FYS 4150 -Computational Physics-Project 4

Studies of phase transitions in magnetic systems with Ising model

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Abstract

The phase transitions in magnetic systems is simulated using two dimensional Ising model with Metropolis algorithm and run with parallelism.First the analytical values for a 2 X 2 lattice is calculated and compared with numerical calculation for 2 X 2 lattice . Thermodynamic parameters such as the energy E, the mean magnetization $\mathscr{M}$, the specific heat C_V and the susceptibility χ of the system is studied as functions of the temperature T for lattice sizes 40 X 40 , 60 X 60 and 80 X80 . The phase transition of the Ising model is studied and the critical temperature T_C is calculated and compared with the analytical value of Onsager [3] at 2.2692kB/J. The value was calculated as 2.26kB/J. The python code is available at github.[1]

1 Introduction

The Ising model[1] is a mathematical model of ferromagnetism in statistical physics. The model consists of discrete variables that represent magnetic dipole moments of atomic "spins" that can be in one of two states ($+1$ or -1). The spins are arranged in a lattice (where the local structure repeats periodically in all directions), allowing each spin to interact with its neighbors. The energy of the lattice is described by the sum of internal magnetic moment interaction between neighbouring dipoles. Heat can disturb this tendency, thus creating the possibility of different structural phases. The two-dimensional square-lattice Ising model is one of the simplest statistical models to show a phase transition. Ising model unders goes second order phase transition when approaching the Curie temperature[3] for infintely large lattice. After this critical point, the lattice becomes a paramagnet.

2 Theory

2.1 Ising Model

The Ising model describes the behavior of a magnetic material depending on its thermal energy and an external magnetic field. It is assumed that our system is represented as a lattice made by a squared grid of atoms, which spin can be either -1 or $+1$.

$$s = \{-1, +1\} \tag{1}$$

Now each particle internal magnetic field can interact with its surrounding particles and the energy given by the interaction of the magnetic spins as

$$E = -J \sum_{<kl>}^{N} s_k s_l - \mathscr{B} \sum_{k}^{N} s_k \tag{2}$$

where J is a constant expressing the strength of the interaction between spins and the notation $< kl >$ means that the sum has to be computed on neighboring particles only. For simplicity , it is assumed that there is no external magnetic field $\mathscr{B}$. The magnetic moment of a certain configuration is then defined as

$$M = \sum_{k}^{N} s_k \tag{3}$$

[1] `https://github.com/jeyalakt/4150COMP_PHY/tree/master/project4`

Suppose we have system $\mathcal{S}$ with a fixed temperature T and no interaction with its surrounding envirorment, meaning no exchange of heat/energy. The system will keep its shape, number of particle and the total energy is conserved. Thus, in other words we have thermal equilibrium at all time. The probability of a state or configruation i for a given energy configruation E_i (in our case E_i is from equation (**??**)), the probability distribution function is defined by boltzmann statistics

$$P(E_i) = \frac{1}{Z} e^{-\beta E_i} \tag{4}$$

where $\beta = 1/(k_b T)$ is inverse of temperature multiplied with Boltzmans constant, and Z is the partition function for the canonical ensemble given by,

$$Z = \sum_{i=1}^{N} e^{-\beta E_i} \tag{5}$$

The expectation value of the energy can then be calculated from the probability distribution with

$$\langle E \rangle = \sum_{i=1}^{N} \frac{1}{Z} e^{-\beta E_i} \tag{6}$$

i indicates all the possible microstate.

The other thermodynamical parameters are given as follows: Mean Magnetisation:

$$\langle M \rangle = \sum_{i=1}^{N} \frac{1}{Z} e^{-\beta M_i} \tag{7}$$

As these involve the partition function,even for a small lattice size of 2 X 2 a sum over 2^{2^4} elements.So we need to explore other ways of calculating it. Other Interesting parameter are given as follows: heat capacity :

$$C_v = \frac{\mathrm{Var}(E)}{kT^2} = \frac{\langle E^2 \rangle - \langle E \rangle^2}{k_b T^2} \tag{8}$$

Where $\langle E^2 \rangle$ is the expectation value of squared energy and $\langle E \rangle$ is the expectation value of energy.

$$C_V = \frac{1}{k_b T^2} \big(\langle E^2 \rangle - \langle E \rangle^2 \big) \tag{9}$$

Susceptibility:

$$\chi = \frac{\mathrm{Var}(M)}{k_b T} = \frac{\langle M^2 \rangle - \langle M \rangle^2}{k_b T} \tag{10}$$

$$\chi = \frac{1}{k_b T} \big(\langle \mathscr{M}^2 \rangle - \langle |\mathscr{M}| \rangle^2 \big) \tag{11}$$

The temperature is taken to be in units of k_b/J, where k_b is Boltzmans constant, and J is the potential energy from magnetic interaction between two spins. The lengths between the lattice elements is assumed to be baked into the dependence of magnetization for the energy.

2.2 Metropolis algorithm

The Metropolis algorithm[2] is based on Markov Chains, where a system evolves from one state to another by transition probabilities. we consider only the probability ratio of two different energy states, the so called acceptance ratio, dentoed as $A_{i \to j}$. Meaning we are looking at a lattice in some state jumping to another state, by flipping a random spin $\mathcal{S}$. Thus

$$A_{i \to j} = \frac{P(E_j)}{P(E_i)} = \frac{e^{-\beta E_j / Z}}{e^{-\beta E_i / Z}} = e^{-\beta (E_j - E_i)} = e^{-\beta \Delta E} \tag{12}$$

To accept this jump and update the thermodynamical quantitites, the acceptance ratio $A_{i \to j}$ must be lower than a random number ζ

$$\zeta \leq e^{-\beta \Delta E} \tag{13}$$

Metropolis algorithm is used to simulate spin flipping. It is implemented as follows: An initial configuration is assumed to begin with , which could be either a random or a all-up configuration (both cases are simulated and tested) and compute the energy of the whole system.

Then a random position in the spin matrix is picked and the energy of the lattice is computed after having flipped the chosen spin.

The energy of the system before and after the flip is compared; if it has decreased, the move is accepted, otherwise it is accepted with a probability of $e^{-\beta\Delta E}$, where ΔE is the difference of the two energies and β is $\frac{1}{kT}$

The final configuration is now taken as the initial configuration and the process is repeated

This algorithm is implemented for different values of temperature between $\frac{k_bT}{J} = 1$ and $\frac{k_bT}{J} = 2.4$ and for different sizes of the lattice from a 2×2 one (for which the analytical values are computed) to a 80×80 one. Periodic boundary conditions have been applied.

The Ising model undergoes a phase transition of second order, i.e. below a critical temperature T_C (Curie temperature) the system has a spontaneous magnetization, being $\langle \mathscr{M} \rangle \neq 0$, while above T_C $\langle \mathscr{M} \rangle = 0$. $\langle \mathscr{M} \rangle$ is normally called the order parameter.

2.3 Studies of phase transitions

As proven later by the famous Norwegian theoretical physcisit and chemist, Lars Onsager, there exist phase transitions in two dimensional Ising model when reaching the curie tempeature[3]. Meaning that for a random confiqurated square lattice (with no external magnetic field exterted on it) for low temperatures the system will be in a ferromagnetic state until it has reached the curie temperature where it undergoes a second order phase transition and become paramagnet where it looses its ability to self magnetize. Near this critical or so called curie temperature, T_C, we can use simple power law approximation to show how different thermodynamical quantities behave. Consider the following mean expressions mean magnetization:

$$\langle M(T) \rangle \sim |T_C - T|^{\beta} \tag{14}$$

Where $\beta = 1/8$. A similar relation can applies also for the heat capacity and magnetic susceptbility Heat capacity:

$$C_V \sim |T - T_C|^{\alpha} \tag{15}$$

Where $\alpha = 0$ Susceptibility:

$$\chi \sim |T - T_C|^{\gamma} \tag{16}$$

$\gamma = 7/4$. The exponent α, β, γ are the so-called critical exponents. The Curie temperature is dependant on the lattice size i.e number of spins/particles, when increasing the the number of spins L and the curie temperature T_C converges to a certain value when $L \to \infty$. Ideally this is impossible to simulate and we have chosen only do simulations from $L = 40$ to $L = 80$ to save time. But through so-called finite scale sizing relations , it is possible to relate the behaviour of finite and infintely large lattice and we can estimate the Curie temperature . The Curie temperature scales then as

$$T_C(L) - T_C(L \to \infty) = aL^{-1/\nu} \tag{17}$$

Where ν can be calculated from $\xi \sim |T_c - T|^{-\nu}$ and a is some constant. In order to find a estimate for $T_C(L)$ we must find out what the constant a is, to do so we can look at the difference for two lattices L_1 and L_2. Consider

$$aL_1^{-1/\nu} - aL_2^{-1/\nu} = (T_C(L_1) - T_C(L_1 \to \infty)) - (T_C(L_2) - T_C(L_2 \to \infty)) \tag{18}$$

Notice when $L_1, L_2 \to \infty$ there basicly identical, thus $T_C(L_1 \to \infty) = T_C(L_2 \to \infty)$. This will cancel each other out. Solving with respect to a, we will obtain the following expression

$$a = \frac{T_C(L_1) - T_C(L_2)}{L_1^{-1/\nu} - L_2^{-1/\nu}} \tag{19}$$

Using this expression for a in (17), and solve it for $L(L \to \infty)$

$$T_C(L \to \infty) = T_C(L) - \frac{T_C(L_1) - T_C(L_2)}{L_1^{-1/\nu} - L_2^{-1/\nu}} L^{-1/\nu} \tag{20}$$

The Curie temperature can be observed when we observe a significant change at which the second order phase transition are characterized by a divergent magnetic susceptibility and heat capacity. A analytical solution has been achieved for ν by Lars Onsager and is of the form:

$$T_C(L \to \infty) = \frac{2}{\ln(1 + \sqrt{2})} \approx 2.269 \tag{21}$$

3 Analytical solution of 2 X 2 lattice

First we consider a system of 2×2 square lattice. We have total of four spins, where each spin have two spin orientation, $\{+1, -1\}$. Meaning we have $2^4 = 16$ lattice configruations. Using periodic boundary conditions we can obtain these lattice configruations states and their corresponding energy and magnetic moment as

Number of ↑	Regeneracity	Energy	Magnetic moment
4	1	$-8J$	4
3	4	0	2
2	2	$8J$	0
2	4	0	0
1	4	0	-2
0	1	$-8J$	-4

The partition function for these configruations is

$$Z = \sum_{i=1}^{16} e^{-\beta E_i} = 2e^{8\beta J} + 2e^{-8\beta J} + 12 = 4\cosh(8\beta J) + 12 \tag{22}$$

The probability distribution function for this system from eqn 4 ,
Mean expaction value, $\langle E \rangle$, and the expectation value of sqaured energy, $\langle E^2 \rangle$. are given as ,
eqrefexpect val, thus

$$\langle E \rangle = \frac{2(-8J)e^{-8\beta J} + 2(8J)e^{8\beta J}}{Z} \tag{23}$$

$$\langle E \rangle = \frac{4(-8J\sinh(8\beta J))}{4\cosh(8\beta J) + 12} \tag{24}$$

$$\langle E \rangle = \frac{-8J\sinh(8\beta J))}{\cosh(8\beta J) + 3} \tag{25}$$

and the squared energy

$$\langle E^2 \rangle = \frac{1}{Z}\sum_{i}^{16} E_i^2 P(E_i) = \frac{64J^2\cosh(8\beta J)}{\cosh(8\beta J) + 3} \tag{26}$$

Using the analytical expression (8) presented in previous section, the solution of the heat capacity becomes

$$C_V = \frac{\sigma_E}{k_b T^2} \tag{27}$$

where variance $\sigma_E = \langle E^2 \rangle - \langle E \rangle^2$.
The expectation value of the magnetic moment is given as

$$\langle M \rangle = \frac{1}{Z}\sum_{i}^{16} M_i P(E_i) = 0 \tag{28}$$

Expectation value of absolute magnetic moment is calculated as

$$\langle |M| \rangle = \frac{1}{Z}\sum_{i}^{16} |M|_i P(E_i) = \frac{2e^{8\beta J} + 4}{\cosh(8\beta J) + 3} \tag{29}$$

and the squared magnetic moment

$$\langle M^2 \rangle = \frac{1}{Z} \sum_{i}^{16} M_i^2 P(E_i) = \frac{8e^{8\beta J} + 8}{\cosh(8\beta J) + 3} \tag{30}$$

Using this and the analytical expression from (10), the magnetic susceptibility becomes

$$\chi = \frac{\sigma_{|M|}}{k_b T} = \tag{31}$$

where variance$\sigma_{|M|} == \langle |M|^2 \rangle - \langle |M| \rangle^2$.

4 Implementation, Results and Discussion

To avoid problems at the boundary the particles on the boundary are allowed to interact with particle on the opposite end, to achieve a continuous force/field exchange and avoid discontinuities. Code for the Ising model using the metropolis algorithm and periodic boundary conditions was written in Python with Parallelization.

Given a size of the lattice grid L , the value of mean energy , mean magnetisation , heat capacity as functions of T $\langle M(T) \rangle$ was calculated

The algorithm for transitioning to a new state is to flip one random spin, check the transition probability due to changes in energy w and comparing this to a random number r between 0 and 1. If the transition probability is higher than the random number w$>$ r then we perform the transition and update the energy, magnetization and spin matrix

4.1 Results and Discussion

4.1.1 2 x 2 Case

The data calculated is tabulated and compared them with the analyticl values :

n	Eexact	Ecalc	CV_exact	CV-calc	sus_exact	sus_calc	Mabs_exact	Mabs_calc
100	-7.983928	-8	0.128329	0	0.016043	0	3.994643	4
1000	-7.983928	-7.992	0.128329	0.063936	0.016043	0.015984	3.994643	3.996
10000	-7.983928	-7.9848	0.128329	0.121369	0.016043	0.011181	3.994643	3.9956
100000	-7.983928	-7.98464	0.128329	0.122644	0.016043	0.018089	3.994643	3.99442
1000000	-7.983928	-7.984352	0.128329	0.124939	0.016043	0.015645	3.994643	3.99478

Figure 1: Data for L 2X 2allup spin

n	Eexact	Ecalc	CV_exact	CV-calc	sus_exact	sus_calc	Mabs_exact	Mabs_calc
100	-7.983928	-7.92	0.128329	0.6336	0.016043	0.1584	3.994643	3.96
1000	-7.983928	-7.992	0.128329	0.063936	0.016043	0.003996	3.994643	3.998
10000	-7.983928	-7.9904	0.128329	0.076708	0.016043	0.011987	3.994643	3.9964
100000	-7.983928	-7.98456	0.128329	0.123282	0.016043	0.013217	3.994643	3.99522
1000000	-7.983928	-7.983856	0.128329	0.128891	0.016043	0.01649	3.994643	3.994556

Figure 2: Data for L 2X 2 random spin

it is observed that for 2X 2 random spin case, the estimated value of all parameters are compatible with analytical values to third leading digit (for susceptiblity,second leading digit) at Montecarlo cycles 10^6 itself.

For all up case , the values for E and Mabs starts agreeing to analtyical value to second leading digit only after Montecarlo cycles 10^6 and the values of heat capacity and susceptibilty are not converging even at that.

4.1.2 Study of transitory states and equilibrium, 20 x 20 case

Now a bigger lattice of size 20 X 20 is chosen. We want to analyze how much time (number of MC cycle) is needed in order to reach an equilibrium position. After equillibrium is reached,some expectation values of the system are computed . The steps for doing this are the following.
First we set $T = 1$ and all the spin of the matrix pointing upwards. Then we make the calculation of Energy and susceptibility as as a function of Monte Carlo cycles. Also the number of accepted cycles is plotted as a function of Monte Carlo cycles. This is repeated with T= 1 and random spin configuration .

In the next step same experiment is repeated setting $T = 2.4$ and using a all up spin and random-spin-matrix configuration
Parallelisation with Numba package was used through out all the codes and experiments as it was not possible to run the codes without parallelisation in Python.
we can observe that after 15000 cycles , the state reaches equilibrium state for all up configuration and there is almost no difference for different temperature values. For random configuration, it reaches equilibrium state earlier at 10^4 cycles for higher temp T =2.4. The number of accepted cycles increase linearly with number of monte carlo cycles. since the metropolis algorithm is based on the comparison between a random number and the factor $e^{-\frac{\Delta E}{T}}$, the number of accepted points will grow with the temperature

For lattice size 20 X 20 , for temperature T =1 and 2.4, for different number of montecarlo cycles , resulting expectation values (energy and magnetisation) were plotted.

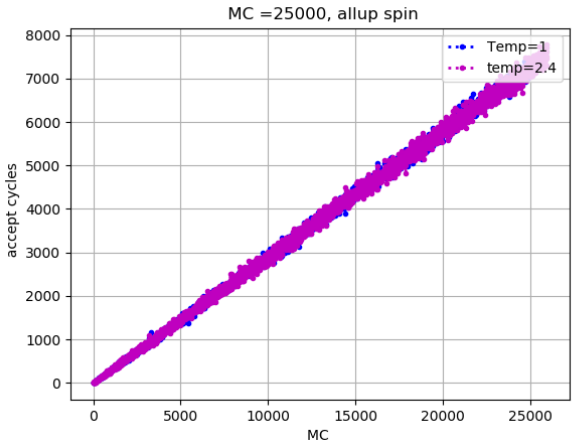

Figure 3: L20 X 20 allup spin

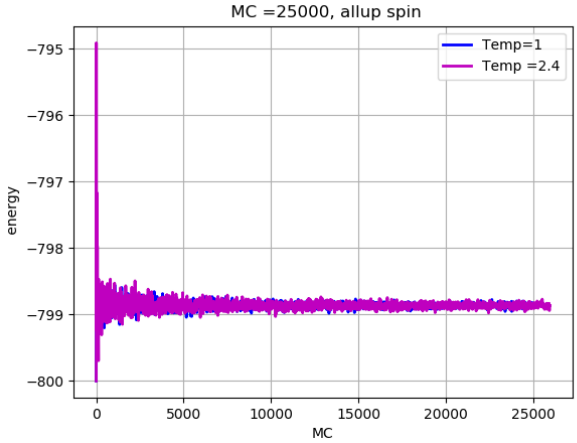

Figure 4: L20 X 20 allup spin

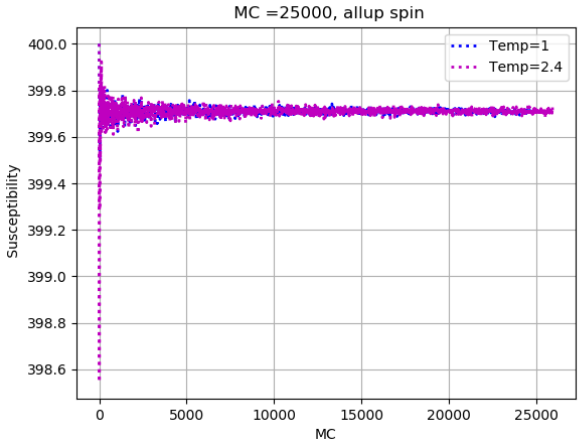

Figure 5: L20 X 20 allup spin

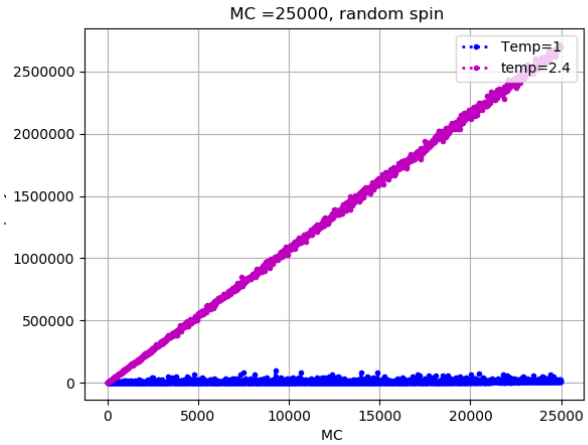

Figure 6: L 20 X 20 random spin

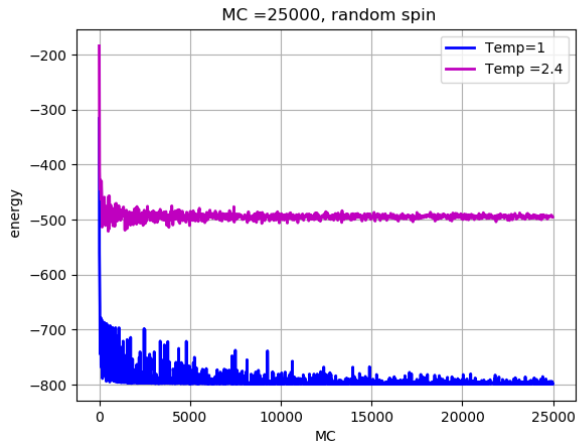

Figure 7: L 20 X 20 random spin

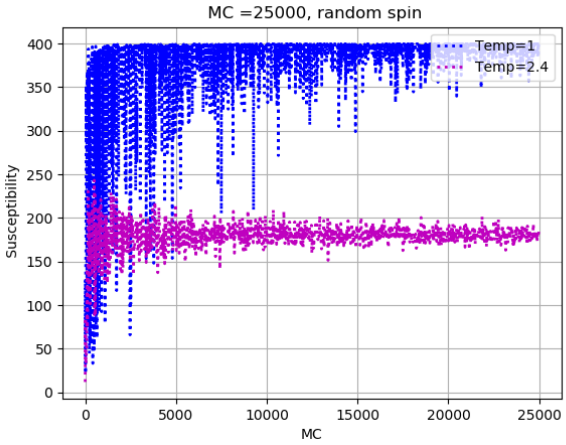

Figure 8: L 20 X 20 random spin

4.1.3 Probability distribution of energy

The probability distribution of energy after reaching steady state condition were recorded. This is done by calculating the number of times the given energy appears in the computation .The histogram is plotted for Lattice size 20 in allup and random spin initial configuration for temperature T= 1 and 2.4 . It is observed that the initial configuration does not have significant impact .

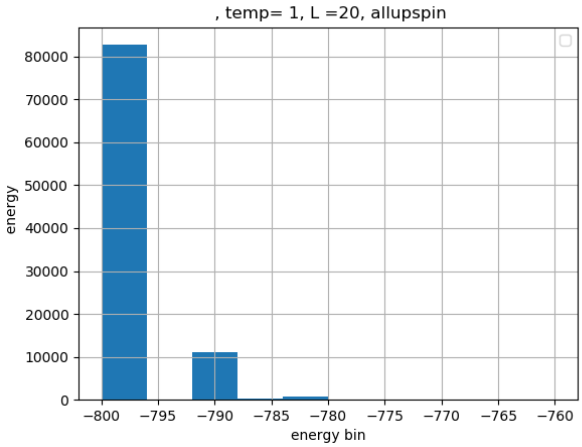

Figure 9: L 20 X 20 allup spin, T=1

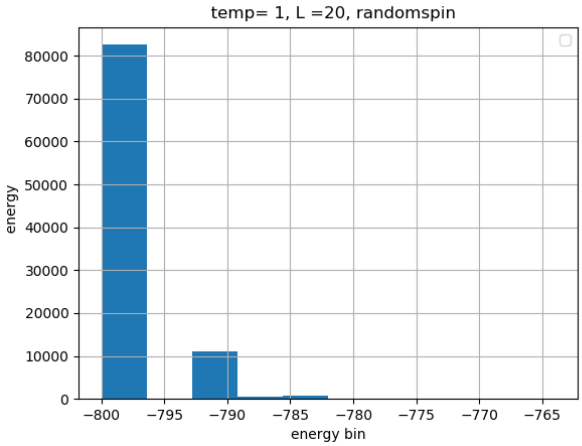

Figure 10: L 20 X 20 random spin, T=1

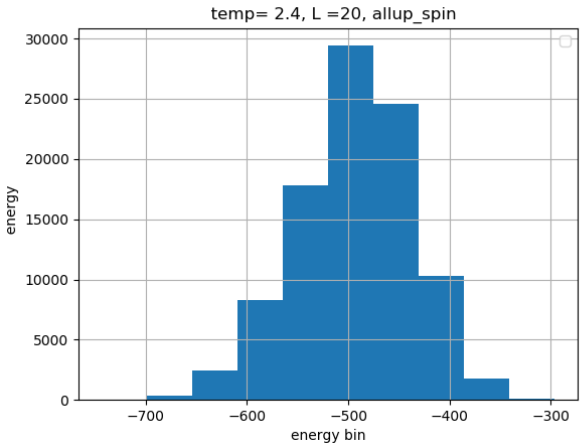

Figure 11: L 20 X 20 allup spin, T=2.4

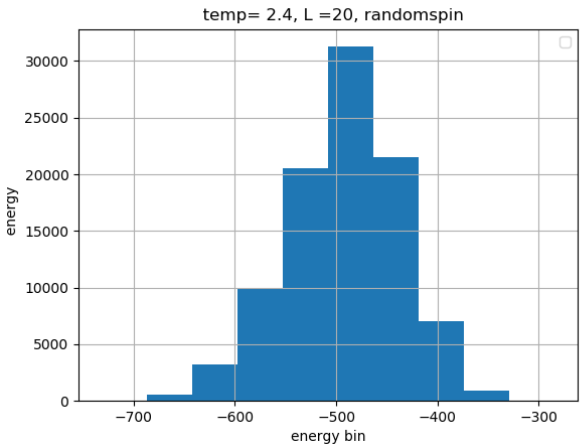

Figure 12: L 20 X 20 random spin, T=2.4

4.2 Bigger dimension matrices- Phase transition and Critical Temperature

4.2.1 Phase Transition

The algorithm is applied to bigger size matrices, respectively 40×40,60×60, 80×80, matrices in order to make our model more realistic and simulate towards infinite lattice size. For each case the values of E, $\mathscr{M}$, C_V, χ are plotted for different values of the absolute temperature $\frac{k_b T}{J}$ in the range between 2.0 and 2.6 in steps of 0.001 .

The phase transition is clearly visible in all plots except the energy plot.

Calculations carried on with bigger matrices resulted in more realistic results, especially for heat capacity and susceptibility, where the peak corresponding to the phase shift gets more sharp as the matrix size grows.

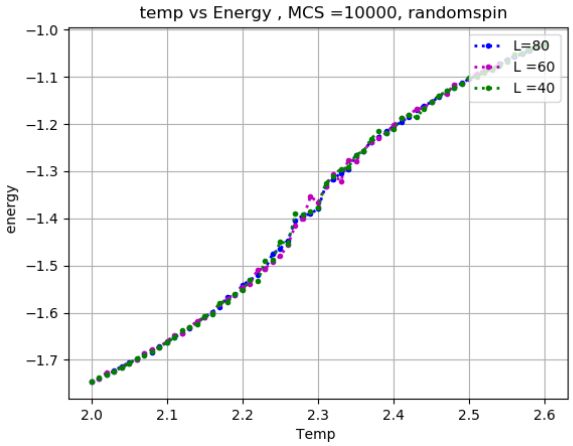

Figure 13: L2X2randomspin

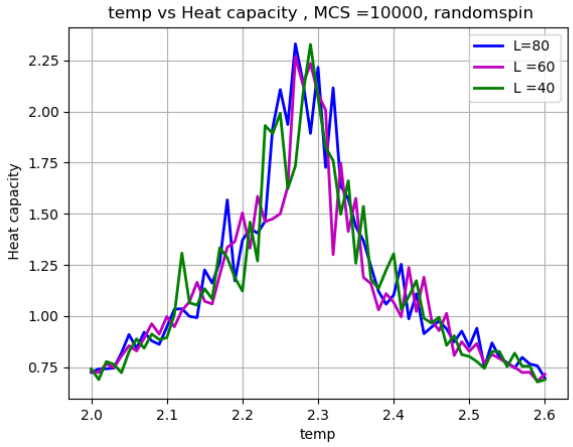

Figure 14: L2X2randomspin

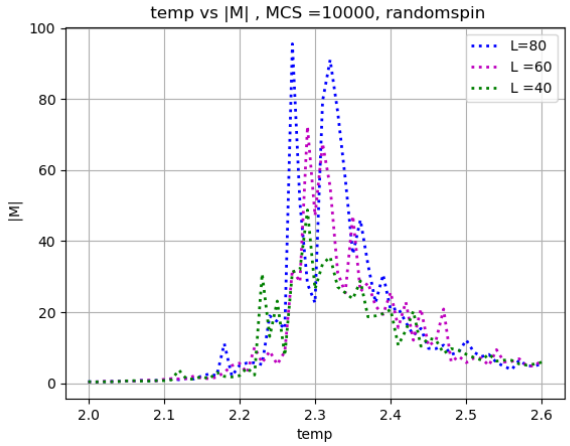

Figure 15: L2X2randomspin

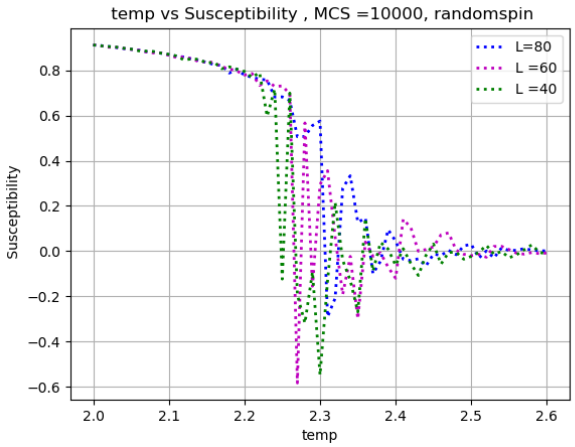

Figure 16: L2X2randomspin

4.2.2 Critical Temperature

Referring to the graphs showing heat capacity and susceptibility , it is clear that the estimate for T_C (i.e. the value of T for which these quantities have their maximum value) decreases as the size of the matrix grows and its value is roughly around the expected value ~ 2.269 [3] The critical temperature was found from the highest value of susceptibility as tabulated below:.

$Latticesize$	$TC(criticaltemp)$
40	2.266
60	2.252
80	2.263

Using the produced result and the constant a in (19)

$$a = \frac{T_C(L_1) - T_C(L_2)}{L_1^{-1/\nu} - L_2^{-1/\nu}} \tag{32}$$

Using $L1 = 80$ and $L2 = 40$ with $\nu = 1$, we can estimate this constant to be

$$a \approx 0.24 \tag{33}$$

And using (17) for $L = 80$, we get that

$$T_C(L \to \infty) = 2.263 - \frac{0.24}{80} \approx 2.26 \tag{34}$$

The theoretical value predicted by Onsager[3] is ≈ 2.269. Using this we can calculate the relative error is

$$\epsilon_{rel} = 100\% \frac{|2.269 - 2.26|}{2.269} \approx 0.396\% \tag{35}$$

Which indicates that the calculated results are towards theoretical value.

5 Parallelization

As the lattice size increased and to calculate the parameters with reasonable number of Monte carlo cycles it was mandatory to use parallelisation in Python . Without parallelisation it was not even possible to run the code for lattice size 40 X 40 in a reasonable amount of time . Attempt to use the `multiprocessing` module and `Process` function resulted in unexplainable frequent hangs of the Computer similar to the experience in Project 3 . But parallelistion was effectiely achieved with `Numba` package with very reliable and faster execution time in a laptop with 8 processors . The execution time with parallelisation is as given below. We can observe a time gain of app.100

$Latticesize$	$MCcycles$	$Processor$	$Exetime(sec)$
20	1000	1	96.437
20	1000	8	2.203
20	5000	1	598.54
20	5000	8	7.684
60	10000	1	impractical to get exe time
60	10000	8	48.6325

6 Conclusions

It looked like an almost impossible task to study a physical system which evolves to equilibrium state whose PDF's normalisation factor is impossible to find, analytical calculations are not possible, transition probability is not known . But this was achieved with Metropolis algorithm as a reliable simulation for a spin lattice experiencing phase transition described by the Ising model, being more realistic as the size of the lattice increases. All physical quantities taken in account have varied as expected in relation to the temperature around T_C and their behavior for larger matrices is reasonably clear.
Estimation of the value of the critical temperature for an infinite dimension lattice also resulted in a value which is compatible with the theoretical one.
Fairly good optimization of the code using parallelization was achieved for higher dimension simulations in reasonable time in Python. Figure 14 shows the clearest example of a second order phase transition in our Ising model, especially for higher grid sizes.

The different errors have not been quantified like the statistical error and also the selection of condition of steady state as 15 $\%$ of total Monte carlo cycles also may be studied further for different values.

Though choice of Python looks unsuitable for higher dimension lattice sizes , i could satisfactorily simulate the expected results using parallelisation with `Numba` Package in Python for lattice size 80 x 80. It could have been attempted to provide a single program for all sections of problems in Project4.

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