A study of phase transitions in magnetic systems

Christina Knudsen, Jessie H. K. Warraich
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We have in this project looked at the Ising model in two dimensions. The Monte Carlo algorithm and Metropolis sampling rule was implemented for the numerical calculations. We obtained expectation values for the mean energy, the mean magnetization, the specific heat and the susceptibility as functions of T using periodic boundary conditions. We reached steady state for a lattice of size $L = 20 \times 20$ at around 500 Monte Carlo cycles for $T = 1.0 k_B T/J$, and 2000 Monte Carlo cycles for $T = 2.4 k_B T/J$. The energy probability for $T = 1.0 k_B T$ had a narrow distribution at only a few of the lowest energy levels, while the distribution was Gaussian for $T = 2.4 k_B T$. We plotted the expectation values for different lattice sizes and were able to extract a critical temperature value $T_c = 2.2905$ for $L \to \infty$ with relative error of 0.95%.

I. INTRODUCTION

In this paper we will study the popular Ising model to study a phase transition in two dimensions. At a given critical temperature, this model exhibits a phase transition from a magnetic phase to a phase with zero magnetization. This is a so-called binary system where the objects at each lattice site can only take two values. In our system we use spins pointing up or down as our model. In one and two dimensions it has analytical solutions to several expectation values, which gives a qualitatively good understanding of several types of phase transitions.

To model this, we will implement a Monte Carlo algorithm in addition to a Metropolis sampling rule. We will use different lattice sizes and temperatures to see the see how the energy and magnetization behave when run over a period of time. The goal is to extract a value for the critical temperature and compare it to the analytical value obtained by Lars Onsager[4].

II. THEORY

A. The Ising Model

The Ising model, named after the german physicist Ernst Ising, is a mathematical model of ferromagnetism in statistical mechanics. As he gave his student the one-dimensional model as a problem[1], the analytical description was first given by Lars Onsager in 1994[4]. In its simplest form, the Ising model is expressed as,

$$E = -J \sum_{\langle kl \rangle}^{N} s_k s_l - \mathscr{B} \sum_{k}^{N} s_k \tag{1}$$

with $s_k = \pm 1$. The quantity N represents the total number of spins and J is a coupling constant expressing the strength of the interaction between neighboring spins and $\mathscr{B}$ is an external magnetic field interacting with the magnetic moment set up by the spins. The symbol $\langle kl \rangle$ indicates that we sum over nearest neighbors only. We will assume that we have a ferromagnetic ordering, viz $J > 0$.

In order to calculate expectation values such as the mean energy $\langle E \rangle$ or magnetization $\langle M \rangle$ in statistical physics at a given temperature, we need a probability distribution given by the Boltzmann distribution

$$P_i(\beta) = \frac{e^{\beta E_i}}{Z} \tag{2}$$

with $\beta = 1/k_B T$ being the inverse of the temperature, k_B is the Boltzmann constant, E_i is the energy of a state i while Z is the partition function of the canonical ensemble defined as

$$Z = \sum_{i=1}^{m} e^{\beta E_i}$$

where the sum extends over all microstates m. In this project we consider a case of the two dimensional Ising model, with $\mathscr{B} = 0$, which leaves equation 1 as

$$E = -J \sum_{\langle kl \rangle}^{N} s_k s_l. \tag{3}$$

The expectation value of the energy and magnetization are therefore given as

$$\langle E \rangle = \sum_{i=1} E_i P_i(\beta) = \frac{1}{Z} \sum_{i=1} E_i e^{-\beta E_i} \tag{4}$$

$$\langle M \rangle = \sum_{i=1} M_i P_i(\beta) = \frac{1}{Z} \sum_{i=1} M_i e^{-\beta E_i} \tag{5}$$

where we sum over all configurations. Other quantities of interest are the heat capacity C_V, defined as

$$C_V = \frac{1}{k_B T^2} \left(\langle E \rangle^2 - \langle E^2 \rangle \right), \tag{6}$$

and the magnetic susceptibility χ

$$\chi = \frac{1}{k_B T} \left(\langle M \rangle^2 - \langle M^2 \rangle \right). \tag{7}$$

In this project we consider the factor J to be in the units of energy, leaving the calculated energy dimensionless. This also leads to the Boltzmann's constant k_B having unit of energy per temperature, and the temperature consequently has a unit of energy.

As figure 1 shows an arbitrary configuration of a 2×2 spin lattice, the energy of the given configuration is given by equation 3

$$E_i = -J\left((+1)(-1) + (+1)(-1) + (+1)(-1) + (+1)(-1)\right) = 8J,$$

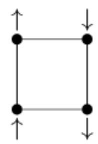

FIG. 1: *An example of a 2 × 2 lattice with spins.*

which is the highest energy possible for this particular system. Similarly, the lowest energy is $-8J$, while the rest of the energies are as tabled in table I.

No. of spins up	Degeneracy	Energy [J]	Magnetization
0	1	-8	-4
1	4	0	-2
2	2	8	0
2	4	0	0
3	4	0	2
4	1	-8	4

TABLE I: *Possible energy states of a 2 × 2 lattice in the Ising model.*

B. Analytical values

To compute the analytical values for a 2×2 lattice for the mean energy $\langle E \rangle$, mean magnetisation $\langle M \rangle$, heat capacity $\langle C_V \rangle$ and susceptibility $\langle \chi \rangle$, we first take a look at the partition function of the system

$$\begin{aligned} Z &= \sum_{i=1}^{m} e^{\beta E_i} = 2e^{8\beta J} + 2e^{-8\beta J} + 2e^{0 \cdot \beta J} \\ &= 12 + 4\cosh(8\beta J). \end{aligned} \tag{8}$$

The expected energy is given as

$$\begin{aligned} \langle E \rangle &= -\frac{\partial}{\partial \beta} \ln Z = -\frac{\partial}{\partial \beta} \ln\left(12 + 4\cosh(8\beta J)\right) \\ &= -\frac{8J\sinh(8\beta J)}{3 + \cosh(8\beta J)}, \end{aligned} \tag{9}$$

The expected magnetization, and the absolute value,

$$\begin{aligned} \langle M \rangle &= \frac{1}{Z}\left(-4e^{8\beta J} - 8e^{0 \cdot \beta J} + 8e^{0 \cdot \beta J} + 4e^{8\beta J}\right) \\ &= 0, \\ |\langle M \rangle| &= \frac{1}{Z}\left(4e^{8\beta J} + 8e^{0 \cdot \beta J} + 8e^{0 \cdot \beta J} + 4e^{8\beta J}\right) \\ &= \frac{8e^{8\beta J} + 16}{12 + 4\cosh(8\beta J)} = \frac{8(e^{8\beta J} + 2)}{4(3 + \cosh(8\beta J))} \\ &= \frac{2e^{8\beta J} + 4}{3 + \cosh(8\beta J)}. \end{aligned} \tag{10}$$

The expected value for the specific heat

$$\begin{aligned} \langle C_V \rangle &= \frac{1}{k_B T^2} \frac{\partial^2}{\partial \beta^2} \ln Z = \frac{1}{k_B T^2} \frac{\partial}{\partial \beta}\left(-\frac{8J\sinh(8\beta J)}{3 + \cosh(8\beta J)}\right) \\ &= \frac{1}{k_B T^2}\left(\frac{64J^2\cosh(8\beta J)}{\cosh(8\beta J) + 3} - \frac{64J^2\sinh^2(8\beta J)}{(\cosh(8\beta J) + 3)^2}\right) \\ &= \frac{1}{k_B T^2} \frac{64J^2}{\cosh(8\beta J) + 3}\left(\cosh(8\beta J) - \frac{\sinh^2(8\beta J)}{\cosh(8\beta J) + 3}\right). \end{aligned} \tag{11}$$

Looking back at equation 7, we see that we can use the variance of the magnetisation to find the susceptibility of the magnetization. The variance is defined as

$$\sigma_x^2 = \left\langle x^2 \right\rangle - \left\langle x \right\rangle^2, \tag{12}$$

which will give the magnetic susceptibility as

$$\begin{aligned} \chi &= \frac{1}{k_B T}\sigma_M^2 = \frac{1}{k_B T}\left(\left\langle M^2 \right\rangle - \left\langle M \right\rangle^2\right) \\ &= \frac{1}{k_B T}\left(\frac{8 + 8e^{8\beta J}}{1 + 3\cosh(8\beta J)} - 0\right) = \frac{1}{k_B T} \frac{8 + 8e^{8\beta J}}{1 + 3\cosh(8\beta J)}. \end{aligned} \tag{13}$$

C. Phase transitions

Near the critical temperature T_C we can characterize the behavior of many physical quantities by a power law behavior. For the Ising class of models, the mean magnetization, heat capacity and the susceptibility scales as

$$\begin{aligned} \langle M(T) \rangle &\sim (T - T_C)^{\beta}, \\ C_V(T) &\sim |T_C - T|^{\alpha}, \\ \chi(T) &\sim |T_C - T|^{\gamma}, \end{aligned} \tag{14}$$

with $\alpha = 0$, $\gamma = 7/4$ and $\beta = 1/8$ as so-called critical exponents[2]. Another important quantity is the correlation length, which is expected to be of the order of the lattice spacing for $T \gg T_C$. Because the spins become more and more correlated as T approaches T_C, the correlation length increases as we get closer to the critical temperature. The divergent behavior of ξ near T_C is

$$\xi(T) \sim |T_C - T|^{-\nu}. \tag{15}$$

A second-order phase transition is characterized by a correlation length which spans the whole system. Since we are always limited to a finite lattice, ξ will be proportional with the size of the lattice. Through so-called finite size scaling relations it is possible to relate the behavior at finite lattices with the results for an infinitely large lattice. The critical temperature scales then as

$$T_C(L) - T_C(L = \infty) = aL^{-1/\nu}, \tag{16}$$

with a a constant and ν defined in equation (15). From Lars Onsager[4], we have the analytical value for the critical temperature when $\nu = 1$

$$\frac{k_B T_C}{J} = \frac{2}{\ln\left(1 + \sqrt{2}\right)} \approx 2.269. \tag{17}$$

III. METHOD

All codes and results are given in the linked github repository [3].

A. Monte Carlo Algorithm and Metropolis sampling

We will use the Monte Carlo algorithm for solving the Ising model with the Metropolis algorithm as a sampling rule and periodic boundary conditions. New configurations are generated using a transition probability that depends on energy differences between initial and final states.

The Monte Carlo algorithm is set up in the following way. First we establish an initial state with energy E at a random configuration. Then we flip this spin and compute the new energy. We calculate ΔE between the new and the old configuration, and if this is less than zero, we accept the new configuration. If it is not, we use the Metropolis algorithm to decide whether we accept or reject the new configuration. This is done by calculating the ratio w between the probabilities in equation (2) of the new and the old configuration. By taking the ratio, the partition function is cancelled out, and we are left with $w = e^{-(\beta \Delta E)}$. We will compare this with a random number r between 0 and 1. If $r \leq w$, the new configuration is accepted, if not we keep the old configuration. Then we update all expectation values. By using the Metropolis algorithm after each flip, we can use precalculated values for ΔE and save computation time. We will repeat this until we get a good representation of states. One such sweep over the lattice is called a Monte Carlo cycle.

We will first run our program for a 2×2 lattice to see how many Monte Carlo cycles are needed in order to get a good agreement with the analytical results. Then we will see how many Monte Carlo cycles are needed to reach an equilibrium state, by plotting the mean energy and magnetization as a function of the number of Monte Carlo cycles for temperature $T = 1.0k_BT/J$ and $T = 2.4k_BT/J$. We will use both a uniform and a random distribution of initial states.

We will also make a histogram of the probabilities by counting the number of times a given energy appears after the system has reached a steady state.

At last we will calculate the expectation values for lattice sizes L=40, 60, 80 and 100, plot these as a function of temperature, and use these plots to extract a value for the critical temperature.

As in the previous project, we will use MPI to speed up our calculations. For this project we divide the number of Monte Carlo cycles on the number of processors, and sum the results at the end of the calculations. We use c++ to calculate the expectation values and Python to plot the results.

IV. RESULTS

A. The simplified 2×2 lattice

A series of runs for a 2×2 lattice with different numbers of Monte Carlo cycles were calculated as shown in table II.

mcs	$\langle E \rangle$	$\langle M \rangle$	C_V	χ
10^2	-2	1	0	0
10^3	-1.998	0.999	0.015984	0.003996
10^4	-1.9964	0.9988	0.0287482	2.49631
10^5	-1.99578	0.998625	0.0336888	3.93652
10^6	-1.99585	0.998621	0.033147	3.99056
Analytical	-7.984	0.0	0.128	5.334

TABLE II: *Table of numerical results of the Ising model for a 2×2 lattice for different number of Monte Carlo cycles mcs. Here $\langle E \rangle$ is the mean energy, $\langle M \rangle$ the mean magnetization, C_V the specific heat and χ is the susceptibility.*

B. Most likely state

We changed our lattice to 20×20 and plotted the expectation values as a function of time (the number of Monte Carlo cycles) for temperatures $T = 1.0k_BT/J$ and $T = 2.4k_BT/J$. This is given in figure 2 and 3. We can see that the most likely state was reached at around 500 cycles for both the magnetization and the energy at $T = 1.0k_BT/J$ and a bit later, around 2000 for $T = 2.4k_BT/J$. The probability distribution was also computed for both temperatures, see figure 4 and 5. For the highest temperature the histogram looks like a Gaussian, while for a low temperature the probability peaks at the the lowest energies. With the same lattice we also calculated a variance of respectively $\sigma_E^2 = 265.93$ and $\sigma_E^2 = 107.02$.

C. Phase transitions

We also studied the expectation values as functions of temperatures for different lattice sizes $L \times L$ with $L = 40, 60, 80$ and 100, over a range of temperatures $T \in [2.0, 2.4]$. The plot of the expectation values for $\langle E \rangle$, expectation values for $\langle M \rangle$, specific heat C_V and magnetic susceptibility χ in these specific lattices are plotted in figure 6. The expression for the critical temperature given in equation (16) has a linear form, which can also be seen from the extremal points in the heat capacity plot. By using this property $T(L \to \infty)$ was approximated to be 2.2905. Comparing to the analytical value from section II C, we get an relative error of 0.95%.

V. DISCUSSION

The expectation values we obtained for a square lattice of size 2×2 are tabulated in table II. As we can see, the analytical values are not even close to the ones we obtained numerically. We assume this is because of our scaling in the code, but we were not able to find the error. We will instead use our result for mcs $= 10^6$ as comparison for the other numerical values. We see now that the expectation values for the mean energy and the magnetization converges at only a few Monte Carlo cycles, mcs $= 10^3$. The expectation values for the heat capacity and magnetic susceptibility on the other hand reach the analytical values at around mcs $= 10^6$.

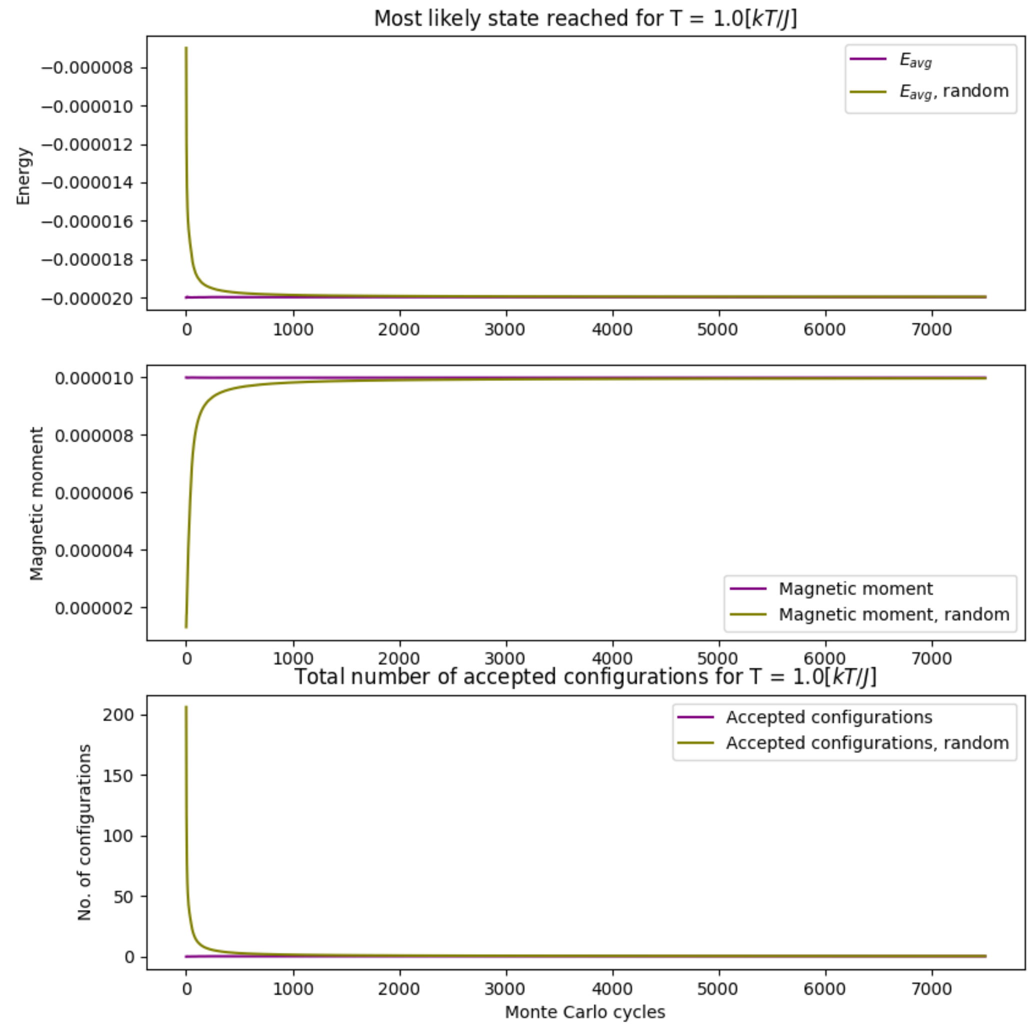

FIG. 2: *Mean energy and magnetic moment over a range of Monte Carlo cycles for the* 20×20 *lattice system with* $T = 1.0k_BT/J$*. We have used both uniform and random distribution on the spins, and the number of accepted configurations are plotted. We see that our system reaches a stable state at around 500 Monte Carlo cycles.*

We calculated the mean energy and the magnetization for a lattice of size $L = 20$ to get a better representation. As we can see from figure 2, the most likely state for the energy and the magnetization at $T = 1.0$ is reached faster for the uniform distribution than the random. As the uniform distribution represents a configuration with the lowest possible energy, this is as expected for low temperatures. The number of accepted configurations is initially higher for the random distribution. This is also in compliance with what we would expect, as the uniform distribution reaches equilibrium faster at this temperature. For temperature $T = 2.4$ in figure 3, it takes more time for the system to reach an equilibrium state. Here the random distribution reaches steady state faster, which is also in accordance with our expectations as we have more thermal energy and more possible energy states. The number of accepted configurations is therefore also much higher at higher temperature, being around 100 for $T = 2.4$ and only around 0.5 for $T = 1.0$.

The probabilities in figure 4 and 5 behave differently for the different temperatures. For $T \to 0$ we get a peak on the lowest energies, with only a few energy levels represented. This is as expected when the temperature goes to zero. For $T = 2.4$, there is a bigger variance. A higher temperature gives a higher thermal energy and therefore more permitted energy states. As the plot for $T = 2.4$ has a Gaussian shape, one can compare this with the calculated standard deviation. Looking at figure 5 and our analytical result, this seems to be a good match.

The Onsager limit for critical temperature is at $T_c = 2.269$ as mentioned in section II C. Therefore, when we plotted the expectation limits for a temperature range from 2.0 to 2.4, we had a system going from a state with magnetization to a state with zero magnetization. This can be seen in the plot for the different expectation values in figure 6. The

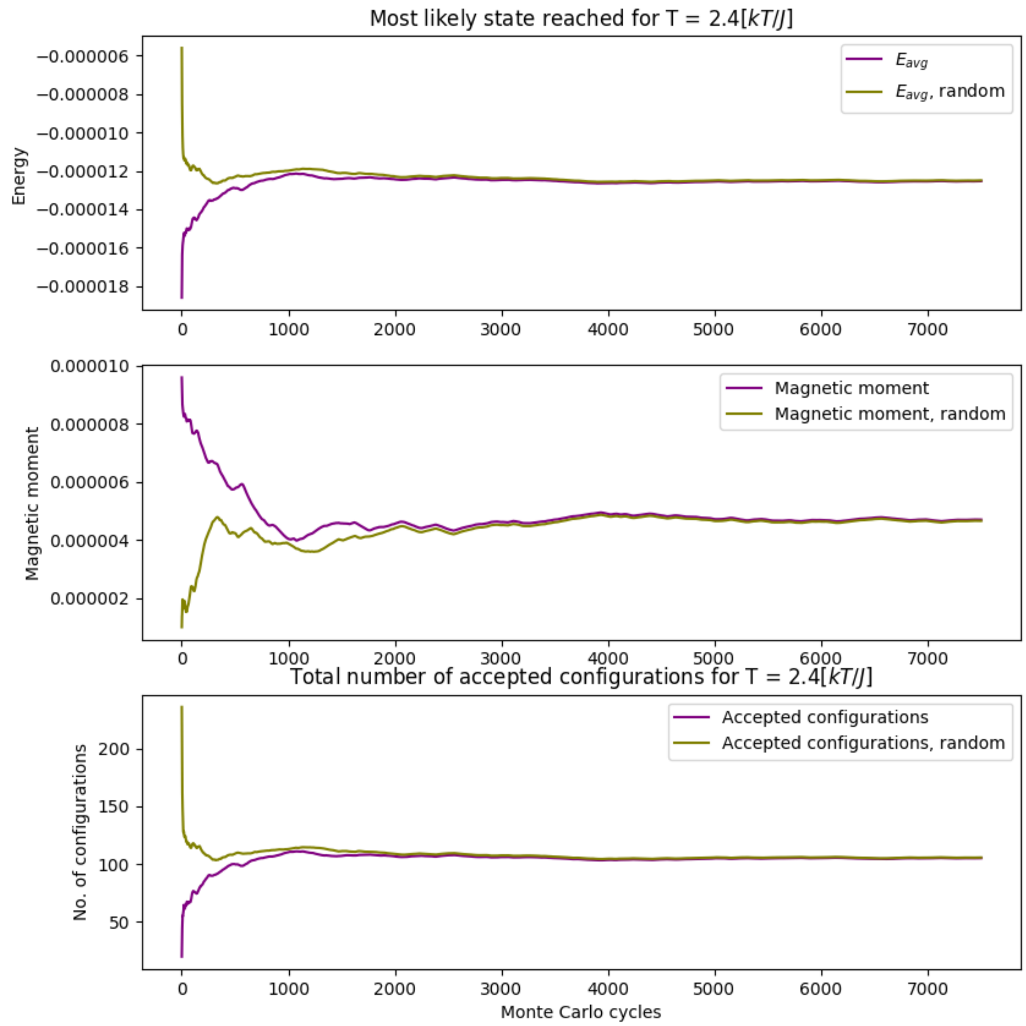

FIG. 3: *Mean energy and magnetic moment over a range of Monte Carlo cycles for the* 20×20 *lattice system with* $T = 2.4k_BT/J$*. We have used both uniform and random distribution on the spins, and the number of accepted configurations are plotted. We see that our system reaches a stable state at around 2000 Monte Carlo cycles.*

specific heat has its peak at the phase transition, with the critical temperature reaching the Onsager limit at increasing lattice sizes. One can also see that the absolute values for the mean magnetization goes to zero with increasing lattice size at this point.

VI. CONCLUSION

We have in this project looked at the Ising model in two dimensions. We obtained numerical and analytical expressions for the mean energy, mean magnetization, the specific heat and the susceptibility as functions of temperature using periodic boundary conditions. The numerical solution was obtained using the Monte Carlo algorithm with Metropolis sampling rule.

The behavior of the system for the different temperatures was as expected, and we were able to extract a value for the critical temperature close to the exact Onsager limit. As our numerical result for $L = 2 \times 2$ did not match the analytical values, we therefore assume there is a scaling problem we did not account for in our analytical calculations.

We could in general have taken a closer look at sources of error. This would give us a better clue as to how exact this model is, and how good our code was.

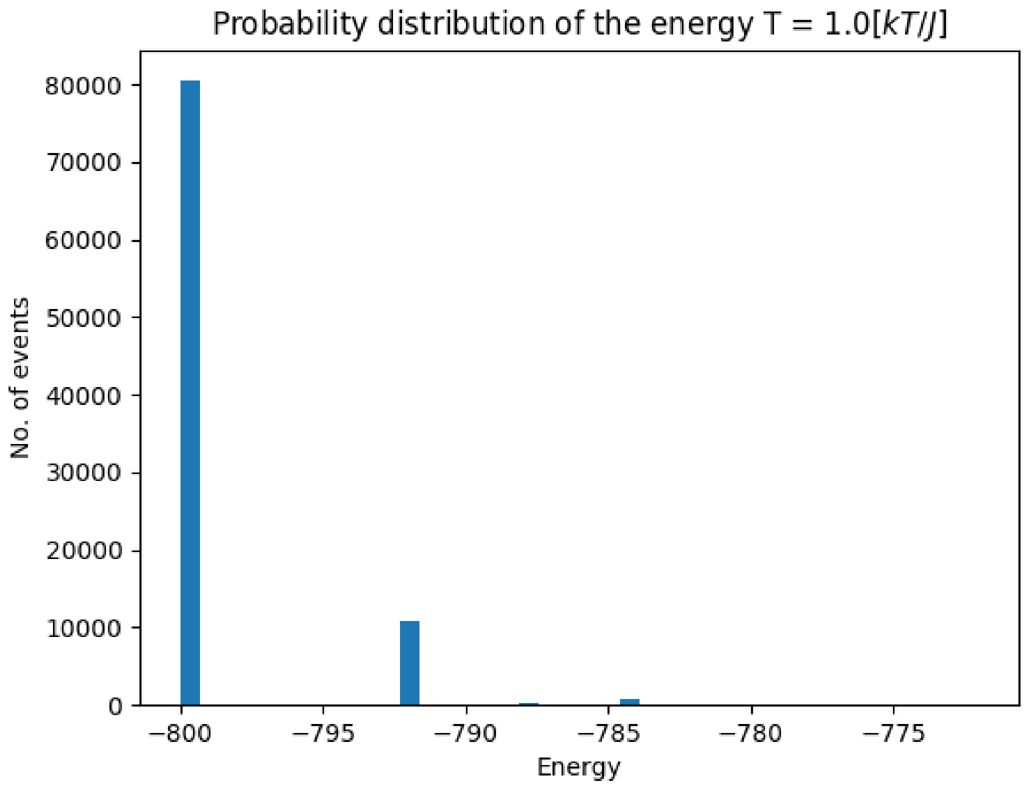

FIG. 4: *Probability distribution $P(E)$ for the 20×20 lattice system with $T = 1.0 k_B T/J$. Here we have used uniformly distributed spins, and variance of 265.93. This is calculated after the system has reached a stable state, from monte carlo cycles number 7500 and up to 10^5.*

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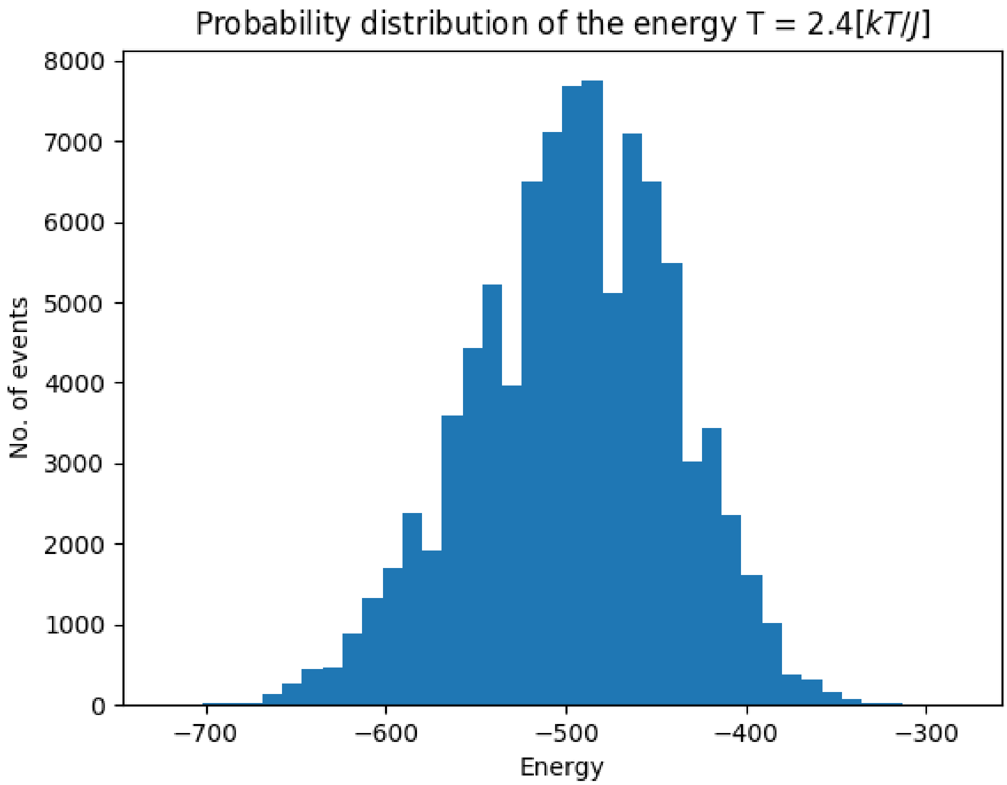

FIG. 5: *Probability distribution $P(E)$ for the 20×20 lattice system with $T = 2.4 k_B T/J$. Here we have used uniformly distributed spins, and variance of 107.02. This is calculated after the system has reached a stable state, from Monte Carlo cycles number 7500 and up to 10^5.*

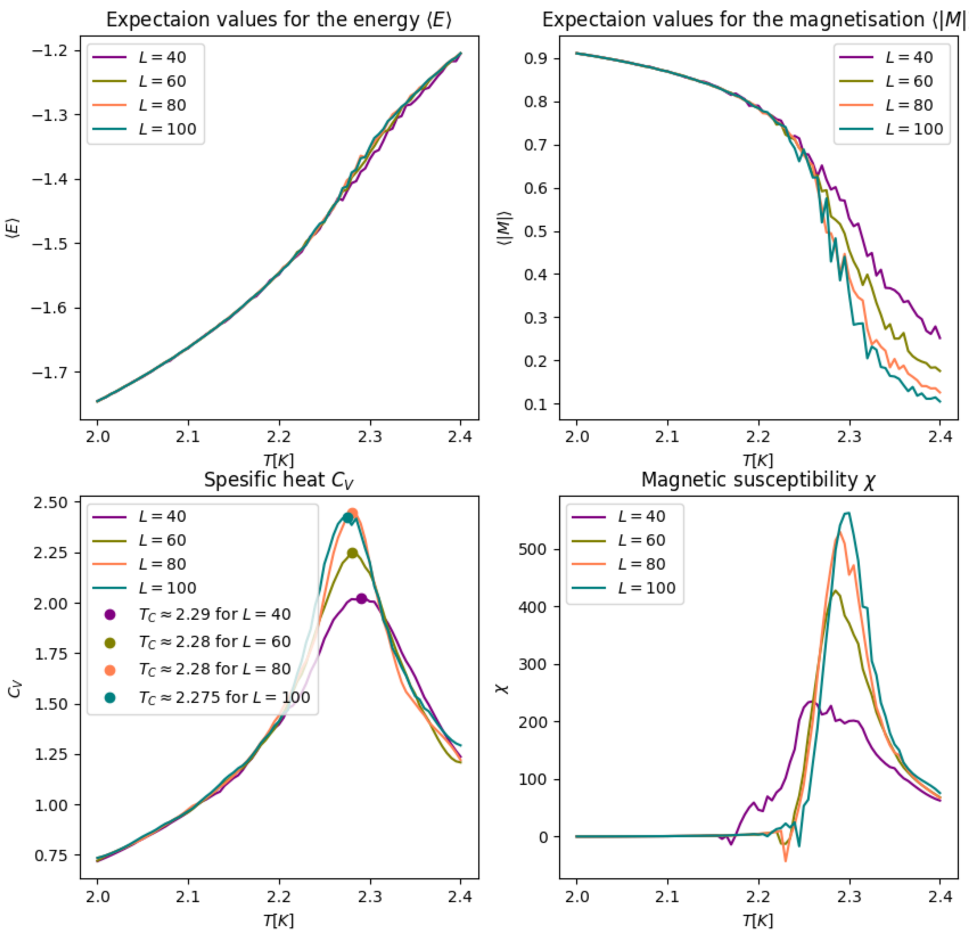

FIG. 6: *Plot of the expectation values for $\langle E \rangle$, expectation values for $\langle M \rangle$, specific heat C_V and magnetic susceptibility χ for four different lattice sizes $L \times L$ with $L = 40, 60, 80$ and 100. This has been calculated with a temperature range of $T \in [2.0, 2.4]$ over 10^5 Monte Carlo cycles with $\Delta T = 0.005$. Also plotted are the peaks of the specific heat in each of the systems.*