FYS4150 - Computational Physics
Project 4

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Introduction

In fields like thermal dynamics, one will experience a phenomena called phase transitions. A phase transition is is when matter changes it's form. An example of a phase transition is when water turns into ice, i.e, liquid transitions into solid matter. We will in this project study a very popular model, the Ising model, to simulate phase transitions.

Method

Simple 2 $\times$ 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. The boundaries for the lattice will be periodic. We will then compare the Ising model with the analytical expressions later.

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, is given by

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

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.

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 $2\times2 = 4$ 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 $2(s_1s_2 + s_2s_3)$ for the point s_1. It does not include s_4 as it is not the closest neighbour to s_1.

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

$$E_i = -2J \sum_{s_1=\pm1} \sum_{s_2=\pm1} \sum_{s_3=\pm1} \sum_{s_4=\pm1} (s_1s_2 + s_1s_3 + s_2s_4 + s_3s_4) \tag{1}$$

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

$$M_i = \sum_{s_1=\pm1} \sum_{s_2=\pm1} \sum_{s_3=\pm1} \sum_{s_4=\pm1} (s_1 + s_2 + s_3 + s_4) \tag{2}$$

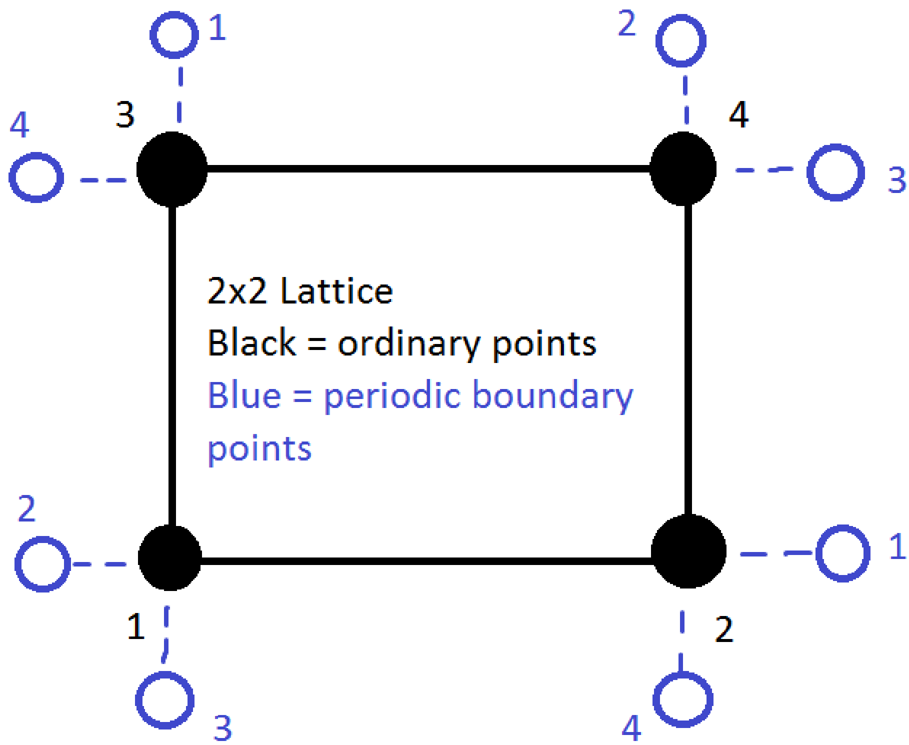

Figure 1: An illustration of the 2×2 lattice. The black points corresponds to the ordinary points s_1, s_2, s_3, s_4 (as point 1, 2, 3, 4 in the figure respectively). The blue points corresponds periodic boundary points.

Let us now determine both the energies and magnetic moments for all microstates. Using table 1, we can determine equation (1) and (2) to their respective microstate. Table 2 and 3 shows the energies and 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. It is defined as

$$Z = \sum_i e^{-\beta E_i}$$

It sums over all microstates i and $\beta = \frac{1}{k_b T}$, with k_b as the Boltzmann constant and T as the temperature. Using the energies given in table 2, the partition

$E_i =$			
-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.

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

$$< E >= \frac{1}{Z}\sum_i E_i e^{-\beta E_i}$$

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

$$\begin{aligned} < E > &= \frac{1}{Z}\left(2(8J)e^{-8\beta J} + 2(-8J)e^{8\beta J} + 12 \times 0 \times e^0\right) \\ &= \frac{-32J\sinh(8\beta J)}{4\cosh(8\beta J) + 12} \\ &= \frac{-8J\sinh(8\beta J)}{\cosh(8\beta J) + 3} \end{aligned}$$

The expectation of the energy squared is then

$$\begin{aligned}
< E^2 > &= \frac{1}{Z}\sum_i E_i^2 e^{-\beta E_i} \\
&= \frac{1}{Z}\left(2(8J)^2 e^{-8\beta J} + 2(-8J)^2 e^{8\beta J} + 12 \times (0)^2 e^0\right) \\
&= \frac{4(8J)^2\cosh(8\beta J)}{4\cosh(8\beta J) + 12} \\
&= \frac{64J^2\cosh(8\beta J)}{\cosh(8\beta J) + 3}
\end{aligned}$$

Implementation

Results

Conclusion

Reference