FYS3150/FYS4150 Computational Physics - Project 4

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This project aims to study the properties of ferromagnetism, such as equilibrium process, probability distribution of energy in two different phases and phase transition behavior near the critical temperature using two-dimensional Ising model and Monte Carlo simulations. Statistical properties of the system for difference lattice sizes were studied with the parallel Ising model. The system reached steady state in lower energy levels and higher magnetization at temperature below the critical temperature, and reached steady state in higher energy levels and lower magnetization at temperature above the critical temperature, with larger variance. Transition of magnetic phase is also included in this study. The Ising model with the parallel simulated the first and the second order phase transition with the range of temperature T = [2.20, 2.36]. It apparently results the more pronounced critical temperature for larger lattice sizes. The critical temperature extracted from the simulations with finite lattices is found to be in fairly well agreement with Onsager's exact value.

I Introduction

Ferromagnetic materials exhibit characteristic phase transition behaviors at the critical temperature(T_C). It is identified with discontinuity of energy and magnetization (first-order phase transition), and divergence of heat capacity(C_v) and magnetic susceptibility (second-order phase transition). The non-equilibrium state of the matter is not fully understood, yet models to simulate the transition behaviors were developed. It is possible to find the analytic expressions of expectation values and variances of energy and magnetization for one or two-dimension model, (Onsager, 1944) but for three and higher dimensions, numerical method is the only possible approach. Therefore, study of ferromagnetism with numerical methods stands in great importance.

In this project, simulation of magnetic phase transition of ferromagnetism is studied with Ising model in two dimensions. The small 2×2 spin lattice is first studied. The numerical

results for mean energy, heat capacity, mean magnetization and susceptibility are compared with the analytical calculations to ensure that the model properly reproduces the expected results. Next we move on to 20×20 system and study the equilibration of physical quantities as functions of time steps, as well as the probability distribution of mean energy at the equilibrium state in two different temperatures, each lying below and above T_C. Phase transition behavior around the critical temperature was reproduced with 20×20, 40×40, 60×60, 80×80 and 100×100 sized lattices. Critical temperature for infinite-sized lattice is estimated with the results from finite-sized lattices, using power law relations.

II Method

2.1 Ising model

The system being studied in the project can be modeled with Ising model with discrete spin variables in a lattice structure. The energy of the system is expressed as

$$E = -\sum_{<kl>}^{N} J_{kl} s_k s_l - \mu \sum_{k}^{N} h_k s_k,$$

while s indicating the spin, J_{kl} being a coupling constant for each spin site, N being the total number of spins, μ being the magnetic moment and h_k indicating the external magnetic field interacting with each spin site. $<kl>$ indicates the summation over the nearest neighbors.

In this project, we take two-dimensional square lattice with periodic boundary condition. We also take the simplest form of the expression above. Namely, the coupling constant J is assumed as the same for all spin sites and the contribution of external magnetic field is ignored. The simplification makes

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

with J now being universal.

The probability of the system being found in a state i is given as the Boltzmann distribution of E_i

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

while E_i indicating the energy at a given spin configuration i and Z being the partition function which sums over all M spin configurations,

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

Expectation value and variance of energy and magnetization can be calculated with the probability expression above. With the expression for magnetization for a given spin configuration i being

$$M_i = \sum_{k=1}^{N} s_k,$$

expectation value of energy $< E >$, specific heat at constant volume C_V, expectation value of absolute magnetization $<|\mathcal{M}|>$ and magnetic susceptibility χ is expressed as below.

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

$$C_v = \frac{\sigma_E}{k_B T^2} = \frac{< E^2 > - < E >^2}{k_B T^2}$$

$$< |\mathcal{M}| > = \frac{1}{Z} \sum_{i=1}^{M} \mathcal{M}_i e^{-\beta E_i}$$

$$\chi = \frac{\sigma_{\mathcal{M}}}{k_B T} = \frac{< \mathcal{M}^2 > - < |\mathcal{M}| >^2}{k_B T}$$

These are the main physical quantities that is studied in this project.

2.2 Markov chain and Monte Carlo method, with Metropolis algorithm

With the model introduced above, we mimic the system behaving with the rule of energy minimization and entropy maximization. In order to do this, the Markov process is implemented using Monte Carlo simulations with Metropolis algorithm.

Markov process is described with normalized probability distribution vector ω and stochastic matrix W. The next probability distribution ω_i is determined by current state ω_j and the stochastic matrix W_{ij}. In this project, the same approach is implemented with spin matrix, which serves as the state matrix, and the Monte Carlo simulation with

Metropolis algorithm, which serves as the stochastic matrix. The first state of spin matrix is given as a guess, either as ground state or random state.

The metropolis algorithm is a useful technique. We do not need to reach all possible microstates in the system. The algorithm allows us to figure out the energy difference between the initial state and a new proposed state, then apply the difference to an acceptance routine.

The Monte Carlo cycles with Metropolis algorithm is implemented as below.

1. Generate a starting state
2. Generate a trial mode
3. Check the energy difference between the proposed state against the starting state
4. Calculate probability $w = e^{-\beta \Delta E}$ and compare with the random number

   if $r \leq w$, we accept the new state, if not keep the old value.
5. Find the new expectation values
6. Repeat the step 1-5 (applying the Monte Carlo cycles)

The expected values from the few first step of the Monte Carlo cycles vary. This cause the large error in the results. In order to get rid of this error, we will accept the values after it reach the most likely state (equilibrium state). The values of interest, energy and magnetization will be plotted as a function of number of the Monte Carlo cycles. Then, we will select the number of cycles where the graph trends to be stable.

2.3 Power-law relation of critical temperature (T_C)

The critical temperature of infinitely large lattice can be calculated with the results from finite-size lattice(L) as below,

$$T_C(L) - T_C\left(L = \infty\right) = aL^{-\frac{1}{\nu}}$$

where a is a constant and the exponent constant ν is given as 1 (Onsager, 1944). We get critical temperature of finite lattice by taking the temperatures where extremum point of energy and magnetization lie, and averaging the two. Then we obtain the value of constant a which generates the least variance of calculated $T_C\left(L = \infty\right)$s. With the constant, we

calculate $T_C\left(L=\infty\right)$ with different lattices and take the average. The estimated value is compared with Onsager's exact calculation, $k_BT_C/J = 2/\ln\left(1+\sqrt{2}\right) \approx 2.269$.

2.4 Implementations

The codes for programs are written in C++ and Fortran. For simulations in 3.4, codes are parallelized in 4 processors using MPI. All relevant codes and data files are available at:

https://github.com/minjukum/FYS3150-Computational-Physics/tree/master/Project4

III Results and discussions

3.1 Ising model of 2x2 lattice

3.1.1 Analytical expressions

Here we find the analytical expressions for 2×2 spin lattice, which will be compared with the numerical results. All the spin configurations are described in Table 1.

Table 1. Spin configurations, degeneracy, energy and magnetization of 2×2 spin lattice. Different configurations with same energy and magnetization is denoted as degenerated.

Configuration	Degeneracy	Energy	Magnetization
↑ ↑ ↑ ↑	1	-8J	4
↓ ↑ ↑ ↑	4	0	2
↓ ↓ ↑ ↑	4	0	0
↓ ↑ ↑ ↓	2	8J	0
↓ ↓ ↓ ↑	4	0	-2
↓ ↓ ↓ ↓	1	-8J	-4

Using formulae in 2.1, we get

$$\boldsymbol{Z} = e^{\frac{8J}{k_BT}} + 4 + 4 + 2\times e^{-\frac{8J}{k_BT}} + 4 + e^{\frac{8J}{k_BT}}$$

$$< \boldsymbol{E} > = \frac{1}{Z}(1\times(-8J)\times e^{\frac{8J}{k_BT}} + 2\times 8J\times e^{-\frac{8J}{k_BT}} + 1\times(-8J)\times e^{\frac{8J}{k_BT}})$$

$$\boldsymbol{C_v} = \frac{1}{k_BT^2}(1\times 64J^2\times\frac{e^{\frac{8J}{k_BT}}}{Z} + 2\times 64J^2\times\frac{e^{-\frac{8J}{k_BT}}}{Z} + 1\times 64J^2\times\frac{e^{\frac{8J}{k_BT}}}{Z} - \frac{1}{Z^2}\left(1\times(-8J)\times e^{\frac{8J}{k_BT}} + 2\times 8J\times e^{-\frac{8J}{k_BT}} + 1\times(-8J)\times e^{\frac{8J}{k_BT}}\right)^2)$$

$$< |\boldsymbol{\mathcal{M}}| > = \frac{1}{Z}(1\times 4\times e^{\frac{8J}{k_BT}} + 4\times 2 + 4\times 2 + 1\times 4\times e^{\frac{8J}{k_BT}})$$

$$\boldsymbol{\chi} = \frac{1}{k_BT}(1\times 16\times\frac{e^{\frac{8J}{k_BT}}}{Z} + 4\times 4\times\frac{1}{Z} + 4\times 4\times\frac{1}{Z} + 1\times 16\times\frac{e^{\frac{8J}{k_BT}}}{Z} - \frac{1}{Z^2}\left(1\times 4\times e^{\frac{8J}{k_BT}} + 4\times 2 + 4\times 2 + 1\times 4\times e^{\frac{8J}{k_BT}}\right)^2)$$

3.1.2 Numerical results

Now we implement the codes for 2x2 spin lattice. The initial state is set as the ground state, namely, all spins in the upward direction. The results for T = 1.0 (in units of k_BT) is compared with the analytical calculation in Table 2 with different number of Monte Carlo cycles. Note that all values are presented in the unit of "per spin," and the energy is dimensionless, namely in units of [energy /J].

Table 2. Comparison of numerical results with analytical calculations. It shows good agreement to the third-fourth leading digit with 10^6 Monte Carlo cycles.

$\boldsymbol{N}$	$< \boldsymbol{E} >$	$\boldsymbol{C_v}$	$< \lvert\boldsymbol{\mathcal{M}}\rvert >$	$\boldsymbol{\chi}$
Analytical	-1.9959821	0.032082332	0.99866073	0.0040107395
$\mathbf{10^2}$	-2	0	1	0
$\mathbf{10^3}$	-2	0	1	0
$\mathbf{10^4}$	-1.9946	0.04308336	0.9982	0.00538704
$\mathbf{10^5}$	-1.9964	0.02874816	0.99882	0.00347443
$\mathbf{10^6}$	-1.995962	0.032238778	0.9986535	0.004033748

10^7	-1.996008	0.031881856	0.99866685	0.004000391

From Table 2, we can see that with 10^6 Monte Carlo calculation, the numerical results show good agreement with the analytical ones to the third leading digit for all quantities. The plot for expectation value of energy with varying N below (Figure 1) shows that the analytical value shows acceptable accordance with numerical results after 10^4 MC cycles. It eventually falls within the error range of numerical result and shows a good agreement from 10^6 cycles.

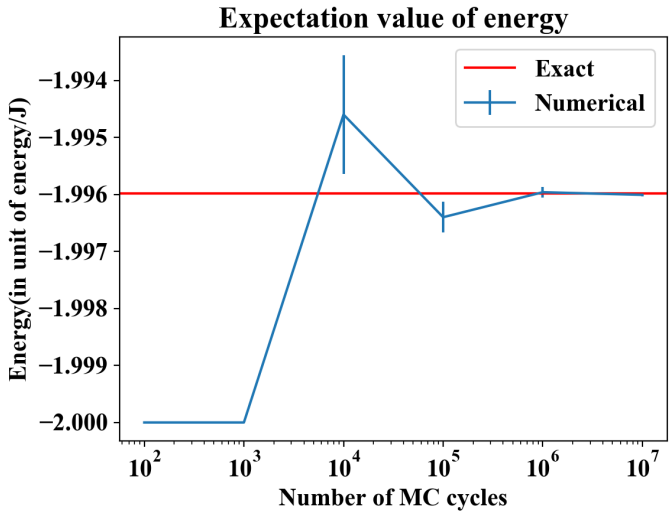


Figure 1. Expectation value of energy with different numbers of Monte Carlo cycles. Error bar indicates the standard deviation of expectation value of energy, calculated based on the central limit theorem. It is shown that the analytical (labeled as "Exact") result shows acceptable accordance with numerical result from 10^4 cycles. It eventually falls within the error range of numerical results and achieves good agreement from N=10^6.

3.2 Equilibration of the system

Here we look more into the equilibration behavior of the system, including the time needed for the system to reach the most likely state, which can be considered proportional to the number of MC cycles. Figure 2 shows the evolution of expectation values of energy and magnetization of 20×20 spin lattice with increasing MC cycles, which denotes time, at two different temperatures; T=1.0 and T=2.4, and from two different initial conditions; ground state and random state. T=1.0 is in fact below the critical temperature which is to

be derived in later section, and T=2.4 is above the critical temperature. It is read that in low temperature(T=1.0), the system evolves to low-energy state close to -2.0, and in most cases the spin configurations are found to be ordered to one direction. In higher temperature(T=2.4) the system evolves to relatively higher-energy state, and the spin configurations are more disordered. The initial state being chosen as a ground state and a random state is physically equivalent to taking an object of 0K(ground state) or infinitely high temperature(random state) to a room at T=1.0 or T=2.4, and the object achieving the thermal equilibrium with the environment.

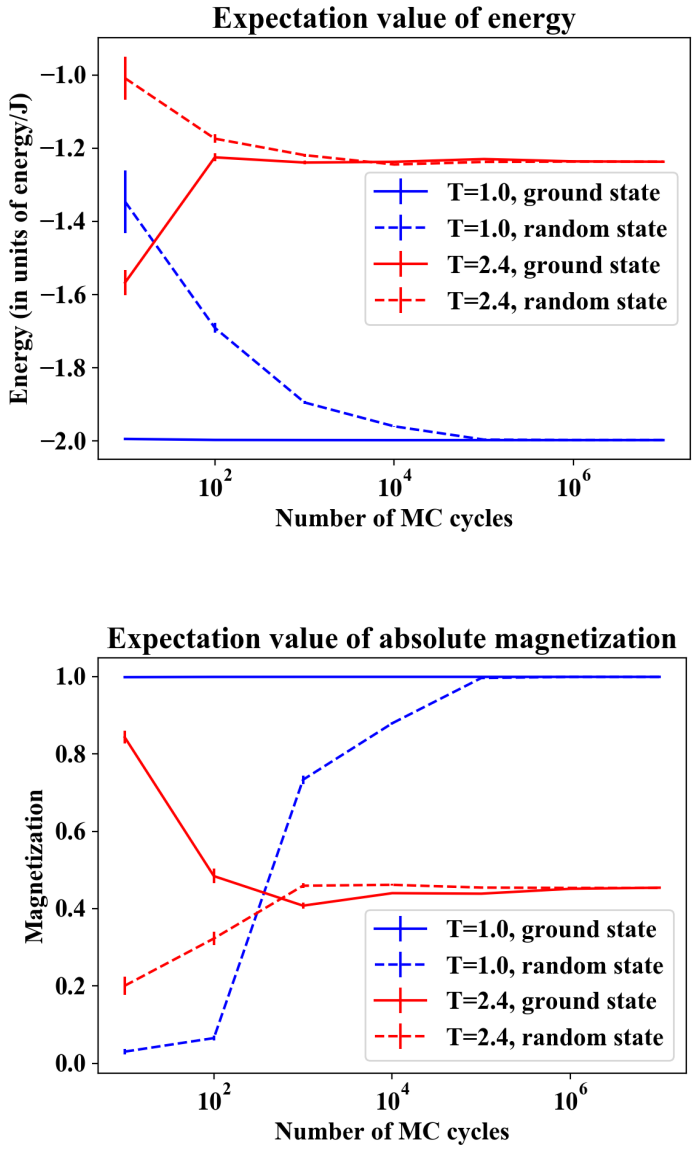


Figure 2. Evolution of expectation values of energy(above) and absolute magnetazation(below) with increasing number of MC cycles. Blue denotes T=1.0 and red denotes T=2.4. Two initial states are tested, ground state(solid line) and random state(dashed line). Error bar denotes the standard deviation of expectation

values, calculated based on the central limit theorem. In the first figure we see that at T=1.0 the system evolves to the low-energy state close to -2.0, and at T=2.4 the system evolves to the higher-energy state around -1.2. Magnetization evloves to near 1.0 at low temperature while it converges to lower value around 0.4 at higher temperature, which indicates higher entropy. Both graph shows good enough convergence from 10^6 Monte Carlo cycles.

3.3 Probability distribution

Here we study the probability distribution of expectation value of energy after the equilibrium is reached. The 20x20 lattice system is simulated at T=1.0 and T=2.4 with 10^7 Monte Carlo cycles, with taking the last 9×10^6 effective Monte Carlo samples. Since the system is studied after the equilibrium state is reached, the initial state, which is set as the ground state in this case, is considered to have no contribution to the result. In Figure 4, probability distribution of total energy of the system is presented. At low temperature, T=1.0, energies are distributed in low-energy states, with mean value being -798.87 and variance being 9.32(STD=3.05). At higher temperature, T=2.4, energies are distributed in higher-energy states and more spread out. The mean value is -494.90 with variance being 3250.72(STD=57.02). The result seems to well reproduce energy distribution following the Boltzmann distribution.

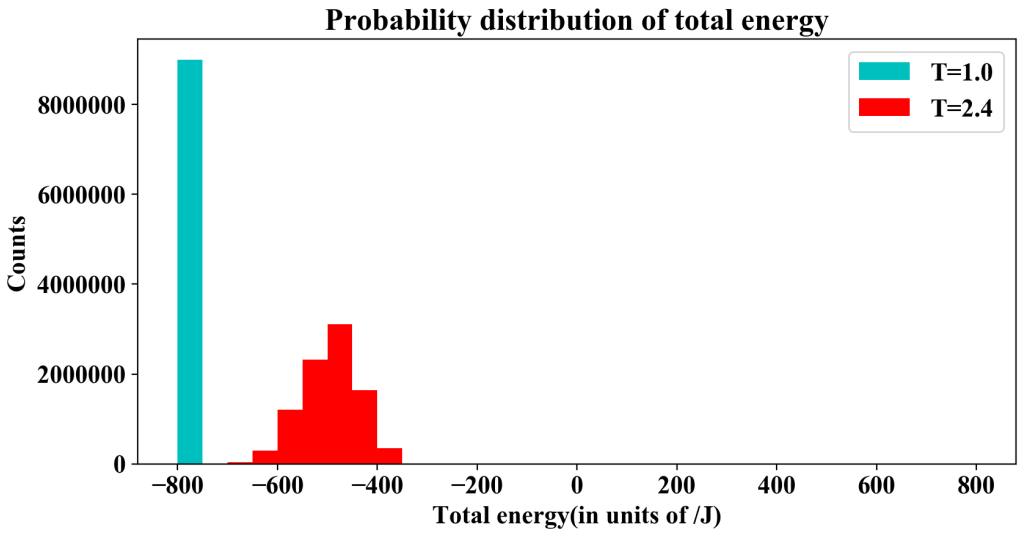
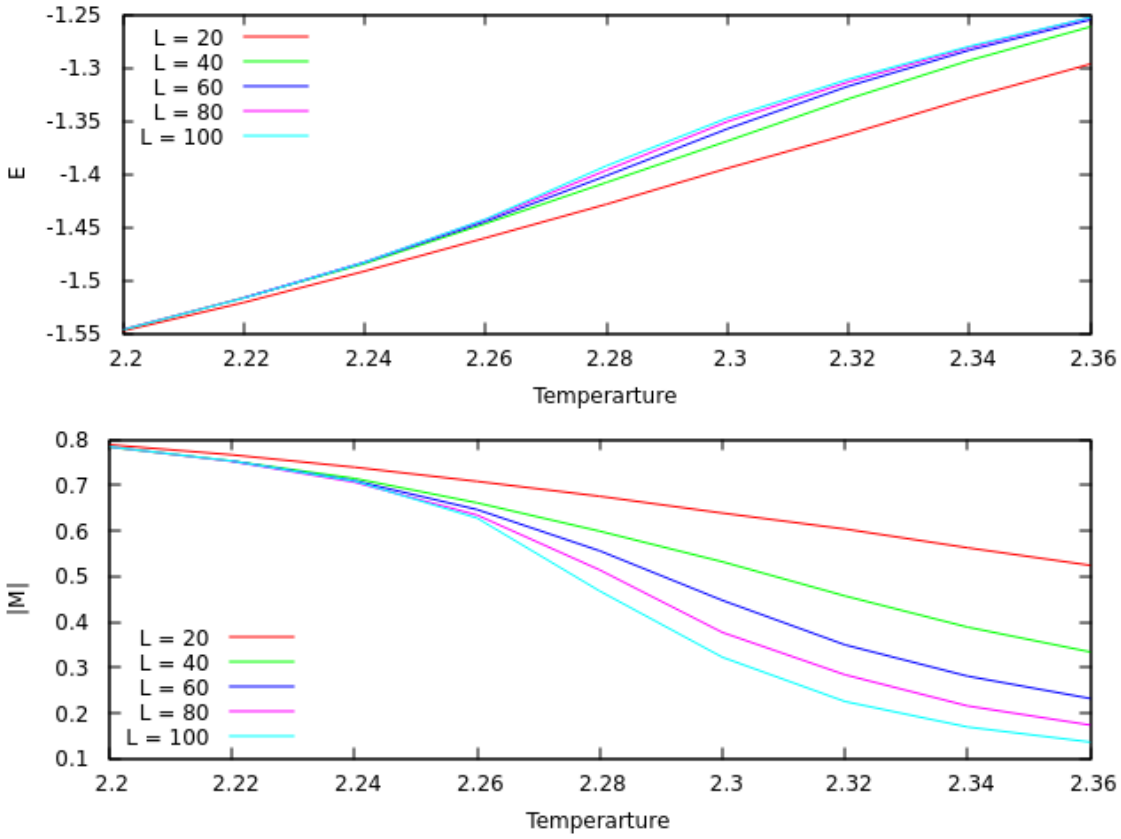


Figure 4. Probability distribution of total energy at T=1.0(cyan) and T=2.4(red). At T=1.0, all energies are falling into a single bin (from -800 to -750), while at T=2.4 the mean is shifted to higher energy level and more spread out. Total counts are 9×10^6 for each case.

3.4 Phase transitions and the critical temperature

Phase transitions analysis was conducted with the Ising model with five difference sizes of lattices (20×20, 40×40, 60×60, 80×80 and 100×100). All expected values were simulated over a temperature range T = [2.20, 2.36] where we expect the critical temperature for phase transition. The step of temperature is 0.02, and each temperature step was simulated with 10^6 Monte Carlo cycles discarding the first 10^4 cycles.



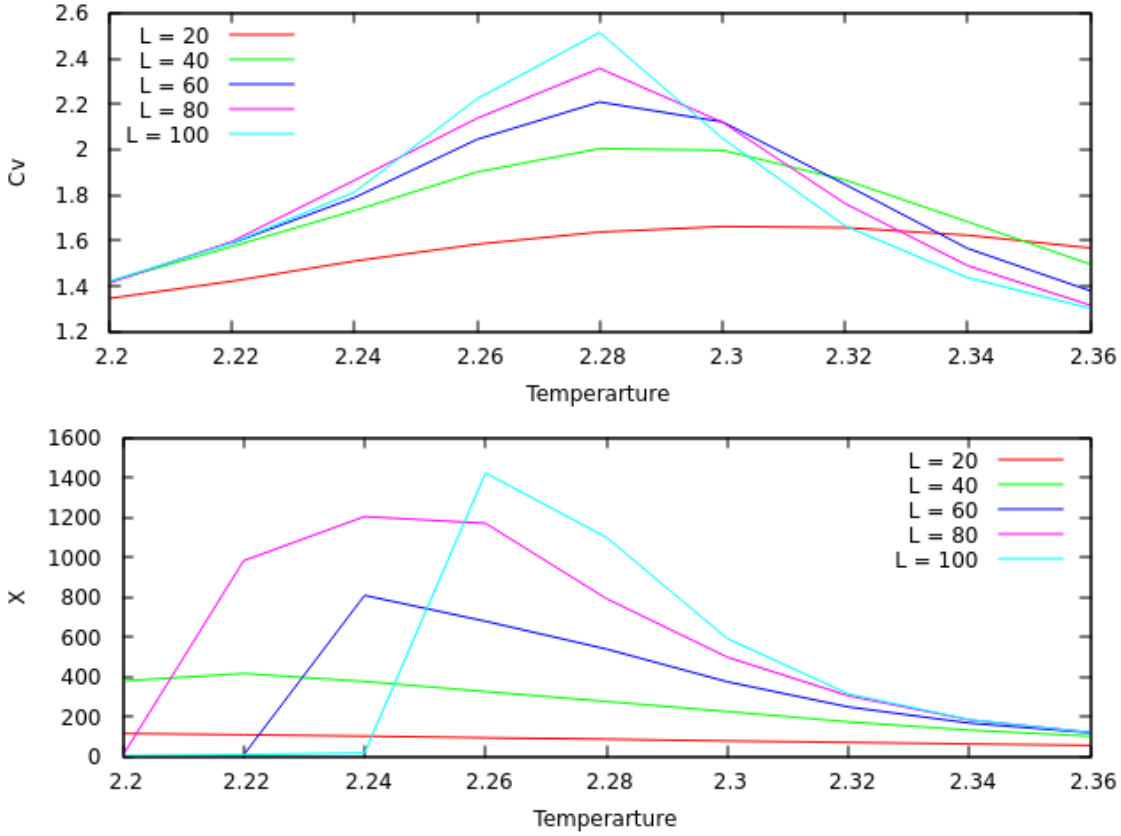


Figure 5. The expected values of energy (E), magnetization(|M|)(above), heat capacity (C_V) and magnetic susceptibility (χ)(below) simulation for T = [2.2,2.36] with step of 0.2. 10^6 Monte Carlo cycles were run discarding the results from first 10^4 cycles. The simulations perform in five different lattices size which are 20X20, 40×40, 60×60, 80×80, and 100×100.

According to Hjort-Jensen (2015), both heat capacity and susceptibility diverge at the critical temperature. This could imply that the critical temperature is at the maximum of heat capacity and susceptibility. As shown in figure 5, the maximum susceptibility for the 100×100 lattices is at T = 2.26 which strongly corresponds with the Onsager's exact approximation of 2.269 (Onsager, 1944). In contrast, the maximum heat capacity is at T = 2.28 where a bit different from the Onsager's exact value about 0.5 % (relative error). We assume the critical temperature for L=100 is about 2.27 by the averaging the values from both heat capacity and susceptibility.

In term of the sizes of lattices, the larger size simulations perform well to estimate the critical temperature. It is difficult to exact the critical temperature from the 20×20 and 40×40 lattices sizes simulations by looking the graph. This apparently represents the effect lattices sizes have for estimation of the critical temperature. For higher accuracy, simulation needs larger size lattices.

Our critical temperatures of finite-size lattices are gradually approaching that of infinite-size lattice with growing L. Here we try to estimate the critical temperature for infinite-size lattice. We have

$$T_C\left(L=\infty\right)=T_C(L)-\frac{a}{L}.$$

while L=20, 40, 60, 80, 100. The constant a was calculated as -1.83, which generated the least variance of calculated $T_C\left(L=\infty\right)$s. With the regression constant, we get the following result.

Table 3. The critical temperature of each finite lattices and estimated critical temperatures for infinite lattice, with $a=-1.83$ and $\nu=1$. The average is 2.289. L=20 was omitted because we couldn't get the proper extremum point from the data.

$\boldsymbol{L}$	$\boldsymbol{T_C(L)}$	$\boldsymbol{T_C(L=\infty)}$
40	2.25	2.30
60	2.26	2.29
80	2.26	2.28
100	2.27	2.29
		Average 2.29

L=20 was omitted because we couldn't get the proper extremum point from the data. By taking the average of four critical temperatures of infinite lattice, we get $\boldsymbol{T_C(L=\infty)}=2.29$, which differs with Onsager's exact result with 0.88%. The error could be reduced by using larger sample size in Monte Carlo simulations, by setting higher threshold for equilibrium and discarding results from the first 10^6 simulations, and obtaining simulation results with more lattices.

IV Conclusion

This project studied the properties of ferromagnetism near critical temperature, using the two dimensional Ising model. The Markov process of Ising model was implemented with Monte Carlo simulation using Metropolis algorithm. The numerical simulations were verified by available analytical solutions using a small lattice. They showed good agreement from 10^6 Monte Carlo simulations at T=1.0.

With 20×20 lattice, the equilibration of energy and magnetization was observed as a

function of number of Monte Carlo cycles, which can be considered proportional to time. Equilibrium was reached after 10^6 Monte Carlo cycles for both quantities. Simulations were done for two different temperatures which belonged to two different phases, namely T=1.0(below T_C) and T=2.4(above T_C). For the lower temperature, the mean energy converged near the ground state (-2.0) and mean magnetization converged near 1.0, which indicated spins normally being ordered in one direction. For the higher temperature, the mean energy converged to higher energy and lower magnetization, which indicated spins being more disordered with higher entropy. Initial state was chosen as ground state and random state, which had no effect after the steady state was reached. The probability distribution of energy was focused after the steady state. The result presented that the energy is distributed with the higher mean with more spreading at the higher temperature, which is consistent with theoretical Boltzmann distribution.

Study of phase transition were conducted through five different lattice sizes, and the behavior of the energy, magnetization, specific heat, and magnetic susceptibility were observed as functions of temperature. The energy and magnetization showed the trend of sharp discontinuity at the critical temperature as the size of the lattice increased. Specific heat and susceptibility also showed the trend of divergence with increasing lattice size. The critical temperature for each lattice was obtained by averaging the temperature point where extremum of energy and magnetization was reached. The critical temperature for infinite-size lattice was extracted from the results of finite-sized lattices, which was T_C=2.29. The result agreed with Onsager's result with the relative error being 0.92%. The error can be reduced with increasing the number of Monte Carlo simulations and setting higher threshold for steady state, but the limit of the Ising model itself is difficult to estimate only from the presented results. Other kinds of model, such as spins interacting with more spins other than the nearest neighbors could be suggested and tested, which is proposed for further studies.

References

Hjort-Jensen, M. (2015), Computational physics, accessible at course github repository. https://github.com/CompPhysics/ComputationalPhysics/tree/master/doc/Lectures

Onsager, L. (1944), Crystal statistics. i. A two-dimensional model with an order-disorder transition, Phys. Rev., 65:117–149