start computing the various expectation values. A rough study is done by plotting the various expectation values

as a function of number of MC cycles, for both $T = 1.0$ kT/J and $T = 2.4$ kT/J, as shown in Fig. 1. For $T = 1.0$ kTJ, we see that the expectation values does not change considerably with MC cycles. Thus, the system quickly reaches an equilibrium state. This is because we set all spin configurations to spin up for temperatures lower than 1.5 kTJ For $T = 2.4$ kTJ, on the other hand, the calculated values shows large variation for small numbers of MC cycles. The system reaches an equilibrium at a much later point.

3.3 The number of accepted configurations

We also study the total number of accepted configurations as a function of the total number of MC cycles, shown in Fig. 2a. The plot shows number of accepted configurations divided by total number of MC cycles. The number of accepted configurations scales approximately linearly with the total number of MC cycles. For $T = 1.0$ kTJ there are no accepted configurations since no spin in the lattice is changed from up to down.

How the total number of accepted configurations vary as a function of temperature is shown in Fig. 2b. The number of accepted configurations increases with higher temperature. We see that this increase is greater with higher lattice size.

3.4 The probability P(E)

By simply counting the number of times a given energy appears in our computation, namely the expectation value for the energy, we can compute the probability $P(E)$ for that energy. We start the counting after the steady state situation has been reached, still looking at the $L = 20$ case. This result is compared with the compute variance in energy σ_E^2.

For $T = 1.0$ kT/J we find that $P(E) = 0.87$ and $\sigma_E^2 = 0.02$, while for $T = 2.4$ kT/J we find that $P(E) = 0.03$ and $\sigma_E^2 = 8.28$ for an ordered initial spin matrix.

DISCUSS.

3.5 Looking for phase transitions

In our study of the behavior of our model close to the critical temperature we look at the various expectation values as a function of T for $L = 20, L = 40, L = 60$ and $L = 80$ for $T \in [2.0, 2.4]$, shown in Fig. 4a-d.

The spin matrix for $L = 80$ in this temperature range is visualized in Fig. 3, where white squares represent upward spins and black squares represent downward spins. It shows clearly that the net magnetization $\langle \mathcal{M} \rangle$ is higher for low T with most spins pointing in the same direction (in this case upwards), while the $\langle \mathcal{M} \rangle$ approaches zero at higher T where the number of spins pointing upward and downward are about the same.

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3.6 Estimating the critical temperature

Lastly, we want to estimate the critical temperature T_C in the thermodynamical limit $L \to \infty$ running simulations for different values of L using Eq. (10).

3.7 Parallelization

As described previously, we parallelized our code using MPI. Here we have gathered some time recordings, using $n = 4$ processes on a 2,5 GHz Intel Core i5 processor:

Lattice size L	Time usage t
$L = 10$	00m 57s
$L = 20$	03m 52s
$L = 40$	15m 23s
$L = 60$	48m 06s
$L = 80$	2h 02m 00s
$L = 100$	8h 46m 22s

These data is plotted in Fig. 5, approximated by a L^2 curve which makes a good fit for lower values of L, and a $e^{L/9.5}$ curve which is a good approximation for higher values of L.

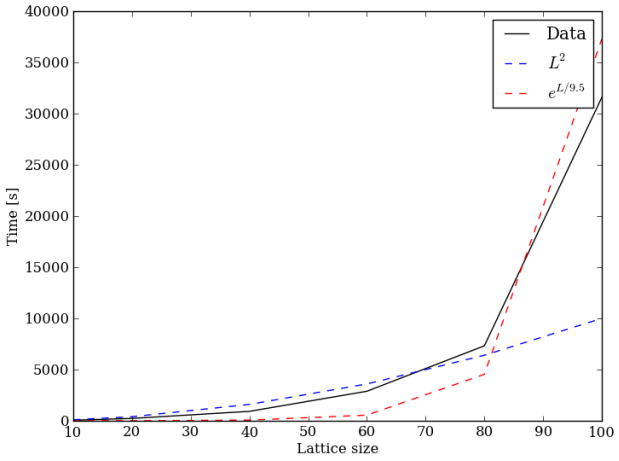

Figure 5: Time needed to run the program as a function of lattice size.

4 Conclusions

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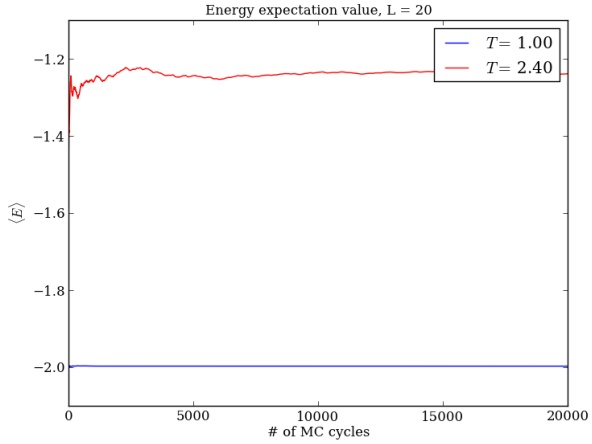
Something about lattice size vs. time vs. results.

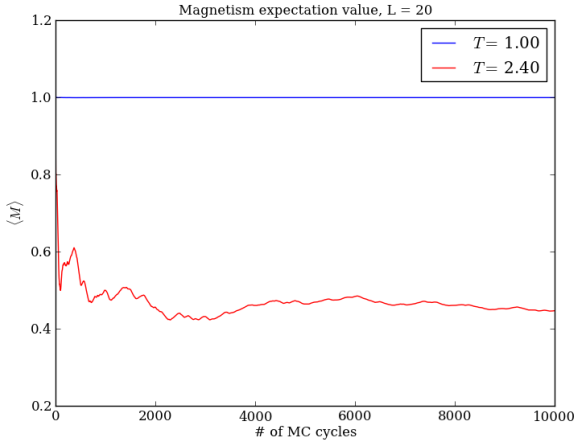
5 List of codes

The codes developed and used for this project are:

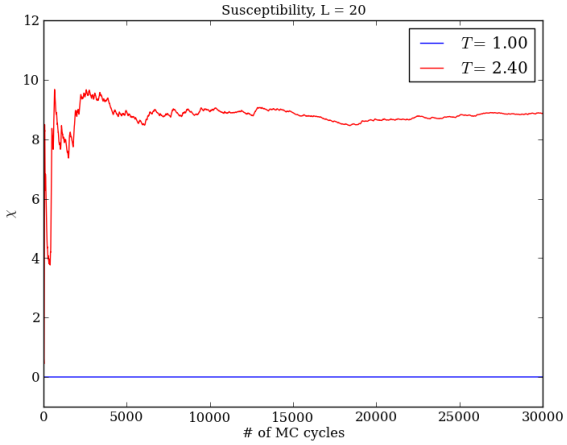
`main.cpp` – main program (C++).
`plotting.py` – plotting program which makes plots to study the total number of accepted configurations as a function of total number of MC cycles and as a function of temperature T (Python).
`visualization.py` – provided program for running the Metropolis algorithm and plotting the spin matrix, as shown in Fig. 3 (Python).



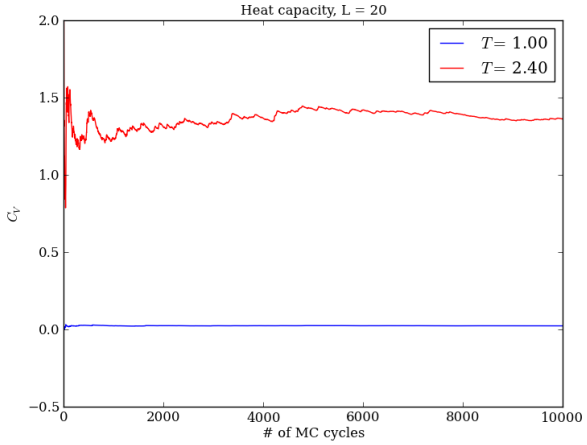
(a) Energy



(b) Magnetization

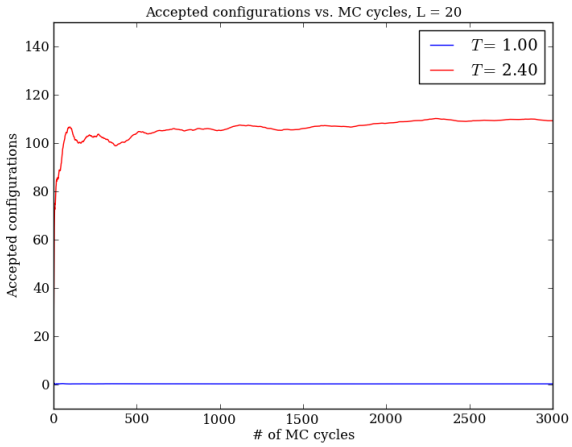


(c) Susceptibility

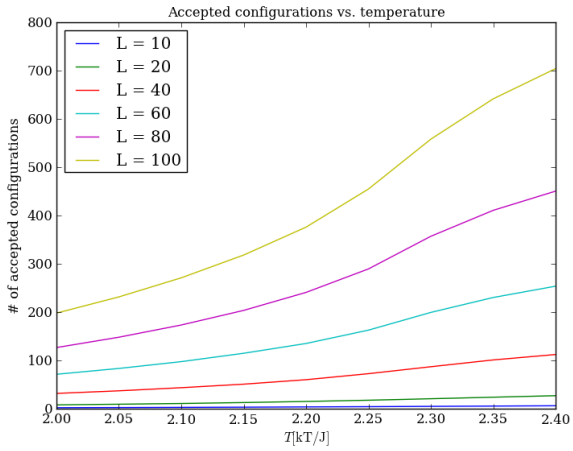


(d) Heat capacity

Figure 1: Expectation values as a function of number of MC cycles with the hottest temperature in red.

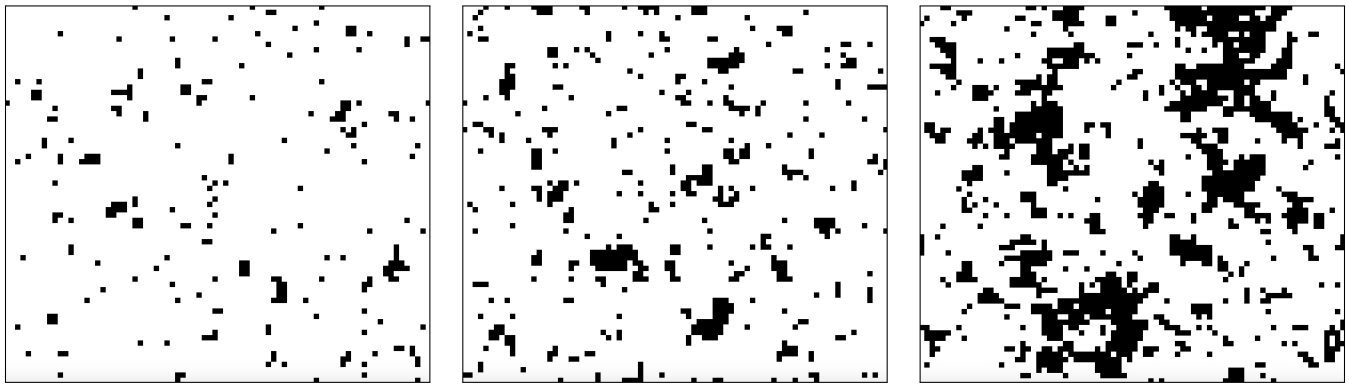


(a) As a function of # of MC cycles.



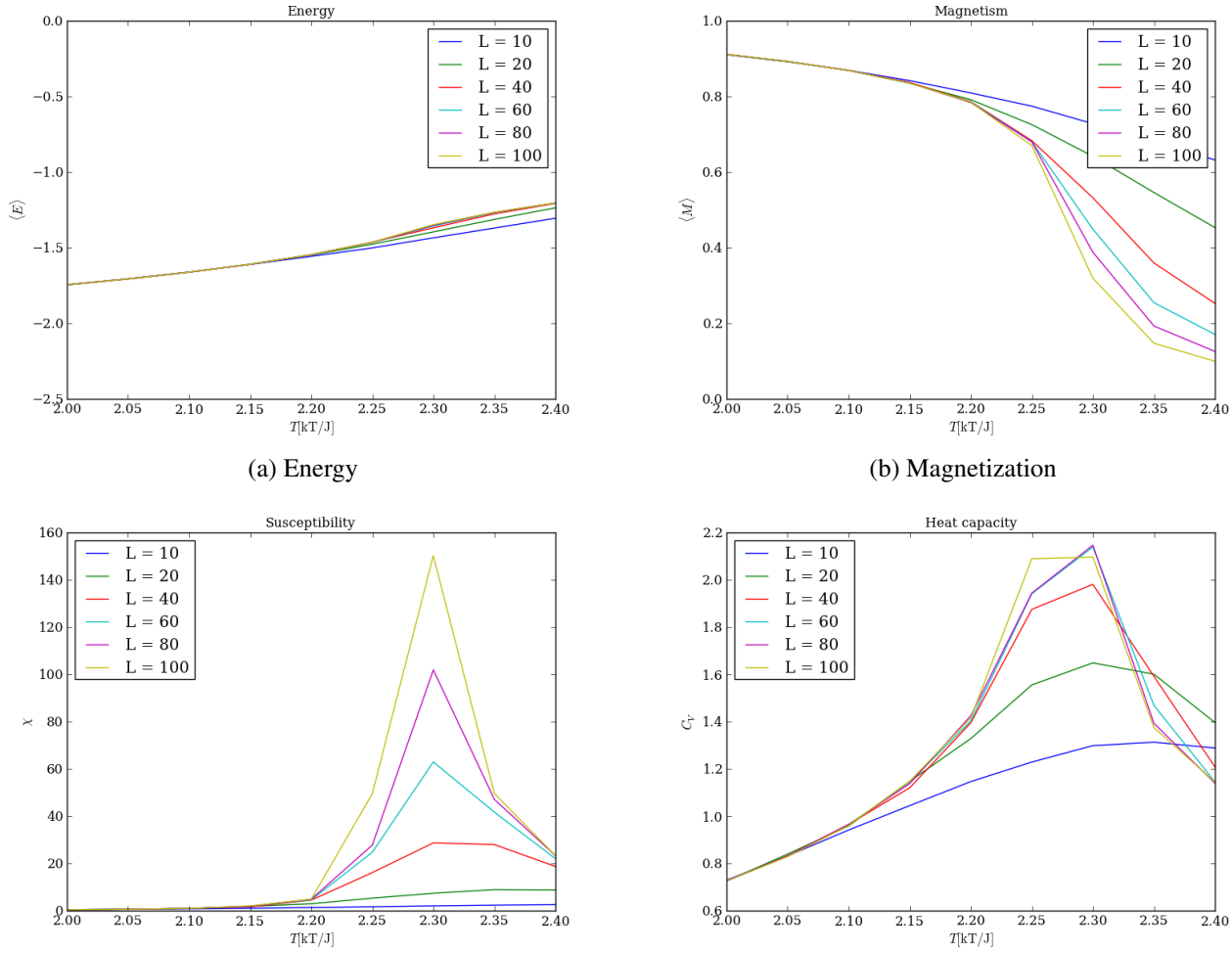
(b) As a function of temperature.

Figure 2: Number of accepted configurations.



(a) $T = 2.0$ (b) $T = 2.2$ (c) $T = 2.4$

Figure 3: Visualization of the spin matrix for a 80×80 lattice for different temperatures T. White = spin up, black = spin down.



(a) Energy (b) Magnetization

(c) Susceptibility (d) Heat capacity

Figure 4: Expectation values as a function of temperature.