Studying second order phase transitions by using the Ising model in two dimentions and the metropolis algorithm

Project 4, FYS-3150

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Abstract

The aim of this project is to numerically solve ..... by using the .... algorithm.
the Ising model in two dimensions, without an external magnetic field
Title: Studying phase transitions (critical T) using the ising model (metropolis alg)?
compare teory, lars onsager

Contents

1 Motivation and purpose

2 Theory

something about phase transitions and therefore chi and heat capacity is relevant

2.1 The Ising model in two dimentions

The Ising model is a simple model for ferromagnetism in statistical physics. The model consists of magnetic spins that are allowed to interact with its neigbours. The magnetic dipole moments are allowed to have two values, 1 and -1.

In this project we will study the ising model i two dimentions wich allows the identification of phase transitions (define). We will also set the external magnetic field to zero troughout this paper.

The Ising model gives that the energy (for the whole system?) can be expressed as

$$E = -J \sum_{<kl>}^{N} s_k s_l \tag{1}$$

where the value of the spins are $s_k = \pm 1$ and N is the total number of spins. The variable J is a coupling constant expressing the strength of the interaction between neighboring spins.

The symbol $< kl >$ indicates that we sum over nearest neighbors only. We will assume that we have a ferromagnetic ordering, viz $J > 0$ and use periodic boundary conditions.

(invlude matrix of spins and define variable L, N and M)

First we assume that there is only two spins in each dimention (x and y), we set $L = 2$. Then the closed form expression for the partition function is given by:

$$Z = \sum_{i=1}^{M} e^{-\beta E_i}$$

where M is the number of microstates or combinations of spins.

2.2 L=2 analytical values

$N = L \cdot L = 4$

There is $M = L^N = 2^N = 16$ microstates, or possible combinations and energies of the spin system. So to calculate the partition function we have to find the energies:

$$Z = e^{-\beta E_1} + ... e^{-\beta E_{16}}$$

The spin system can be visualized as 16 matrices on the form: $\begin{bmatrix} s(0,0) & s(0,1) \\ s(1,0) & s(1,1) \end{bmatrix}$ with corresponding energies.

Periodic boundaryconditions give that every spin has a neighbour. The neighbours of the spin $s(1,1)$ is $s(0,1)$ twice (above and below) and $s(1,0)$ twice (above and below). To find the energy we have to sum over the nearest neighbours for all the spins in the system. The product $s_l s_k$ of two neighbours should only be calculated once. This is solved if the index of s_l is fixed while s_k has one higher index in each direction at a time:

$$E = -J\left(s(0,0) \cdot \big[s(1,0) + s(0,1)\big] + s(0,1) \cdot \big[s(1,1) + s(0,0)\big]\right.$$
$$\left. + s(1,0) \cdot \big[s(0,0) + s(1,1)\big] + s(1,1) \cdot \big[s(0,1) + s(1,0)\big]\right) \tag{2}$$

The 16 states with corresponding energies calculated with equation 2 is then:

$$E_1 = 0 \qquad E_2 = 0 \qquad E_3 = 0 \qquad E_4 = 0$$
$$\begin{bmatrix} 1 & 1 \\ -1 & -1 \end{bmatrix} \quad \begin{bmatrix} 1 & -1 \\ 1 & -1 \end{bmatrix} \quad \begin{bmatrix} -1 & 1 \\ -1 & 1 \end{bmatrix} \quad \begin{bmatrix} -1 & -1 \\ 1 & 1 \end{bmatrix}$$
$$E_5 = 0 \qquad E_6 = 0 \qquad E_7 = 0 \qquad E_8 = 0$$
$$\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \quad \begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix} \quad \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix} \quad \begin{bmatrix} -1 & 1 \\ 1 & 1 \end{bmatrix}$$
$$E_9 = 0 \qquad E_{10} = 0 \qquad E_{11} = 0 \qquad E_{12} = 0$$
$$\begin{bmatrix} -1 & -1 \\ -1 & 1 \end{bmatrix} \quad \begin{bmatrix} -1 & -1 \\ 1 & -1 \end{bmatrix} \quad \begin{bmatrix} 1 & -1 \\ -1 & -1 \end{bmatrix} \quad \begin{bmatrix} -1 & 1 \\ -1 & -1 \end{bmatrix}$$
$$E_{13} = 8J \qquad E_{14} = 8J \qquad E_{15} = -8J \qquad E_{16} = -8J$$
$$\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \quad \begin{bmatrix} -1 & 1 \\ 1 & -1 \end{bmatrix} \quad \begin{bmatrix} -1 & -1 \\ -1 & 1 \end{bmatrix} \quad \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$$

We then see that there is only three possible values for the energies, $E \in \{-8J, 0, 8J\}$ with corresponding multiplicity $\{2, 12, 2\}$. The partition function can then be calculated:

$$Z = 2e^{-\beta(-8J)} + 12e^{-\beta \cdot 0} + 2e^{-\beta \cdot 8J} = 2(e^{\beta \cdot 8J} + e^{-\beta \cdot 8J}) + 12$$
$$= 4\cosh(8J\beta) + 12$$

using that $\cosh(x) = \frac{1}{2}(e^{-x} + e^x)$.

Now that we have the partition function various expectation variables can be calculated. We start with the expectation value for the energy:

$$\langle E \rangle = \frac{1}{Z}\sum_{i=1}^{M} E_i e^{-\beta E_i} = \frac{1}{Z}\big[2 \cdot (-8J)e^{8J\beta} + 0 + 2 \cdot 8Je^{-8J\beta}\big] = \frac{1}{Z}\big[-16Je^{8J\beta} + 16Je^{-8J\beta}\big]$$

$$= -\frac{16J}{Z}\big[-e^{-8J\beta} + e^{8J\beta}\big] = -\frac{32J}{Z}\sinh(8J\beta) = -\frac{8J\sinh(8J\beta)}{\cosh(8J\beta) + 3}$$

using that $\sinh(x) = \frac{1}{2}(-e^{-x} + e^x)$. We will now calculate the heat capacity

$$C_v = \frac{1}{k_b T}\sigma_E^2 = \frac{1}{k_b T}\big(\langle E^2 \rangle - \langle E \rangle^2\big)$$

where

$$\langle E^2 \rangle = \frac{1}{Z}\sum_{i=1}^{M} E_i^2 e^{-\beta E_i} = \frac{1}{Z}\big[2 \cdot (-8J)^2 e^{8J\beta} + 0 + 2 \cdot (8J)^2 e^{-8J\beta}\big] = \frac{128J^2}{Z}\big[e^{8J\beta} + e^{-8J\beta}\big]$$

$$= \frac{128J^2 \cdot 2\cosh(8J\beta)}{4\cosh(8J\beta) + 12} = \frac{64J^2\cosh(8J\beta)}{\cosh(8J\beta) + 3}$$

so that

$$C_v = \frac{1}{k_bT}\left[\frac{64J^2\cosh(8J\beta)}{\cosh(8J\beta)+3} - \left(-\frac{8J\sinh(8J\beta)}{\cosh(8J\beta)+3}\right)^2\right] = \frac{1}{k_bT}\left[\frac{64J^2\cosh(8J\beta)}{\cosh(8J\beta)+3} - \frac{64J^2\sinh^2(8J\beta)}{(\cosh(8J\beta)+3)^2}\right]$$

$$= \frac{64J^2}{k_bT}\left[\frac{\cosh(8J\beta)(\cosh(8J\beta)+3)-\sinh^2(8J\beta)}{(\cosh(8J\beta)+3)^2}\right] = \frac{64J^2}{k_bT}\left[\frac{\cosh^2(8J\beta)+3\cosh^2(8J\beta)-\sinh^2(8J\beta)}{(\cosh(8J\beta)+3)^2}\right]$$

$$= \frac{64J^2\beta}{T}\left[\frac{1+3\cosh(8J\beta)}{(\cosh(8J\beta)+3)^2}\right]$$

We define the magnetization $\mathcal{M}$ as the sum of all the spins s. It is easy to see that for the 2×2 system there are only 5 possible values for the magnetization, $\mathcal{M} \in \{-4,-2,0,2,4\}$. The corresponding energy and multiplicity is given in table 2.2.

# spins up	Multiplicy	Energy	Magnetization
4	1	-8J	4
3	4	0	2
2	4	0	0
2	2	8J	0
1	4	0	-2
0	1	-8J	-4

The expectation value of the magnetization and the magnetization squared can be calculated as

$$\langle\mathcal{M}\rangle = \frac{1}{Z}\sum_{i=1}^{M}\mathcal{M}e^{-\beta E_i} \tag{3}$$

$$\langle\mathcal{M}^2\rangle = \frac{1}{Z}\sum_{i=1}^{M}\mathcal{M}^2 e^{-\beta E_i}$$

which we can use to calculate the suceptibility, the parameter of special interest:

$$\chi = \frac{1}{k_bT}\sigma_{\mathcal{M}} = \frac{1}{k_bT}\left(\langle\mathcal{M}^2\rangle - \langle\mathcal{M}\rangle^2\right).$$

When looking at equation 3 and table 2.2 we quicly see that the expectation value of the magnetization is zero for all temperatures. The microstates whith oposite magnetization have the same multiplicity so they cancel each other out. When running numerical calculations on large systems, for large L, the numerical value of $\langle\mathcal{M}\rangle$ will not reach zero unless the simulation is run for a (extremely) long time. This is because it takes a long time for the simulation to go through all the possible microstates after the simulation have reached a very probable state. But we want to have a reasonable measure of the magnetization and suceptibility for large systems and at the same time minimize the excecution time of the numerical simulation. To do this we choose to use the absolute value of the magnetization in the definition of the suceptibility.

There are 3 possible values for the absolute value of the magnetization, $|\mathcal{M}| \in \{0,2,4\}$. The corresponding energy and multiplicity is given in table 2.2.

Absolute Magnetization	Energy	Multiplicy
4	-8J	2
2	0	8
0	0	4
0	8J	2

We are then ready to calculate the expectation value of the absolute value of the magnetization by using the multiplicity for each energy and corresponding magnetization:

$$\langle |\mathcal{M}| \rangle = \frac{1}{Z} \sum_{i=1}^{M} |\mathcal{M}| e^{-\beta E_i} = \frac{1}{Z}\left(2 \cdot 4 e^{-\beta(-8J)} + 8 \cdot 2 e^0 + 0 \cdot 4 e^0 + 0 \cdot 2 e^{-\beta 8J} \right)$$

$$= \frac{8}{Z}\left(e^{8J\beta} + 2 \right) = \frac{8(e^{8J\beta} + 2)}{4\cosh(8j\beta) + 12} = \frac{2(e^{8J\beta} + 2)}{\cosh(8j\beta) + 3}. \tag{4}$$

We also obtain the expectation value of the square of the magnetization:

$$\langle \mathcal{M}^2 \rangle = \frac{1}{Z} \sum_{i=1}^{M} \mathcal{M}^2 e^{-\beta E_i} = \frac{1}{Z}\left(2 \cdot 4^2 e^{-\beta(-8J)} + 8 \cdot 2^2 e^0 + 0 + 0 \right) = \frac{32}{Z}\left(e^{8J\beta} + 1 \right)$$

$$= \frac{8\left(e^{8J\beta} + 1 \right)}{\cosh(8J\beta) + 3}.$$

And finally the suceptibility is given by

$$\chi = \frac{1}{k_b T}\left(\langle \mathcal{M}^2 \rangle - \langle |\mathcal{M}| \rangle^2 \right) = \frac{1}{k_b T}\left[\frac{8(e^{8J\beta} + 1)}{\cosh(8J\beta) + 3} - \left(\frac{2(e^{8J\beta} + 2)}{\cosh(8j\beta) + 3} \right)^2 \right]$$

$$= \frac{1}{k_b T}\left[\frac{8(e^{8J\beta} + 1)(\cosh(8j\beta) + 3) - 4(e^{8J\beta} + 2)^2}{(\cosh(8j\beta) + 3)^2} \right]$$

$$= 4\beta\left[\frac{2(e^{8J\beta} + 1)(\cosh(8j\beta) + 3) - (e^{8J\beta} + 2)^2}{(\cosh(8j\beta) + 3)^2} \right]$$

2.3   Units, scaled parameters

We will now write the equations for the expectation values, the heat capacity and the susceptibility in terms of a scaled temperature

$$T' = T\frac{k_b}{J}$$

$$\Rightarrow T = T'\frac{J}{k_b}$$

$$\Rightarrow \beta = \frac{1}{k_b T} = \frac{1}{k_b \cdot T'\frac{J}{k_b}} = \frac{1}{T'J}$$

We then set $J = 1$ so that:

$$\beta = \frac{1}{T'}$$

We will use this new temperature T' in the numerical calculations. We also scale the heat capacity as:

$$C_v' = \frac{C_v}{k_b} = \frac{64}{T'^2}\frac{1 + 3\cosh(8/T')}{(\cosh(8/T') + 3)^2}$$

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In terms of T' the expectation values and the susceptibility for the 2×2 system can be written as:

$$\langle E \rangle = -\frac{8 \sinh(8/T')}{\cosh(8/T') + 3} \tag{5}$$

$$\langle E^2 \rangle = \frac{64 J^2 \cosh(8/T')}{\cosh(8/T') + 3} \tag{6}$$

$$\langle |\mathcal{M}| \rangle = \frac{2(e^{8/T'} + 2)}{\cosh(8/T') + 3} \tag{7}$$

$$\langle \mathcal{M}^2 \rangle = \frac{8(e^{8/T'} + 1)}{\cosh(8/T') + 3} \tag{8}$$

$$\chi = \frac{4}{T'} \frac{2(e^{8/T'} + 1)(\cosh(8/T') + 3) - (e^{8/T'} + 2)^2}{(\cosh(8/T') + 3)^2} \tag{9}$$

These theoretical values will be used to test the implementation of the numerical method for the $L = 2$ system.

3 Numerical methods

bla bla theory and the programs

3.1 Metropolis algorithm

See notes?

Start out with an initial state, random or ordered

1. The system are in a spin state with energy E

2. Create a trial state with the trial energy E_t by flipping one spin

3. Compute $\Delta E = E_t - E$

    - If $\Delta E \leq 0$
        - Accept the trial state as the new state
    - If $\Delta E > 0$ calculate $w = e^{-\beta \Delta E}$ and create a random number r
        - If $r \leq w$ (the metropolis test): Accept the trial state as the new state
        - Else discard the trial state (do nothing with the state)

4. Do 1.-3. $L \times L$ times (one MC cycle)

5. Update mean values

6. Reapeat 1.-6. untill enough statistics is sampled, the desired number of MC cycles

   Psedocode:

```
for numberOfTemperatures:
{
        //create initial state here
        //calculate initial energy and magnetization here
        for numberoOfMCcycles:
        {
                for numberOfspins:
                {
                        //do one spin flip here
                }
                //update mean values here
                //print mean values to file here
        }
        //or print values to file here
}

//then read data from file and plot in python
```

for some of the files temperature loop is left in python code, which also compiles and runs the cpp code

should discard contributions to mean vals before equilibrium

3.2   Coding ΔE, $\Delta \mathcal{M}$ and w efficiently

We wish to run the simulations for large numbers of Monte Carlo cycles 10^5. It is therefore very important to code the calculation of ΔE efficiently because it will be calculated N times each Monte Carlo cycle.

The difference in the energy can be expressed as:

$$\Delta E = E_2 - E_1 = -J \sum_{<kl>}^{N} s_{k,2} s_{l,2} + J \sum_{<kl>}^{N} s_{k,1} s_{l,1}$$

where the l index is the spin that was flipped and k the neighbours of l. We only flip one spin at a time, so the neighbours of s_l are unchanged meaning that $s_{k,2} = s_{k,1} = s_k$. The difference in energy can then be written as:

$$\Delta E = J \sum_{<kl>}^{N} s_k s_{l,1} - J \sum_{<kl>}^{N} s_k s_{l,2} = J \sum_{<kl>}^{N} s_k (s_{l,1} - s_{l,2})$$

The spin can only take two values, so $s_{l,1}$ is either 1 or -1. If $s_{l,1} = 1$ then after the flip $s_{l,2} = -1$ and $s_{l,1} - s_{l,2} = 1 - (-1) = 2$. If $s_{l,1} = -1$ then after the flip $s_{l,2} = 1$ and $s_{l,1} - s_{l,2} = -1 - 1 = -2$. We can therefore write $s_{l,1} - s_{l,2} = 2s_{l,1}$ and then we obtain:

$$\Delta E = J \sum_{<kl>}^{N} s_k \cdot 2s_{l,1} = 2J s_{l,1} \sum_{<k>}^{N} s_k$$

which is the same as in theory????when doing by hand energy?

Similarly for the magnetization:

$$\Delta \mathcal{M} = \mathcal{M}_2 - \mathcal{M}_1 = \sum_i^N s_{i,2} - \sum_i^N s_{i,1} = \sum_i^N (s_{i,2} - s_{i,1}) = s_{l,2} - s_{l,1} = -2s_{l,1}$$

$$\Rightarrow \mathcal{M}_2 = \mathcal{M}_1 - 2s_{l,1}$$

This way of calculating the difference in energy and magnetization makes the algorithm for flipping one spin run faster than orther solutions. We also want to avoid to calculate the exponential of $DeltaE$, the value of $w = e^{-\beta \delta E}$ for every time the trial energy is higher than the current energy. We can avoid this by noticing that there are only 5 possible values ΔE can take when we only flip one spin at a time (in the two dimentional case) $\Delta E \in \{-8, -4, 0, 4, 8\}$. So the energy minimum have to change in steps of 4, and maximum in steps of 8 when we flip one spin at a time. Then there are also only 5 possible values of w for a given temperature. We can exploit this further by realizing that we only use w when $\Delta E > 0 \Rightarrow \Delta E \in \{4, 8\}$. For a given temperature we then calculate the two values of w once and pass it on to the metropolis test which uses the value corresponding to ΔE.

something something random initial state ??? p. 439, dependence T

4 "Experiment"

4.1 Testing the implementation of the model and algorithm

4.2 Studying the number of Monte Carlo cycles

4.3 Studying .... close to the critical temp

4.4 Calculations to find T_c

5 Results and output

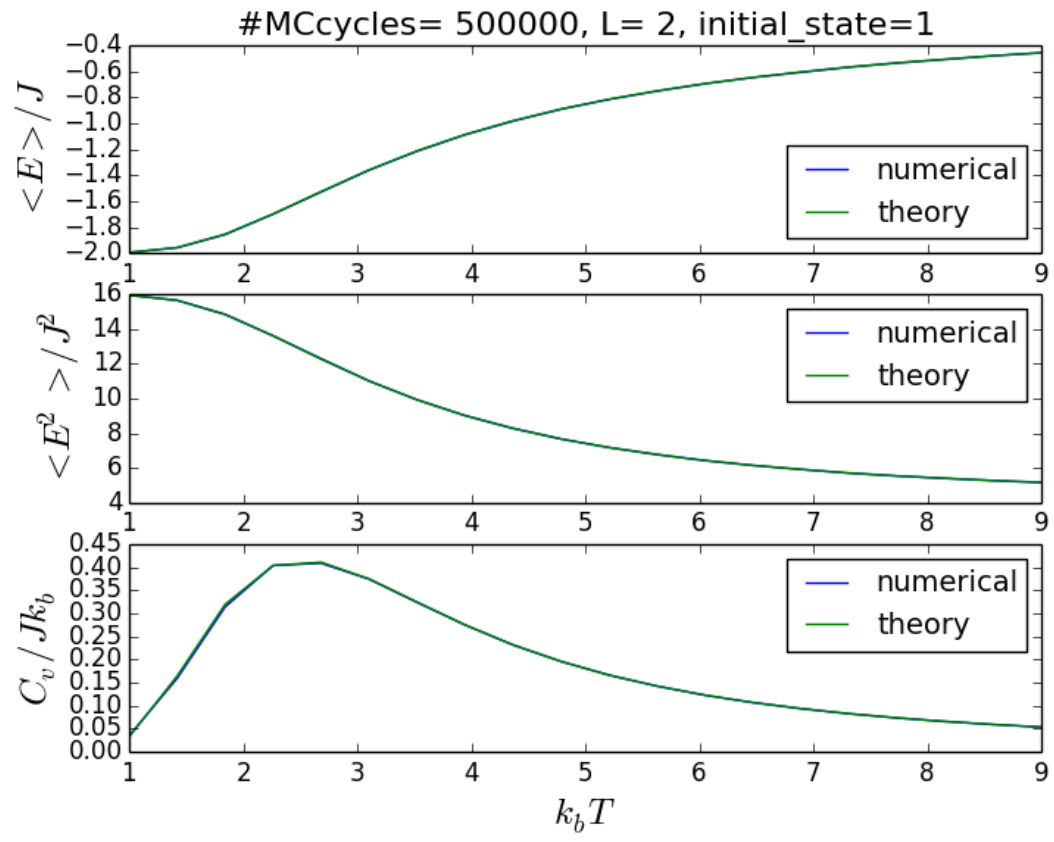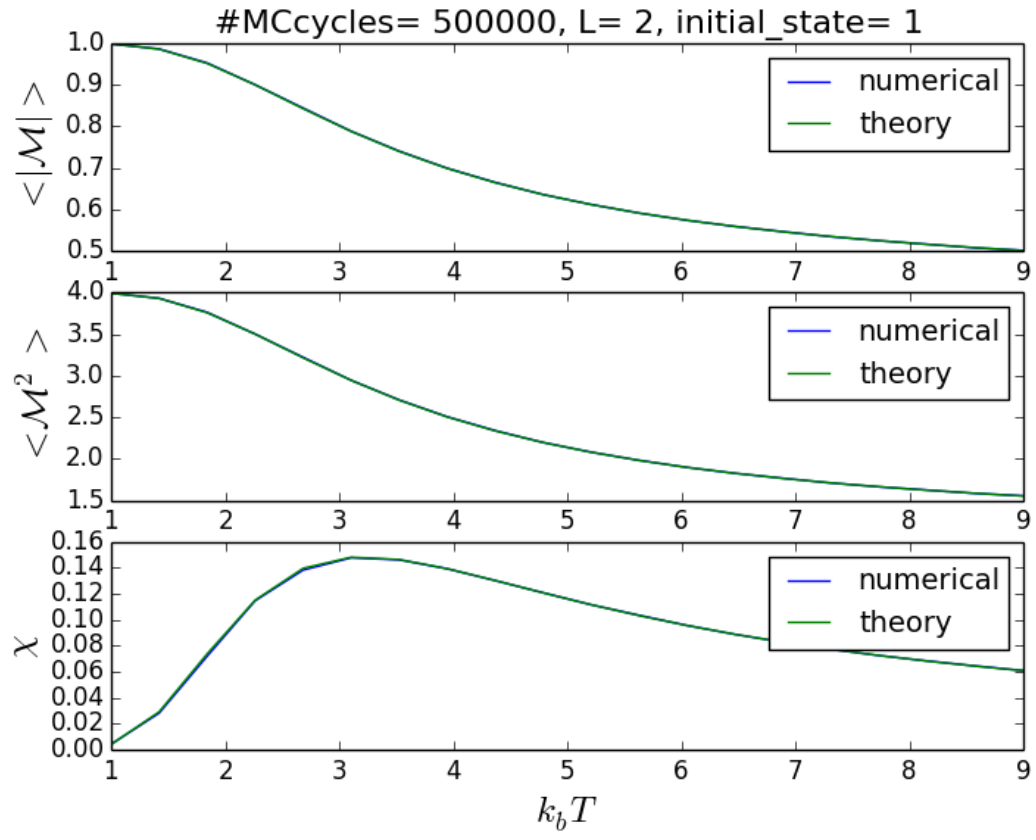# 6 Discussion and experiences

Figure 1: noe? everything per spin

Figure 2: noe? everything per spin

a) Assume we have only two spins in each dimension, that is $L = 2$. Find the closed form expression for the partition function and the corresponding expectations values for for E, $|\mathcal{M}|$, the specific heat C_V and the susceptibility χ as functions of T using periodic boundary conditions.

b) Write now 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 $L = 2$ in the x and y directions. Compare your results with the expressions from a) for a temperature $T = 1.0$ (in units of kT/J).

   How many Monte Carlo cycles do you need in order to achieve a good agreeement?

c) We choose now a square lattice with $L = 20$ spins in the x and y directions.

   In [b) we did not study carefully how many Monte Carlo cycles were needed in order to reach the most likely state. Here we want to perform a study of the time (here it corresponds to the number of Monte Carlo cycles) one needs before one reaches an equilibrium situation and can start computing various expectations values. Our first attempt is a rough and plain graphical one, where we plot various expectations values as functions of the number of Monte Carlo cycles.

   Choose first a temperature of $T = 1.0$ (in units of kT/J) and study the mean energy and magnetisation (absolute value) as functions of the number of Monte Carlo cycles. Use both an ordered (all spins pointing in one direction) and a random spin orientation as starting configuration. How many Monte Carlo cycles do you need before you reach an equilibrium situation? Repeat this analysis for $T = 2.4$.

   Make also a plot of the total number of accepted configurations as function of the total number of Monte Carlo cycles. How does the number of accepted configurations behave as function of temperature T?

d) Compute thereafter the probability $P(E)$ for the previous system with $L = 20$ and the same temperatures. You compute this probability by simply counting the number of times a given energy appears in your computation. Start the computation after the steady state situation has been reached. Compare your results with the computed variance in energy σ_E^2 and discuss the behavior you observe.

Near T_C we can characterize the behavior of many physical quantities by a power law behavior. As an example the mean magnetization is given by

$$\langle \mathcal{M}(T) \rangle \sim (T - T_C)^\beta, \tag{10}$$

where $\beta = 1/8$ is a so-called critical exponent. A similar relation applies to the heat capacity

$$C_V(T) \sim |T_C - T|^\alpha, \tag{11}$$

and the susceptibility

$$\chi(T) \sim |T_C - T|^\gamma, \tag{12}$$

with $\alpha = 0$ and $\gamma = 7/4$. Another 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

$$\xi(T) \sim |T_C - T|^{-\nu}. \tag{13}$$

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 scales then as

$$T_C(L) - T_C(L = \infty) = aL^{-1/\nu}, \tag{14}$$

with a a constant and ν defined in Eq. (13). We set $T = T_C$ and obtain a mean magnetisation

$$\langle \mathcal{M}(T) \rangle \sim (T - T_C)^{\beta} \to L^{-\beta/\nu}, \tag{15}$$

a heat capacity

$$C_V(T) \sim |T_C - T|^{-\gamma} \to L^{\alpha/\nu}, \tag{16}$$

and susceptibility

$$\chi(T) \sim |T_C - T|^{-\alpha} \to L^{\gamma/\nu}. \tag{17}$$

e) We wish to study the behavior of the Ising model in two dimensions close to the critical temperature as a function of the lattice size $L \times L$. Calculate the expectation values for $\langle E \rangle$ and $\langle |\mathcal{M}| \rangle$, the specific heat C_V and the susceptibility χ as functions of T for $L = 20$, $L = 40$, $L = 60$ and $L = 80$ for $T \in [2.0, 2.4]$ with a step in temperature $\Delta T = 0.05$ or smaller. Plot $\langle E \rangle$, $\langle 1\mathcal{M}1 \rangle$, C_V and χ as functions of T. Can you see an indication of a phase transition?

Use the absolute value $\langle |\mathcal{M}| \rangle$ when you evaluate χ.

You should parallelize the code using either OpenMP or MPI.

f) Use Eq. (14) and the exact result $\nu = 1$ in order to estimate T_C in the thermodynamic limit $L \to \infty$ using your simulations with $L = 20$, $L = 40$, $L = 60$ and $L = 80$ The exact result for the critical temperature (after Lars Onsager) is $kT_C/J = 2/ln(1+\sqrt{2}) \approx 2.269$ with $\nu = 1$.

Background literature

If you wish to read more about the Ising model and statistical physics here are two suggestions.

1. M. Plischke and B. Bergersen, Equilibrium Statistical Physics, Prentice-Hall, see chapters 5 and 6.

2. M. E. J. Newman and T. Barkema, Monte Carlo methods in statistical physics, Oxford, see chapters 3 and 4.