FYS4150 - Computational Physics
Project 4

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Abstract

Contents

1   Introduction

In fields like thermal dynamics, one will study the phenomena called a *phase transition*. Not only do we study it, but we experience this phenomena on a day-by-day basis. An example of a phase transition is when water turns to steam when we boil the water. More general, a phase transition is when matter changes it's form, either from gas to liquid, or liquid to solid (and vice versa).

We will in this project use a very popular model, the Ising model, to look at the statistical properties of phase transitions analytically. After that, we will use the Metropolis algorithm to see how well it works with the analytical solution and how our system will be for many spins per dimension.

All relevant files can be found in this GitHub page:

`https://github.com/AHo94/FYS3150_Projects/tree/master/Project4`

2   Method

2.1   The Ising model

The Ising model is a mathematical model for magnetic systems in statistical mechanics. We will in this project consider phase transitions at finite temperatures. The energy, for a specific microstate i, is expressed as

$$E_i = -J \sum_{<kl>}^{N} s_k s_l - \mathcal{B} \sum_{k}^{N} s_k \tag{1}$$

With the spins s_k which can take values $s_k = \pm 1$. N is the total number of spins in the system and J is a coupling constant, which we will assume to be $J > 0$. The symbol $< kl >$ indicates that we only sum over the nearest neighbouring spin. That is, we only the spin s_k with the closest spin s_l. $\mathcal{B}$ is an external magnetic field that is interacting with the magnetic moment between neighbouring spins. For simplicity of this project, we will set $\mathcal{B} = 0$.

We also have the magnetization (or magnetic moment) defined as

$$\mathcal{M} = \sum_{j=1}^{N} s_j \tag{2}$$

What we are interested in is the expectation values of the energy $\langle E \rangle$ and the magnetization $\langle \mathcal{M} \rangle$. In order to do that, we will need a probability distribution

$$P_i(\beta) = \frac{e^{-\beta E_i}}{Z} \tag{3}$$

where $\beta = 1/k_b T$, the inverse temperature with k_b as the Boltzmann constant. The partition function Z is given as

$$Z = \sum_{i=1}^{M} e^{-\beta E_i} \tag{4}$$

which sums over all possible microstates M. With these, we can calculate the expectation value of an arbitrary variable x

$$\langle x \rangle = \frac{1}{Z} \sum_i x_i e^{-\beta E_i}$$

$$\langle x^2 \rangle = \frac{1}{Z} \sum_i x_i^2 e^{-\beta E_i}$$

The variance for this variable is then

$$\sigma_x^2 = \langle x^2 \rangle - \langle x \rangle^2$$

We can now use these properties to calculate the heat capacity C_v and susceptibility χ, which are given as

$$C_v = \frac{\sigma_E^2}{k_B T}$$

$$\chi = \frac{\sigma_M^2}{k_B T}$$

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2.2 Metropolis algorithm

In this project, we will use the Monte Carlo algorithm known as the Metropolis algorithm to solve our 2 dimensional lattice numerically.

The algorithm is as following. For each Monte Carlo cycle we do:

- **1)** We start with an arbitrary microstate for the given lattice. We use that microstate to calculate the energy E_b

- **2)** Choose a random spin in the microstate and flip it (e.g, from $\uparrow$ to $\downarrow$). Now we use that state to calculate the energy E_t.

- **3)** Calculate the energy difference $\Delta E = E_t - E_b$.

- **4)** If $\Delta E <= 0$, we accept the new spin configuration and use the energy E_t. What this means is that the energy has been lowered and we are in a lower state.

- **5)** If $\Delta E > 0$, pick a random number r that is given from a uniform distributor in the range $r \in [0, 1]$. Now we have to consider these two cases

- **5a)** If $r <= e^{-\beta \Delta E}$, we accept the new spin configuration and use the energy E_t.

- **5b)** If $r > e^{-\beta \Delta E}$, we reject this new configuration and flip the chosen spin back to it's original state and use the energy E_b.

- **6)** Once that is done, we use the given microstate (depending on the cases given above) to calculate the magnetic moment M_i.

- **7)** Finally, we add the calculated energy and magnetic moment to E_{sum} and M_{sum} respectively. These will the one sample of the Monte Carlo cycle.

We repeat this process N_{mc} times (with N_{mc} as the number of Monte Carlo cycles) and multiple samplings which will be summed into E_{sum} and M_{sum}. Once that is done, we get the mean energies as

$$\langle E \rangle = \frac{1}{N_{mc}} E_{sum} = \frac{1}{N_{mc}} \sum_i E_i$$

With E_i is energy sample of the i'th Monte Carlo cycle. Similar expressions are used for the magnetic moment and their squares.

Combinations of	(s_1, s_2, s_3, s_4)	$s_j = \{\uparrow, \downarrow\} = \{1, -1\}$	
$(\uparrow,\uparrow,\uparrow,\uparrow)$	$(\uparrow,\uparrow,\uparrow,\downarrow)$	$(\uparrow,\uparrow,\downarrow,\uparrow)$	$(\uparrow,\downarrow,\uparrow,\uparrow)$
$(\downarrow,\uparrow,\uparrow,\uparrow)$	$(\uparrow,\uparrow,\downarrow,\downarrow)$	$(\uparrow,\downarrow,\uparrow,\downarrow)$	$(\downarrow,\uparrow,\uparrow,\downarrow)$
$(\downarrow,\uparrow,\downarrow,\uparrow)$	$(\downarrow,\downarrow,\uparrow,\uparrow)$	$(\uparrow,\downarrow,\downarrow,\uparrow)$	$(\uparrow,\downarrow,\downarrow,\downarrow)$
$(\downarrow,\uparrow,\downarrow,\downarrow)$	$(\downarrow,\downarrow,\uparrow,\downarrow)$	$(\downarrow,\downarrow,\downarrow,\uparrow)$	$(\downarrow,\downarrow,\downarrow,\downarrow)$

Table 1: All the microstates possible.

2.3   Simple 2×2 lattice

We will first consider a 2×2 lattice, find the analytical expression for partition function Z and find the corresponding expectation value of energy E, mean magnetization $|M|$, specific heat C_V and susceptibility ξ as functions of temperature T. We also consider periodic boundary condition for this lattice. Once we have the analytical expressions, we will compare them to the numerical values from the Metropolis algorithm.

For this system, we will assume that every spin has two directions, i.e. our states can be either be in spin up state or spin down state (shorthand notation as $\uparrow$ or $\downarrow$ respectively).

The energy of the Ising model, without an external magnetic field $\mathcal{B}$, is given by

$$E_i = -J \sum_{<kl>}^{N} s_k s_l$$

Where $J > 0$ is a coupling constant and N is the total number of spins. The symbol $< kl >$ indicates that we only sum over the neighbours only. The values $s_k = \pm 1$ depends on which state it is in. We let $s_\downarrow = -1$ and $s_\uparrow = 1$. We also have the magnetic moment is given as

$$M_i = \sum_{<k>}^{N} s_k$$

Since we have a $2 \times 2 = 4$ lattice, and we have two spin directions, then the number of microstate (or configuration) is $2^4 = 16$. What this means is that our we can have 16 different energies, as well as 16 different magnetic moment, for each respective microstate. Table 1 shows all the possible microstates.

Figure 1 shows a 2×2 lattice. We see that the point s_1 has s_2 and s_3 as the closest neighbours. Since we are considering periodic boundary conditions, then s_1 will connect to s_2 and s_3 twice. The energy term will then give the term $2(s_1 s_2 + s_2 s_3)$ for the point s_1. It does not include s_4 as it is not the closest neighbour to s_1.
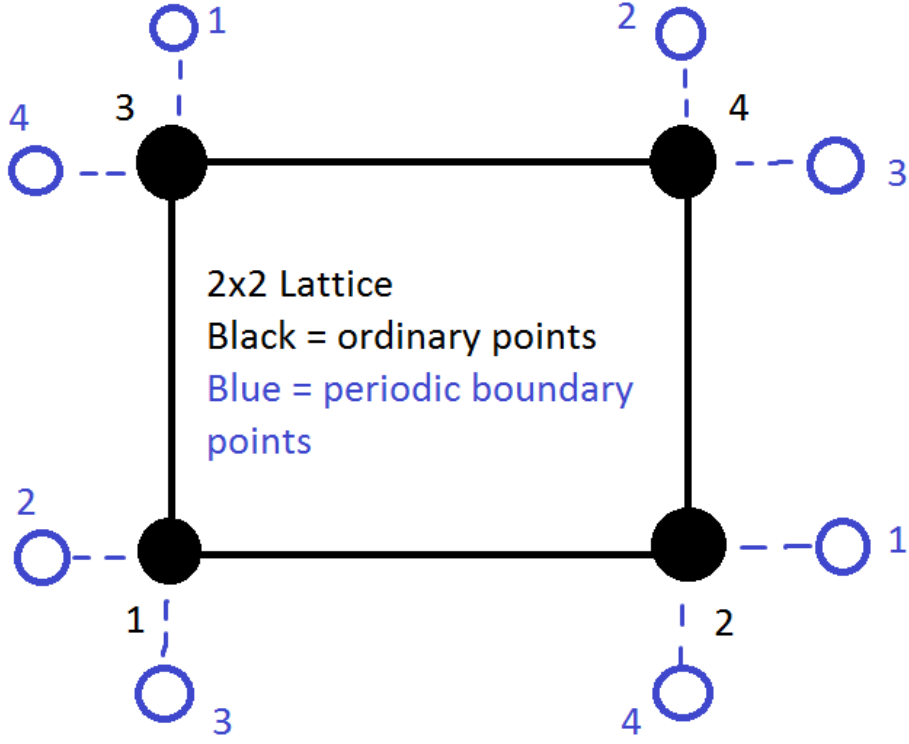
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Figure 1: An illustration of the 2×2 lattice. The black points corresponds to the ordinary points s_1, s_2, s_3, s_4 (as point 1, 2, 3, 4 in the figure respectively). The blue points corresponds periodic boundary points.

We can then continue to add more terms using the three other points, but we need to be careful to not include the connections of the points we previously have considered, which is to prevent double counting. Doing this, the energy for each microstate i will be

$$E_i = -2J \sum_{s_1 = \pm 1} \sum_{s_2 = \pm 1} \sum_{s_3 = \pm 1} \sum_{s_4 = \pm 1} (s_1 s_2 + s_1 s_3 + s_2 s_4 + s_3 s_4) \tag{5}$$

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$E_i =$			
-8J	0	0	0
0	8J	0	0
0	8J	0	0
0	0	0	-8J

Table 2: Energies for each respective microstate.

$M_i =$			
4	2	2	2
2	0	0	0
0	0	0	-2
-2	-2	-2	-4

Table 3: Magnetic moments for each respective microstate.

Similarly for the magnetic moment we get when we sum over all microstates

$$M_i = \sum_{s_1=\pm 1} \sum_{s_2=\pm 1} \sum_{s_3=\pm 1} \sum_{s_4=\pm 1} (s_1 + s_2 + s_3 + s_4) \tag{6}$$

Let us now determine both the energies and magnetic moments for all microstates. Using table 1, we can determine equation (5) and (6) to their respective microstate. Table 2 and 3 shows the energies and magnetic momenta (using the same combinations in table 1) respectively.

Now that we have the energies of each microstate, we can find an analytical expression for the partition function Z given in 4. Using the energies given in table 2, the partition function becomes

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

With the partition function, we can calculate the expectation value of the energy

$$\langle E \rangle = \frac{1}{Z} \sum_i E_i e^{-\beta E_i}$$

Summing over all states i, with the given energies in table 2, we get

$$\langle E \rangle = \frac{1}{Z} \left(2(8J)e^{-8\beta J} + 2(-8J)e^{8\beta J} + 12 \times 0 \times e^0 \right)$$
$$= \frac{-32J\sinh(8\beta J)}{4\cosh(8\beta J) + 12}$$
$$= \frac{-8J\sinh(8\beta J)}{\cosh(8\beta J) + 3}$$

The expectation of the energy squared is then

$$\langle E^2 \rangle = \frac{1}{Z} \sum_i E_i^2 e^{-\beta E_i}$$
$$= \frac{1}{Z} \left(2(8J)^2 e^{-8\beta J} + 2(-8J)^2 e^{8\beta J} + 12 \times (0)^2 e^0 \right)$$
$$= \frac{4(8J)^2 \cosh(8\beta J)}{4\cosh(8\beta J) + 12}$$
$$= \frac{64J^2 \cosh(8\beta J)}{\cosh(8\beta J) + 3}$$

The standard deviation of the energy then becomes

$$\sigma_E^2 = \langle E^2 \rangle - \langle E \rangle^2$$
$$= \frac{64J^2 \cosh(8\beta J)}{\cosh(8\beta J) + 3} - \left(\frac{-8J\sinh(8\beta J)}{\cosh(8\beta J) + 3} \right)^2$$
$$= \frac{64J^2}{\cosh(8\beta J) + 3} \left(\cosh(8\beta J) - \frac{\sinh^2(8\beta J)}{\cosh(8\beta J) + 3} \right)$$
$$= \frac{64J^2}{\cosh(8\beta J) + 3} \left(\frac{\cosh^2(8\beta J) + 3\cosh(8\beta J)}{\cosh(8\beta J) + 3} - \frac{\sinh^2(8\beta J)}{\cosh(8\beta J) + 3} \right)$$
$$= \frac{64J^2}{\cosh(8\beta J) + 3} \left(\frac{1 + 3\cosh(8\beta J)}{\cosh(8\beta J) + 3} \right)$$
$$= \frac{64J^2}{(\cosh(8\beta J) + 3)^2} (4 + \cosh(8\beta J))$$

Dividing by $k_B T$ gives us the specific heat C_V

$$C_V = \frac{1}{k_B T} \left(\langle E^2 \rangle - \langle E \rangle^2 \right) = \frac{64J^2}{k_B T} \frac{(1 + 3\cosh(8\beta J))}{(\cosh(8\beta J) + 3)^2} \tag{7}$$

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We can do similar calculations to obtain the mean magnetization (or the mean absolute value of the magnetic moment), which then gives us

$$\langle |M| \rangle = \frac{1}{Z} \sum_i |M_i| e^{-\beta E_i} = \frac{2(e^{8\beta J} + 2)}{\cosh(8\beta J) + 3}$$

$$\langle M^2 \rangle = \frac{1}{Z} \sum_i M_i^2 e^{-\beta E_i} = \frac{8(e^{8\beta J} + 1)}{\cosh(8\beta J) + 3}$$

Which we can use to calculate the susceptibility χ

$$\chi = \frac{1}{k_B T} \left(\langle M^2 \rangle - \langle |M| \rangle^2 \right) = \frac{8}{k_B T} \frac{(e^{8\beta J} + \cosh(8\beta J) + \frac{3}{2}))}{(\cosh(8\beta J) + 3)^2} \tag{8}$$

Now that we have the analytical expressions, we will later compare it to the numerical values (for a given temperature) from the Metropolis algorithm.

3 Implementation

All programming are done in C++ and data will be saved in a text file. The plotting part will be done in Python.

4 Results

Comparing with the analytical solution

We will now compare the numerical values for C_v and χ with their respective analytical values given in equation 7 and 8. For this case, we will use the temperature $T = 1.0$ in units of kT/J. Running this in C++, with 10^6 Monte Carlo cycles we obtain the following output (Note that the numerical values has not been divided by the number of spins):

```
Number of Monte Carlo cycles = 1000000
Analytic C_v = 0.128329, Numerical C_v = 0.128445
Analytic Chi = 0.016043, Numerical Chi = 0.0162828
```

As we can see, the values are almost identical. The numerical values may change a little bit when we run this multiple times, but still remains fairly close to the analytical values. An example of this can be found in the output below

```
Running multiple times, using MC_cycles = 1000000
Analytic C_v = 0.128329, Numerical C_v = 0.123027
Analytic Chi = 0.016043, Numerical Chi = 0.0156212

Analytic C_v = 0.128329, Numerical C_v = 0.127936
Analytic Chi = 0.016043, Numerical Chi = 0.0154724

Analytic C_v = 0.128329, Numerical C_v = 0.130357
Analytic Chi = 0.016043, Numerical Chi = 0.0164741

Analytic C_v = 0.128329, Numerical C_v = 0.125385
Analytic Chi = 0.016043, Numerical Chi = 0.0152174

Analytic C_v = 0.128329, Numerical C_v = 0.126915
Analytic Chi = 0.016043, Numerical Chi = 0.0156962

Analytic C_v = 0.128329, Numerical C_v = 0.124365
Analytic Chi = 0.016043, Numerical Chi = 0.0159204
```

Using 10^5 Monte Carlo cycles can also give a good numerical result, but it is not as consistent compared to 10^6 Monte Carlo cycles. What that means is that the difference between the analytical and numerical values (for both C_v and χ) may be larger for a lower number of Monte Carlo cycles. The output below shows an example with $N_{mc} = 10^5$. Notice how, for example, the numerical values of C_v can be as low as 0.112442 and as high as 0.160237.

```
Running multiple times, using MC_cycles = 100000
Analytic C_v = 0.128329, Numerical C_v = 0.125194
Analytic Chi = 0.016043, Numerical Chi = 0.0163315

Analytic C_v = 0.128329, Numerical C_v = 0.112442
Analytic Chi = 0.016043, Numerical Chi = 0.0130196

Analytic C_v = 0.128329, Numerical C_v = 0.123282
Analytic Chi = 0.016043, Numerical Chi = 0.0152538

Analytic C_v = 0.128329, Numerical C_v = 0.137304
Analytic Chi = 0.016043, Numerical Chi = 0.0180454
```

```
Analytic C_v = 0.128329, Numerical C_v = 0.125832
Analytic Chi = 0.016043, Numerical Chi = 0.0161317

Analytic C_v = 0.128329, Numerical C_v = 0.160237
Analytic Chi = 0.016043, Numerical Chi = 0.0194764
```

Lattice with L = 20

For the square lattice with $L = 20$ spins, we

The probability distribution

5   Conclusion

References

[1] M. Hjorth-Jensen, *Computational Physics*, 2015, 551 pages