Computational Physics - Project 4

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Contents

Introduction

In project 4 we are dealing with the Ising model in two dimensions without an external magnetic field. We are looking at a lattice of L times L particles, which have spinvalues ± 1. In order to compute different interesting values, we want to use the metropolis algorithm. With our computations, we want to calculate the Energy, the absolute value of the magnetisation, the heat capacity and susceptibility of the system as a function of time. We also want to compare our solutions with the theoretical closed solution. This project may also show the link from statistical physics to macroscopic properties of a given physical system, which is a very interesting relation.

1 Theory

1.1 General properties of physical systems and their link to statistical physics

1.1.1 physical ensembles

Canonical ensemble is a statistical way to represents the possible states in a system with fixed temperature, whereas the system exchange energy, the energy follows as an expectation value. The probability distribution is given by the Boltzmann distribution.

$$P_i(\beta) = \frac{e^{-\beta E_i}}{Z} \tag{1}$$

$\beta = 1/k_B T$ where T is the temperature, k_B is the Bolztmann constant,E_i is the energy of microstate i and Z is the partition function for the canonical ensemble is the sum over all the microstates M.

$$Z = \sum_{i=1}^{M} e^{-\beta E_i} \tag{2}$$

1.1.2 General properties of canonical ensembles

the canonical ensemble pursuit towards an energy minimum and higher entropy expressed by Helmholtz' free energy.

$$F = -k_B T lnZ = <E> - TS \tag{3}$$

where the entropy S is given by

$$S = -k_B lnZ + k_B T \frac{\partial lnZ}{\partial T} \tag{4}$$

after running the system for long time the canonical ensemble is uniquely determined and does not depend on the arbitrary choices for a given temperature, having a steady state without being affected by the equilibrium continuous motion. the system uncertainty due the Energy fluctuations in the canonical ensemble give the variance of the energy.

from equation 3, 4 and probability distribution P_i

$$<E> = k_b T^2 \frac{\partial lnZ}{\partial T} = \sum_{i=1}^{M} E_i P_i(\beta) = \frac{1}{Z} \sum_{i=1}^{M} E_i e^{-\beta E_i} \tag{5}$$

The heat capacity is how much the energy change due to the change in the temperature. The heat capacity C_V can be defined as

$$C_V = \frac{\partial E}{\partial T} \tag{6}$$

$$\frac{\partial}{\partial T}\frac{1}{Z} = \frac{\partial}{\partial T}\frac{1}{\sum_{i=1}^{M} e^{-\frac{1}{k_B T}E_i}} = -\frac{1}{k_B T^2}\frac{\sum_{i=1}^{M} E_i e^{-E_i \frac{1}{k_B T}}}{\left(\sum_{i=1}^{M} e^{-E_i \frac{1}{k_B T}}\right)^2} = -\frac{1}{k_B T^2}\frac{\sum_{i=1}^{M} E_i e^{-E_i \frac{1}{k_B T}}}{(Z)^2} \tag{7}$$

$$\frac{\partial}{\partial T}\sum_{i=1}^{M} E_i e^{-\frac{1}{k_B T}E_i} = \frac{1}{k_B T^2}\sum_{i=1}^{M} E_i^2 e^{-\frac{1}{k_B T}E_i} \tag{8}$$

$$C_V = \frac{\partial < E >}{\partial T} = \frac{\partial}{\partial T}\left(\frac{1}{Z}\sum_{i=1}^{M} E_i e^{-\frac{1}{k_B T}E_i}\right) = -\frac{1}{k_B T^2}\frac{\sum_{i=1}^{M} E_i e^{-E_i \frac{1}{k_B T}}}{Z^2}\sum_{i=1}^{M} E_i e^{-\frac{1}{k_B T}E_i} + \frac{1}{Z}\frac{1}{k_B T^2}\sum_{i=1}^{M} E_i^2 e^{-\frac{1}{k_B T}E_i} \tag{9}$$

$$= -\frac{1}{k_B T^2}\left(\frac{\sum_{i=1}^{M} E_i e^{-E_i \frac{1}{k_B T}}}{Z}\right)^2 + \frac{1}{Z}\frac{1}{k_B T^2}\sum_{i=1}^{M} E_i^2 e^{-\frac{1}{k_B T}E_i} = \frac{1}{k_B T^2}\left(< E >^2 - < E^2 >\right) \tag{10}$$

The magnetic susceptibility is a measurable quantity which indicate if the material is attracted or repelled out of a magnetic field. magnetic materials can be classified as paramagnetic, diamanetic or ferromagnetic based on their susceptibility.

$$\chi = \frac{\partial < M >}{\partial H} \tag{11}$$

we can evaluate the mean magnetization through

$$< M >= \sum_{i}^{M} M_i P_i(\beta) = \frac{1}{Z}\sum_{i}^{M} M_i e^{-\frac{E_i}{k_B T}} \tag{12}$$

The total energy of the system in addition of external magnetic field H

$$E = -\sum_{i,j} J_{s_i s_j} - H\sum_{i} s_i \tag{13}$$

the magnetization is the sum of all spin for a given configuration.

$$\frac{\partial E_i}{\partial H} = -\sum_{i} s_i = -M_i \tag{14}$$

$$\frac{\partial}{\partial H}\frac{1}{Z} = \frac{\partial}{\partial H}\frac{1}{\sum_{i=1}^{M} e^{-\frac{1}{k_B T}E_i}} = -\frac{1}{k_B T}\frac{\sum_{i=1}^{M} M_i e^{-E_i \frac{1}{k_B T}}}{\left(\sum_{i=1}^{M} e^{-E_i \frac{1}{k_B T}}\right)^2} = -\frac{1}{k_B T}\frac{\sum_{i=1}^{M} M_i e^{-E_i \frac{1}{k_B T}}}{(Z)^2} \tag{15}$$

$$\frac{\partial}{\partial H}\sum_{i=1}^{M} M_i e^{-\frac{1}{k_B T}E_i} = \frac{1}{k_B T}\sum_{i=1}^{M} M_i^2 e^{-\frac{1}{k_B T}E_i} \tag{16}$$

$$\chi = \frac{\partial < M >}{\partial H} = \frac{\partial}{\partial H}\left(\frac{1}{Z}\sum_{i=1}^{M} M_i e^{-\frac{1}{k_B T}E_i}\right) = -\frac{1}{k_B T}\frac{\sum_{i=1}^{M} M_i e^{-E_i \frac{1}{k_B T}}}{Z^2}\sum_{i=1}^{M} M_i e^{-\frac{1}{k_B T}E_i} + \frac{1}{Z}\frac{1}{k_B T}\sum_{i=1}^{M} M_i^2 e^{-\frac{1}{k_B T}E_i} \tag{17}$$

$$= -\frac{1}{k_B T}\left(\frac{\sum_{i=1}^{M} M_i e^{-E_i \frac{1}{k_B T}}}{Z}\right)^2 + \frac{1}{Z}\frac{1}{k_B T}\sum_{i=1}^{M} M_i^2 e^{-\frac{1}{k_B T}E_i} = \frac{1}{k_B T}\left(< M >^2 - < M^2 >\right) \tag{18}$$

1.1.3 Ferromagnetic order

A ferromagnet have a spontaneous magnetic moment even with the absence of an external magnetic field. Due the existence of a spontaneous moment the electron spin and magnetic moments must be arranged in a regular manner. ferromagnet all spin aligned, antiferromagnet all spin align with neighboring pointing in opposite directions, ferrimagnet the opposing moments are unequal , etc.

1.1.4 link from the Macroscopic values to statistical physics

1.2 theoretical numerical solutions

1.2.1 Ising model

Ising model is a mathematical model for ferromagnetism studies of phase transitions for magnetic system at given a temperature. The model consists the interaction between two neighbouring spins is related by the interaction energy

$$-Js_k s_l \tag{19}$$

where the sin s can be in two states +1 or -1,where s_k and s_l are the nearest neighbors. Which give a low energy (-J) if the two spin aligned and high energy (j) for spin pointing in opposite direction. The total energy to a system with N number of spins and with the absence of magnetic field can be expressed as

$$E = -J \sum_{<kl>}^{N} s_k s_l \tag{20}$$

...probability distribution with expectation value <E> ...

1.2.2 Periodic boundary conditions

Periodic boundary conditions is used for approximating a large or infinite system by using smaller repeating system, we will impose PBCs on our spin lattice in x and y directions. satisfied s(L+1,y) = s(1,y)
s(x,L+1) = s(X,1)

1.2.3 Metropolis algorithm in the two dimensional Ising model

The Ising model with Metropolis algorithm generates a sequence of states with Monte Carlo path, where the transition between states depends on the transition probability between the next and current state. The probability distribution is given by the Boltzmann distribution which is the probability for finding the system in a state s.

$$Ps = \frac{e^{-\beta E_i}}{\sum_{i=1}^{M} e^{-\beta E_i}} \tag{21}$$

It is difficult to compute since we need the sum over all states. If we have a 10 x 10 spin lattice interacting in our Ising model, there are 2^{100} possible states. Computing the sum seems to be not that efficient, but luckily the Metropolis algorithm needs only the ratios between the state probabilities and we do not need to compute the sum of all the states after all. The Metropolis algorithm in this case can be implement by establishing two dimensional Ising model with random lattice configuration. Then we flip a randomly chosen spin and compute the energy difference ΔE. If $\Delta E \le 0$ we accept the flip, otherwise we compute the transition probability $w = e^{-}\beta\Delta E$ and compare with a random number r.
If $r \le w$ we accept the flip otherwise we keep the old configuration. We can keep choosing new random spins until we are satisfied with a good representation of the states.(compare to"lecture notes Computational physics 2015 at University of Oslo by Morten Hjorth-Jensen page 435)"

1.2.4 critical temperature (Lars Onsager)

in 1944 the Norwegian chemist Lars Onsager made very important discovery in theoretical physics, namely the exact solution of the Ising spin model in two dimensions. His work is up to now a valid theoretical description of the two dimensional Ising model. Onsager's solutions achieved the thermodynamic properties of interaction systems and phase transitions at T_c. However in 1942 Lars Onsager solved the two dimensional model for zero field energy, which has been published two years after. In 1948, he wrote the solution for the zero field magnetization in a conference at Cornell. Onsager showed how to derive the partition function for the canonical ensemble with zero external magnetic field Z(B = 0,T)with N spins.

$$Z_N = \left(2cosh(\beta J)e^I\right)^N \tag{22}$$

where $I = \frac{1}{2\pi}\int_0^\pi d\phi ln\left[\frac{1}{2}\left(1+\sqrt{1-\kappa^2 sin^2\phi}\right)\right]$ where $\kappa = \frac{2sinh(2\beta J)}{cosh^2(2\beta J)}$ and the energy is given by

$$< E >= -Jcoth(2\beta J)\left[1 + \frac{2}{\pi}(2tanh^2(2\beta J) - 1)K_1(q)\right] \tag{23}$$

where $q = sinh(2\beta J)/cosh^2(2\beta J)$ and the complete elliptic integral of the first kind is:

$$k_1(q) = \int_0^{\frac{\pi}{2}} \frac{d\phi}{\sqrt{1-q^2 sin^2\phi}} \tag{24}$$

and differentiating the energy with the respect to temperature we obtain the specific heat:

$$C_v = \frac{\partial < E >}{\partial T} = \frac{4K_B}{\pi}(\beta Jcoth(2\beta J))^2\left\{K_1(q) - K_2(q) - (1 - tanh^2(2\beta J))\left[\frac{\pi}{2} + (2tanh^2(2\beta J) - 1)K_1(q)\right]\right\} \tag{25}$$

where

$$k_2(q) = \int_0^{\frac{\pi}{2}} d\phi \sqrt{1 - q^2 sin^2\phi} \tag{26}$$

Near the critical temperature T_c the specific heat behaves as:

$$C_v \approx -\frac{2}{\pi}\left((\frac{2J}{K_B T_c} \right)^2 ln\left[1 - \frac{T}{T_c} \right] + const. \tag{27}$$

$$C_v \sim \left[1 - \frac{T}{T_c} \right]^{\alpha} \tag{28}$$

the limiting form of the function

$$\lim_{\alpha \to 0} \frac{1}{\alpha}(Y^{-\alpha} - 1) = -lnY \tag{29}$$

can be used to infer that closed-form result in low singularity with $\alpha = 0$. Onsager's result can be written as:

$$< \frac{M(T)}{N} >= \left[1 - \frac{(1 - tanh^2(\beta J))^4}{16 tanh^4(\beta J)} \right]^{\frac{1}{8}} \tag{30}$$

for $T < T_c$. otherwise the magnetization is zero "lecture notes Computational physics 2015 at University of Oslo by Morten Hjorth-Jensen page 435)"

1.3 Closed solution for a 2 dimensional 2 x 2 lattice

We want now to look at a 2 x 2 lattice and we want to calculate the partition function, the energy, magnetisation, heat capacity and susceptibility of the system dependent of T. The partition function for a canonical ensemble with periodic boundary conditions can be computed by:

$$Z = \sum_{i=1}^{M} e^{-\beta E_i} \tag{31}$$

Here, β is $\frac{1}{k_b \cdot T}$, where k_b is the Bolzmann constant. In this expression we sum over all microstates m. The Energy of the system in configuration i is then:

$$E_i = -J \sum_{<kl>}^{N} s_k s_l \tag{32}$$

The sum over $< kl >$ means that we only sum over nearest neighbours. In our 2 x 2 case, we have for each "particle" two possible values ± 1. This means that we have all in all $2^{2 \cdot 2} = 2^4 = 16$ micro states. We have to compute the Energy of the micro states in order to compute the partition function. We also want to introduce the magnetisation, which is simply the sum over all the spins of the system:

$$M_i = \sum_{j=1}^{N} s_j \tag{33}$$

We want also to introduce the so called degeneracy, which counts the number of micro states for a given micro energy. We get the following table: We can now write the expression of the partition function as in equation 36. We used the

Figure 1: Energy of the different micro states

Number of spins up (+1)	Degeneracy	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

Table 1 to calculate the sum over the micro states.

$$Z = \sum_{i=1}^{M} e^{-\beta E_i} = 12 \cdot e^{-\beta \cdot 0} + 2 \cdot e^{-8J\beta} + 1 \cdot e^{8J\beta} + 1 \cdot e^{8J\beta} \tag{34}$$
$$= 12 + 2 \cdot e^{-8J\beta} + 2 \cdot e^{8J\beta} \tag{35}$$
$$= 12 + 4 \cdot \cosh\left(8J\beta\right) \tag{36}$$

We can now calculate the expectation value of the energy. There are two possible ways of calculating it. the first way of calculating the expectation value of the energy can be seen in equation 38.

$$< E > = -\frac{\partial ln(Z)}{\partial \beta} = -\frac{1}{Z} \cdot 32J \cdot \sinh(8J\beta) \tag{37}$$
$$= -\frac{32J \cdot \sinh((8J\beta)}{Z} \tag{38}$$
$$= -\frac{8 \cdot J \cdot \sinh(8J\beta)}{3 + \cosh(8J\beta)} \tag{39}$$

Alternatively, we can calculate the expectation value of the Energy by looking at the micro states:

$$< E >= -\frac{1}{Z} \sum_{i=1}^{M} E_i e^{-\beta E_i} = -\frac{8 \cdot J \cdot \sinh(8J\beta)}{3 + \cosh(8J\beta)} \tag{40}$$

Both expressions are equal. Next, we want to determine the expectation value of the magnetisation. We use the formula 42. We can see that we get 0 for the expectation value of the magnetisation.

$$< M > = \frac{1}{Z} \sum_{i}^{M} M_i \cdot e^{-\beta E_i} \tag{41}$$
$$= \frac{1}{Z} \cdot \left(4 \cdot 1 \cdot e^{-8J\beta} + 2 \cdot 4 + (-2) \cdot 4 + (-4) \cdot 1 \cdot e^{-8J\beta}\right) \tag{42}$$
$$= 0 \tag{43}$$

However, we are interested in the expectation value of the absolute value of magnetisation, which is $< |M| >$. This expression can be determined as follows:

$$< |M| > = \frac{1}{Z} \sum_{i}^{M} |M_i| \cdot e^{-\beta E_i} \tag{44}$$
$$= \frac{1}{Z} \cdot \left(|4| \cdot 1 \cdot e^{-8J\beta} + |2| \cdot 4 + |(-2)| \cdot 4 + |(-4)| \cdot 1 \cdot e^{-8J\beta}\right) \tag{45}$$
$$= \frac{1}{Z} \cdot \left(8 \cdot e^{-8J\beta} + 8\right) \tag{46}$$
$$= \frac{2 \cdot e^{-8J\beta} + 2}{3 + \cosh(8J\beta)} \tag{47}$$

In order to describe how the temperature will change when thermal energy is added to the system, we want to look at a quantity called heap capacity. (C_v) The bigger this quantity is the less heats the system up by a given amount of thermal energy, which is added to the system.

$$C_v = \frac{1}{k_b T^2} \left(\frac{1}{Z} \sum_{i=1}^{M} E_i^2 e^{-\beta E_i} - \left(\frac{1}{Z} \sum_{i=1}^{M} E_i e^{-\beta E_i} \right)^2 \right) \tag{48}$$
$$= \frac{1}{k_b T^2} \left(\frac{1}{Z} \left(2 \cdot (8J)^2 \cdot e^{8J\beta} + 2 \cdot (-8J)^2 \cdot e^{-8J\beta}\right) - \left(\frac{8 \cdot J \cdot \sinh(8J\beta)}{3 + \cosh(8J\beta)} \right)^2 \right) \tag{49}$$
$$= \frac{1}{k_b T^2} \left(\frac{64 \cdot J \cdot \cosh(8J\beta)}{3 + \cosh(8J\beta)} - \left(\frac{8 \cdot J \cdot \sinh(8J\beta)}{3 + \cosh(8J\beta)} \right)^2 \right) \tag{50}$$
$$= \frac{1}{k_b T^2} \left(\frac{64 \cdot J + 3 \cdot J \cdot 64\cosh(8J\beta)}{\left(3 + \cosh(8J\beta)\right)^2} \right) \tag{51}$$
$$= \frac{64}{k_b T^2} \left(\frac{J + 3J \cdot \cosh(8J\beta)}{\left(3 + \cosh(8J\beta)\right)^2} \right) \tag{52}$$
$$\tag{53}$$

At last, we wan to have a look at the magnetic susceptibility. This quantity is a magnetic property of the material. The magnetic susceptibility describes the response of the material to an applied magnetic field.

$$\chi = \frac{1}{k_b T} \cdot \left(\frac{1}{Z} \sum_{i=1}^{M} M_i^2 e^{-\beta E_i} - \left(\frac{1}{Z} \sum_{i=1}^{M} M_i e^{-\beta E_i} \right)^2 \right) \tag{54}$$

$$= \frac{1}{k_b T} \cdot \left(\frac{1}{Z} \cdot \left(4^2 \cdot 1 \cdot e^{-8J\beta} + 2^2 \cdot 4 + (-2)^2 \cdot 4 + (-4)^2 \cdot 1 \cdot e^{-8J\beta} \right) - (0)^2 \right) \tag{55}$$

$$= \frac{1}{k_b T} \cdot \frac{32 e^{-8J\beta} + 32}{12 + 4 \cdot \cosh(8J\beta)} \tag{56}$$

$$= \frac{1}{k_b T} \cdot \frac{8 e^{-8J\beta} + 8}{3 + \cdot \cosh(8J\beta)} \tag{57}$$

$$\tag{58}$$

1.4 infinite size effect

1.5 everything related to parts c and later

This part is not structured yet

2 Execution

3 Comparison and discussion of results

4 source code