The Lenz-Ising model

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We use Markov Chain Monte Carlo method to explore temperature-dependent behavior in a system of two-state spins, namely the 2D Lenz-Ising model. We approximate a Boltzmann distribution for $\langle\epsilon\rangle$ at $T = 1J/k_B$ and $T = 2.4J/k_B$ for $L = 40$. However, the distribution approaches a Gaussian distribution for $T = 2.4J/k_B$. For $L = \{40, 60, 80, 100\}$ we find the critical temperatures $T_c = \{2.28, 2.28, 2.29, 2.27\}$ J/k_B for our best fit. A numerically estimated value of the critical temperature of an Lenz-Ising model with $L = \infty$ is found to be $T_c(L = \infty) = 2.28$ J/k_B when deduced from the heat capacity of the system, and $T_c(L = \infty) = 2.31$ J/k_B when deduced from the susceptibility.

I. INTRODUCTION

In 1920, German physicist Wilhelm Lenz (not to be confused with Heinrich Lenz, from whom the Lenz' law got its name), introduced a theory regarding a model of ferromagnetism [1]. This model was the exact solution of a two-dimensional problem regarding ferromagnetism and atomic alignment in the context of statistical mechanics [2]. In 1922, Lenz gave this theoretical model as a problem for his doctorate student Ernst Ising, hoping he could solve the complicated mathematical model. Sure enough, when Ernst Ising published his thesis in 1925 (after submission in 1924), he had calculated an exact partition function for the model, although in the case of a one-dimensional lattice [2]. Somewhat disappointed that his conclusion for the linear model did not apply to higher dimensional problems, Ising left the thoughts of his paper for many years. However, in 1947 he "rediscovered" his paper again, where he realized that in the meantime, Werner Heisenberg had used his solution to develop an even more sophisticated model for ferromagnetism [3]. Hence had Ising's calculations been extremely useful after all, and the model was named the Ising model. To recognize both main contributors to the model, we will refer to it as the Lenz-Ising model.

The Lenz-Ising model can also be used to model many different phenomena in science. In this paper, we will use it to model a spin system that can take one out of two values: $+1$ ($\uparrow$) or -1 ($\downarrow$). We will let the system exchange heat with a thermal bath of temperature T, which can lead to a change in the energy of the system due to thermal fluctuations. We use the Markov chain Monte Carlo method to sample spin states according to the Boltzmann distribution, to compute quantities we are interested in. Our particular goal is to estimate the critical temperature T_c, which is the temperature where our system undergoes a phase transition from a magnetized phase to a phase with no net magnetization.

The paper is structured as follows. In section section II we investigate the methods used in this experiment and present the equations used to calculate our quantities of interest, including the analytical solution for a 2×2 lattice grid Lenz-Ising model. In section III we will present our results and analysis, as well as a discussion of our findings. Lastly, in section IV, we will provide a conclusion, and discuss future work. An appendix is found in section A. The code developed for this paper can be found on our GitHub repository[1].

II. METHODS

A. The Lenz-Ising Model in 2D

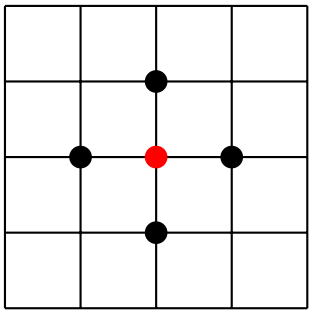
We consider a 2D Lenz-Ising model of two-state spins and periodic boundaries. Each spin s_i has two possible states: $s_i = \pm 1$. The model is a lattice[2] of length L and contains N spins in total, i.e.

$$N = L^2. \tag{1}$$

The spin configuration (also referred to as microstate) is represented as a matrix

$$\mathbf{s} = \begin{bmatrix} s_{1,1} & \cdots & s_{1,L} \\ \vdots & \ddots & \vdots \\ s_{L,1} & \cdots & s_{L,L} \end{bmatrix} \tag{2}$$

We use periodic boundaries for our lattice as illustrated in the figure below. Thus, each spin (red dot) has four neighbors (black dots): top, bottom, left and right.



[1] https://github.uio.no/rebeccng/FYS4150/tree/main/project_4
[2] We only model square lattices in this report.

The total energy of the system is given by

$$E(\mathbf{s}) = -J\sum_{\langle kl\rangle}^{N} s_k s_l \quad [J], \tag{3}$$

where $\langle kl\rangle$ means that the sum goes over all neighboring spin pairs without double-counting and J is the coupling constant. In a system with no magnetic interaction, the total energy of the system is fully determined by the interaction between neighboring spin pairs. The total magnetization of the system is simply the sum over all the spins in the system

$$M(\mathbf{s}) = \sum_{i}^{N} s_i. \tag{4}$$

To compare total energy and magnetization for different lattice sizes, these quantities are normalized to the number of spins

$$\epsilon(\mathbf{s}) = \frac{E(\mathbf{s})}{N} \quad [J], \tag{5}$$

$$m(\mathbf{s}) = \frac{M(\mathbf{s})}{N}. \tag{6}$$

The Boltzmann distribution describes the probability for the system state $\mathbf{s}$ at a given temperature T

$$p(\mathbf{s};T) = \frac{1}{Z}e^{-\beta E(\mathbf{s})}, \tag{7}$$

where Z is the partition function, β is the "inverse temperature"

$$\beta = \frac{1}{k_B T} \quad [1/J], \tag{8}$$

and $k_B = 1.380649 \cdot 10^{-23}$ J/K is the Boltzmann constant. The partition function is given by

$$Z = \sum_{\text{all possible } \mathbf{s}} e^{-\beta E(\mathbf{s})}. \tag{9}$$

The heat capacity of the system normalized to the number of spins is

$$C_V(T) = N\frac{1}{k_B T^2}[\langle \epsilon^2\rangle - \langle\epsilon\rangle^2] \quad [k_B], \tag{10}$$

given in units k_B. Lastly, the susceptibility of the system is

$$\chi(T) = N\frac{1}{k_B T}[\langle m^2\rangle - \langle m\rangle^2] \quad [1/J]. \tag{11}$$

The Monte Carlo simulation (see section II C) requires the Boltzmann factor of the energy difference for a single spin flip

$$e^{-\beta\Delta E}, \quad \Delta E = \Delta E_{\text{after}} - \Delta E_{\text{before}}. \tag{12}$$

There are only five possible values ΔE can take as each spin only has four neighboring spins contributing to the total energy. These five values can be calculated once in our code and used directly to avoid repeatedly calling `exp()`. For a given spin s_k, the total energy from the contribution of its four neighbors is given by

$$E(s_k) = -Js_k\sum_{\langle l\rangle} s_l, \tag{13}$$

where a spin flip is $s_k \to -s_k$. The energy difference ΔE is given by

$$\begin{aligned}\Delta E &= Js_k\sum_{\langle l\rangle} s_l - (-Js_k)\sum_{\langle l\rangle} s_l \\ &= 2Js_k\sum_{\langle l\rangle} s_l.\end{aligned} \tag{14}$$

The five possible values for s_l are

$$s_l = \{-4,-2,0,2,4\}, \tag{15}$$

thus the five possible values for ΔE are

$$\Delta E = \{-8,-4,0,4,8\}J. \tag{16}$$

The same thought process is valid for magnetization where

$$\begin{aligned}\Delta M &= \sum_{i}^{N} s_i - (-\sum_{i}^{N} s_i) \\ &= 2\sum_{i}^{N} s_i.\end{aligned} \tag{17}$$

For $s_i = \{-1,+1\}$ we have $\Delta M = \{-2,+2\}$.

B. Analytical Solution of 2×2 Lattice

Derivation for all quantities in this subsection can be found in more detail in section A. For a 2×2 lattice, $2^4 = 16$ microstates exist for the system and they are presented in Table I

TABLE I. Summary of possible microstates in an $L = 2$ Lenz-Ising model. The number of degeneracies adds up to 16 microstates. ↑ and ↓ denotes spin up and down, respectively.

↑	↓	Total energy	Total magnetization	Degeneracy
4	0	-8J	4	1
3	1	0J	2	4
2	2	0J	0	4
2	2	8J	0	2
1	3	0J	-2	4
0	4	-8J	-4	1

Given the values for total energy and total magnetization from Table I, we derive analytical expressions for Z, $\langle\epsilon\rangle$, $\langle\epsilon^2\rangle$, $\langle|m|\rangle$ and $\langle m^2\rangle$ which will be used to test the implementation of the Markov Chain Monte Carlo method. In this section, we only state the results.

The partition function Z for $L = 2$ is

$$Z = 12 + 4\cosh(8J\beta). \tag{18}$$

The expectation value for energy per spin ϵ is

$$\langle\epsilon\rangle = \sum_{\mathbf{s}} \epsilon(\mathbf{s})p(\mathbf{s}) = \frac{-8J}{Z}\sinh(8J\beta), \tag{19}$$

and ϵ^2

$$\langle\epsilon^2\rangle = \sum_{\mathbf{s}} \epsilon^2(\mathbf{s})p(\mathbf{s}) = \frac{16J^2}{Z}\cosh(8J\beta). \tag{20}$$

The expectation value for the absolute value of magnetization per spin $|m|$

$$\langle|m|\rangle = \sum_{\mathbf{s}} |m|(\mathbf{s})p(\mathbf{s}) = \frac{4 + 2e^{8J\beta}}{Z}, \tag{21}$$

We calculate $\langle|m|\rangle$ rather than $\langle m\rangle$ because we are interested in the strength of magnetization at a given temperature. The expectation value for m^2 is given by

$$\langle m^2\rangle = \sum_{\mathbf{s}} m^2(\mathbf{s})p(\mathbf{s}) = \frac{2}{Z}(1 + e^{8J\beta}). \tag{22}$$

Lastly, the heat capacity $C_{\mathrm{V}}(T)$, normalized to the number of spins is given by

$$\frac{C_{\mathrm{V}}(T)}{N} = N\frac{1}{k_B T^2}\left[\frac{16J^2}{Z}\cosh(8J\beta) - \left(\frac{-8J}{Z}\sinh(8J\beta)\right)^2\right] \tag{23}$$

and susceptibility $\chi(T)$, normalized to the number of spins is given by

$$\frac{\chi(T)}{N} = N\frac{1}{k_B T}\left[\frac{2}{Z}(1 + e^{8J\beta}) - \left(\frac{4 + 2e^{8J\beta}}{Z}\right)^2\right]. \tag{24}$$

C. Markov Chain Monte Carlo

The evolution of the Lenz-Ising model depends on the probability of a chosen random spin to flip. We choose Markov Chain Monte Carlo (MCMC) as the method for drawing spin samples in the lattice. The general idea is starting from a state $\mathbf{s}_i$ we sample a candidate $\mathbf{s}'$ according to the proposal pdf $T(\mathbf{s}_i \to \mathbf{s}')$. We apply the Metropolis-Hastings acceptance rule so that

$$\mathbf{s}_{i+1} = \begin{cases} \mathbf{s}', & \text{if accepted} \\ \mathbf{s}_i, & \text{if rejected.} \end{cases} \tag{25}$$

Assuming a symmetric proposal pdf $T(\mathbf{s}_i \to \mathbf{s}') = T(\mathbf{s}' \to \mathbf{s}_i)$, the acceptance probability is given by

$$\begin{aligned} A(\mathbf{s}_i \to \mathbf{s}') &= \min\left(1, \frac{p(\mathbf{s}')}{p(\mathbf{s}_i)}\right) \\ &= \min\left(1, \frac{\frac{1}{z}e^{-\beta E(\mathbf{s}')}}{\frac{1}{z}e^{-\beta E(\mathbf{s}_i)}}\right) \\ &= \min(1, e^{-\beta\Delta E}). \end{aligned} \tag{26}$$

As energy tends to minimize it is a natural choice to accept proposed states with energy lower than the initial state. A simple outline of the algorithm is as follows:

Algorithm 1 Markov Chain Monte Carlo

```
s ← [s_{1,1}, s_{1,2}, ..., s_{N,N}]          ▷ Generate initial states
E ← [E_{1,1}, E_{1,2}, ..., E_{N,N}]   ▷ Calculate initial total energy
M ← [M_{1,1}, M_{1,2}, ..., M_{N,N}]          ▷ Calculate initial total magnetization
for number of Monte Carlo cycles do
    for N spins do
        s_i                                   ▷ Pick a random spin in lattice
        ΔE                                    ▷ Compute ΔE if spin flip
        r ∈ U(0,1)                ▷ Random number between 0 and 1.
        A = min(1, exp(−βΔE))                 ▷ Acceptence rule
        if r < A then
            s_i ← −s_i                        ▷ Flip spin
            E ← E + ΔE                        ▷ Update energy
            M ← M + ΔM                        ▷ Update magnetization
        else
            s_i ← s_i
```

Double-counting is unavoidable for $L = 2$ with periodic boundary conditions. We want to use our analytical results from section II B to test our code, therefore we allow for double-counting in this special case.

D. Burn-in Time

When executing a Monte Carlo simulation, one must choose a starting point. If our starting point happens to be an improbable value according to $p(x)$, the resulting distribution can be heavily influenced by and significantly biased towards this region. Including all points from the starting point will therefore result in an unreasonable approximation for $p(x)$. It may also lead to expectation values and other quantities being heavily biased by this starting point and region. The solution to this is what we call **burn-in**. This is the practice of disposal of all values that are biased towards this starting point, and instead start analyzing at a value where we can assume that the average of all our samples equals the expectation value. The burn-in time is defined as the time (e.g. measured in cycles) it takes to reach these higher probability regions, where we can use this assumed relation between sample average and expectation value [4].

E. Critical Temperature

The critical temperature defines where our system transitions from a magnetized phase to a phase with no net magnetization. For an infinite ($L = \infty$) 2D Lenz-Ising model the critical temperature is given by

$$T_c(L = \infty) = \frac{2}{\ln\left(1 + \sqrt{2}\right)} J/k_B \approx 2.269 J/k_B, \quad (27)$$

found analytically by Lars Onsager in 1944 [5]. We can numerically estimate the value for $T_c(L = \infty)$ by using the scaling relation

$$T_c(L) - T_c(L = \infty) = aL^{-1} \quad (28)$$

for different lattice sizes and their corresponding critical temperature. This expression can be written on a linear form $y = mx + b$, which yields

$$T_c(L) = aL^{-1} + T_c(L = \infty). \quad (29)$$

In this case, $T_c(L)$ represents y, a represents m, L^{-1} represents x, and $T_c(L = \infty)$ represents b. Hence can a linear regression of observed values for $T_c(L)$ be used to solve $T_c(L = \infty)$ numerically.

Tools

We have utilized GitHub copilot to explain our code and help debug. We used the Python library `matplotlib` [6] to produce all illustrations in this report. In addition to using Grammarly to rewrite and check grammar. We have also used ChatGPT as a tool to help with small code snippets.

III. RESULTS AND DISCUSSION

To calculate the values for $\langle\epsilon\rangle$, $\langle|m|\rangle$, $C_V(T)/N$, and $\chi(T)/N$, we run the entire program 100 times before an average is calculated. This procedure is done for various number of cycles. These results are presented in Table II It is clear that when running the MCMC algorithm with 10^6 cycles, the numerical results agree very well with the analytical results, down to a precision of 4 decimals. $\langle\epsilon\rangle$ and $\langle|m|\rangle$ gives a correct value to this precision already at 10^4. A cycle number of 10^4 also gives an acceptable value for the heat capacity, but to the 3rd decimal precision. It is clear that below a cycle number of 10^4 the values for the quantities start to diverge further away from the analytical result. This is most prominent for the heat capacity and the susceptibility. This makes sense considering they both depend on two quantities, so an increase in error is expected.

TABLE II. Comparison of numerically deduced values versus analytical values, for various cycle numbers. Acceptable results are found from 10^5 cycles. The numerically deduced values are calculated by finding the average of 100 runs.

N_{cycles}	$\langle\epsilon\rangle$ [J]	$\langle\|m\|\rangle$	$C_V(T)/N$ [k_B]	$\chi(T)/N$ [1/J]
Analytical	-1.9960	0.9987	0.0321	0.0040
1	-0.98	0.688	0.0	0.0
10	-1.78	0.9255	1.0464	0.1441
10^2	-1.9822	0.9941	0.1386	0.0172
10^3	-1.9946	0.9982	0.0428	0.0053
10^4	-1.9960	0.9987	0.0317	0.0039
10^5	-1.9960	0.9987	0.0320	0.0040
10^6	-1.9960	0.9987	0.0321	0.0040

A. Burn-in time

Figure 2 shows ϵ and $\langle\epsilon\rangle$ as functions of the number of Monte Carlo cycles, at temperatures 1.0 J/k_B and 2.4 J/k_B. Both cases where the initial lattice spins are ordered and unordered are represented. To decide on the burn-in time, we examine where ϵ and $\langle\epsilon\rangle$ stabilize. For a temperature 1.0 J/k_B, these values seem to be $\epsilon = -2$, and $\langle\epsilon\rangle \approx 1.99$. We recognize this as the same result as for the 2×2 lattice case for $T = 1.0$ J/k_B. For a temperature $T = 2.4$ J/k_B, we see a much stronger variation in $\langle\epsilon\rangle$ than for $T = 1.0$ J/k_B, when the initial lattice is unordered. However, the ordered lattice case seems to imply that the stabilizing value is somewhere a bit above $-1.25J$.

When measuring by eye, we can see that at 10^3 cycles, all the graphs display acceptable values regarding the stabilization value. At 10^4, we can safely say that the burn-in time has been reached. Hence can we set the burn-in time to be a number of cycles between 10^3 and 10^4. We see that $\langle\epsilon\rangle$ and ϵ for $T = 2.4$ J/k_B probably would benefit from running the MCMC-algorithm with a higher number of cycles. However, considering computational power and time available, the maximum of cycles ran for the purpose of determining the burn-in time was 10^5, as we believe the graphs for $\langle\epsilon\rangle$ and ϵ for $T = 2.4$ J/k_B are sufficiently close to a stabilization.

B. Probability function

In Figure 1 we approximate the probability function $p(\epsilon; T)$ for $T = 1.0J/k_B$ and $T = 2.4J/k_B$, respectively. The probability function for $T = 1.0J/k_B$ resembles a Boltzmann distribution. In addition to the peak at $\langle\epsilon\rangle = -2$, there appears a relatively smaller peak at $\langle\epsilon\rangle = -1.98$. We suspect it is due to the initial state of the system, though this requires further investigation. For $T = 2.4J/k_B$ the probability function seems to resemble a Gaussian distribution rather than Boltzmann.

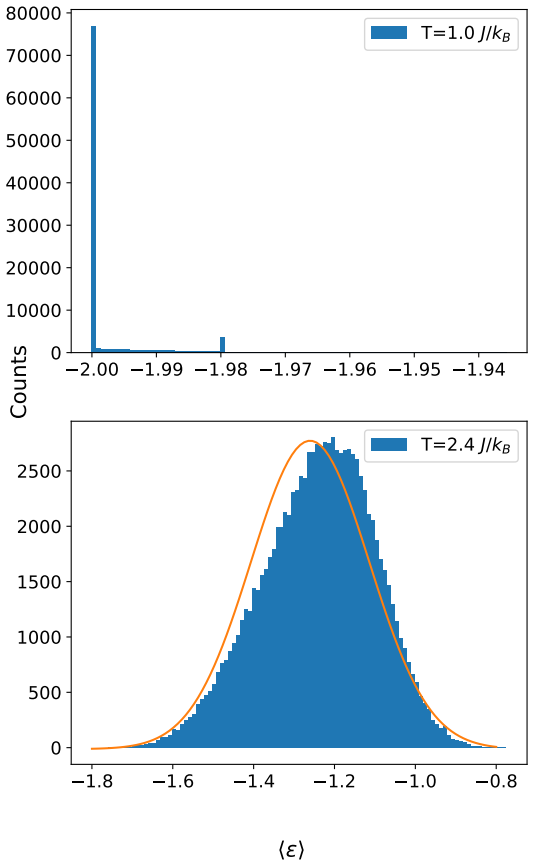


FIG. 1. Probability distribution of $\langle\epsilon\rangle$ at $T = 1.0J/k_B$ (upper panel) and $T = 2.4J/k_B$ (lower panel) generated from 10^5 Markov Chain Monte Carlo cycles. The orange line is the fitted Gaussian distribution $f(x) = 2500\exp^{-\frac{(x+1.2)^2}{2\cdot 0.1^2}}$.

We are unsure if lower temperatures give Boltzmann distribution and higher temperatures approaching Gaussian distribution is a common trend or something that only occurs in our data. This statement would be more reliable if we estimated the probability function for more than two temperatures.

As the temperature increases, the variance increases and higher energies become more probable. This is to be expected as the temperature is a measure of kinetic energy, i.e. $\langle\epsilon\rangle$ should increase/decrease with T. Since higher energies become more probable with higher temperatures, there are more energies to be distributed among the same amount of spins. This is reflected in the increased standard deviation from $T = 1.0J/k_B$ to $T = 2.4J/k_B$.

C. Critical Temperature

In an attempt to identify a phase transition, we create plots of $\langle\epsilon\rangle$, $\langle|m|\rangle$, C_v/N, and χ/N as a function of temperature. We do this for lattices of $\mathrm{L} = \{40, 60, 80, 100\}$, using a cycle number of 10^5. The results can be seen in Figure 3. We have now implemented the burn-in time of 10^4 cycles, so our results are based on 10^5 cycles after the burn-in time is reached. We have chosen to remove the first data point for $L = 100$, as this was clearly an outlier.

We discuss the lower left plot first: the magnetization as a function of temperature. As explained in section II E, the critical temperature is where the system goes from a magnetized phase to a phase of zero net magnetization. We see from the subplot for the magnetization that the graphs seem to undergo a transition between $\sim 2.25 - 2.35J/k_\mathrm{B}$, before flattening out close to zero. Thus this subplot hints that the critical temperature lies somewhere in this range. With this hint from the magnetization phase transition, we will utilize the subplot for the heat capacity C_v/N (upper right subplot in Figure 3) to deduce one value for the critical temperature. We identify that the graphs display a peak. This peak in the heat capacity occurs at the critical temperature. We assume that the accuracy increases for larger lattices, as we are getting closer to infinity, which has an analytical solution, as seen in section II E. Hence will we use the peak for the $L = 100$, with a value of $\sim 2.27J/k_\mathrm{B}$ as our initial guess. We will also generate an average of the four peaks with the values $T = \{2.28, 2.28, 2.29, 2.27\}\ J/k_\mathrm{B}$ for $L = \{40, 60, 80, 100\}$. Hence the average result is which results in a value of 2.28 J/k_B.

In addition to our analytical result for $T_c(L = \infty)$ given in Equation 27, we have also estimated this value numerically, by using Equation 29. The visual results first obtained can be seen in Figure 4. It is clear to see that these results are not satisfactory. From the relation given in Equation 28, one would expect the critical temperature to either decrease or increase linearly with L, depending on whether a is negative or positive. This is not the results we obtain from reading the peaks. However, surprisingly enough, the linear fit shown in Figure 4 yields a function $y = 0.1928x + 2.277$, meaning that our value for $T_c(L = \infty)$ is estimated by $T_c(L = \infty) = 2.277 \approx 2.28J/k_\mathrm{B}$, by using Equation 29. This is exactly the same value we predicted from taking the average of the four heat capacity peaks (with precision to the 2nd decimal), hence our poor fit has resulted in a good estimate for $T_c(L = \infty)$ regardless. Our result of $T_c(L = \infty) = 2.277 \approx 2.28J/k_\mathrm{B}$ does also agree quite well with the analytical value of $2.269J/k_\mathrm{B}$ obtained in Equation 27. However, these results are not very trustworthy due to the relationship between the data points used to deduce them.

As we initially wanted the observed values for T_c to fall in a straight line, we do a second attempt, now using the subplot for susceptibility χ/N in Figure 3. We see from

this plot that the peaks for $L = 60$ and $L = 80$ clearly peak in on the same temperature. We will therefore not get a straight line from this plot either, but the points will appear more ordered than in Figure 4. For the lattice with $L = 40$, we also use the second-highest value, with the benefit of ordering the points. This decision is based on the fact that the smaller lattices are believed to be less accurate, and have larger uncertainties. From this we yield the values $T = \{2.28, 2.29, 2.29, 2.30\}\ J/k_{\mathrm{B}}$ for $L = \{40, 60, 80, 100\}$ respectively. The results are shown in Figure 5. The observed values for T_c yield a linear function $y = -1.157x + 2.309$. From this function we can readily read that $T_c(L = \infty) = 2.309 \approx 2.31 J/k_{\mathrm{B}}$. This value is further away from our initial guess than the results obtained when using the heat capacity results, in spite of the points looking more ordered in this case. Hence can we conclude that our results from the heat capacity data were more correct than the results from the susceptibility, although this might be because of coincidences.

A large source of uncertainty in estimating the critical temperature in this paper is our step size in temperature when calculating the values for C_v/N and χ/N. When estimating $T_c(L = \infty)$ from both the heat capacity and the susceptibility, we obtain peaks with the same temperature, despite different values for L. This is a problem that possibly could have been solved by increasing the step size on the temperature, to distinguish better between the temperatures of the peaks.

IV. CONCLUSION

We have in this paper investigated the two-dimensional Lenz-Ising model; a lattice with periodic boundaries containing two-state spins, with value $+1$ or -1. To generate new states for our lattice and evolve the model, we have used a Markov Chain Monte Carlo algorithm as a tool to draw random samples from our system. The spin of the sample is flipped if the probability of flipping is larger than not flipping, a probability that is decided by calculating the Boltzmann factor for a certain change in energy. We calculate that the only possible values for change in energy after flipping a state is $\Delta E = \{-8, -4, 0, 4, 8\}J$.

The Markov Chain Monte Carlo algorithm is repeated a certain amount of cycles to generate more correct results. We introduce burn-in, to dispose of all values that are biased to an improbable starting point. After running the algorithm for 10^5 cycles, we see a stabilization between $10^3 - 10^4$ cycles, which means that we can conclude that the burn-in time is somewhere in this range. For certainty, when investigating phase transitions of the system, we use a burn-in time of 10^4 cycles. The phase transitions of the system gives us insight into the behavior of various quantities like average state energy $\langle\epsilon\rangle$, average state magnetization $\langle|m|\rangle$, heat capacity C_v/N, and susceptibility χ/N. From our results for the heat capacity, we deduce a critical temperature $T_c = \{2.28, 2.28, 2.29, 2.27\}J/k_{\mathrm{B}}$ for lattices of $L = \{40, 60, 80, 100\}$, and from the susceptibility results we deduce a critical temperature $T_c = \{2.28, 2.29, 2.29, 2.30\}J/k_{\mathrm{B}}$ for the same sized lattices. Although the last set of temperatures is more ordered according to what we would expect, it is the first set that gives us a better value compared to the analytically derived value, with a numerical value of $T_c(L = \infty) = 2.28 J/k_{\mathrm{B}}$ versus an analytical value of $T_c(L = \infty) = 2.269 J/k_{\mathrm{B}}$. However, uncertainties in these calculations must be taken into account if more correct results are desired.

For the case of a 2×2 lattice case we have derived analytical expressions, used to test our code for Markov Chain Monte Carlo. Numerically calculated values for $\langle\epsilon\rangle$, $\langle|m|\rangle$, C_v/N, and χ/N are compared to the analytical solution. We conclude that 10^5 cycles are enough to obtain trustworthy results from our algorithm, as we at this point obtain results with precision to the 4th decimal for $\langle\epsilon\rangle = -1.9969$, $\langle|m|\rangle = 0.9987$, and $\chi/N = 0.0040$, and precision to the 3rd decimal for $C_v/N = 0.0321$.

Future work with the Markov Chain Monte Carlo algorithm and the Lenz-Ising model would include optimizing our code to obtain results with a higher number of cycles, as well as implementing smaller step sizes when examining the change of the system for a temperature range. This, along with an increase in the number of temperature points would allow us to estimate the probability function with greater precision. Implementing burn-in time would create a smoother histogram with no relatively small peaks due to the initial state of the system. This remains a topic for future work.

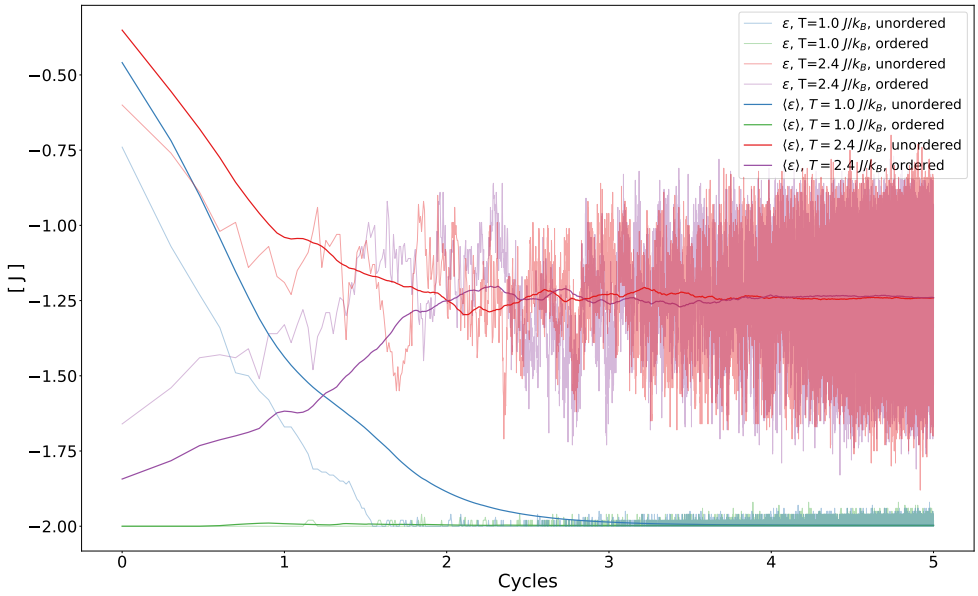


FIG. 2. The average state energy $\langle\epsilon\rangle$ per spin and energy per spin ϵ as a function of number of cycles. Note that the x-scale is logarithmic.

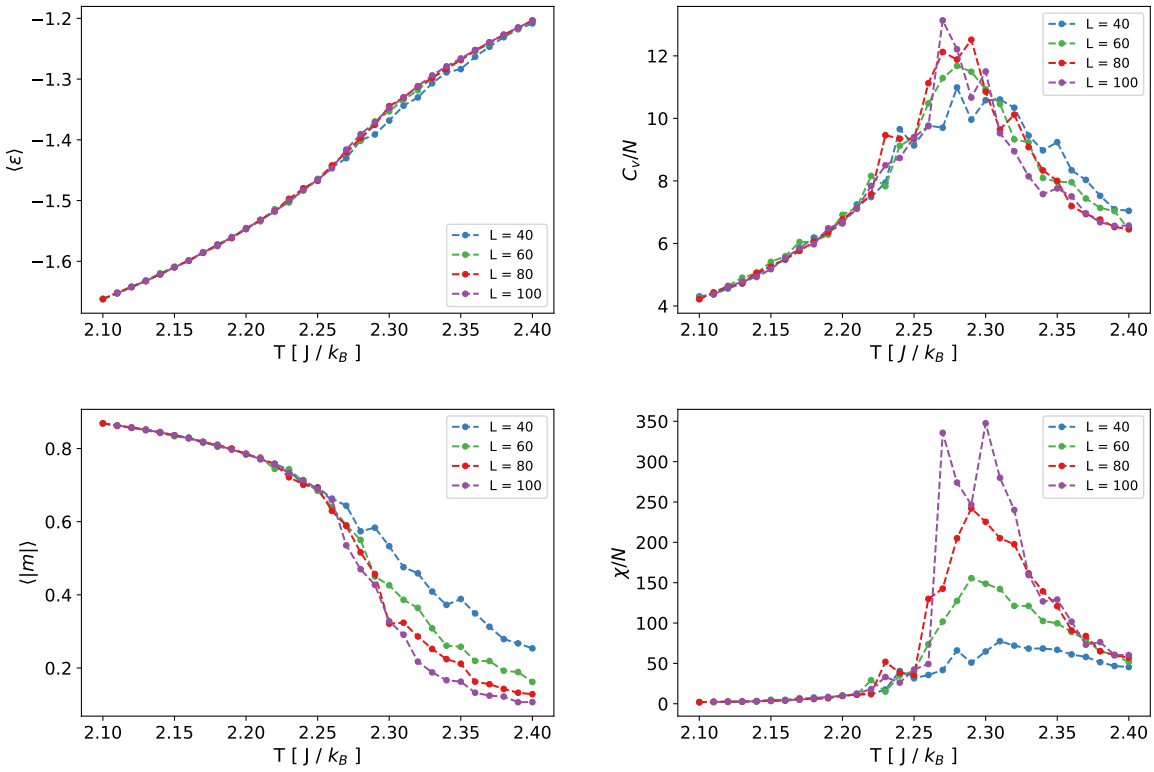


FIG. 3. Values for $\langle\epsilon\rangle$, $\langle|m|\rangle$, C_v/N, and χ/N as function of temperature T in a range $T \in [2.1, 2.4]$. A cycle number of 10^5 is used. The critical temperature T_c is inferred from the upper right panel, with values $T_c = \{2.28, 2.28, 2.29, 2.27\}$ for $L = \{40, 60, 80, 100\}$, and from the lower right panel with values $T_c = \{2.28, 2.29, 2.29, 2.30\}$ for the same values of L.

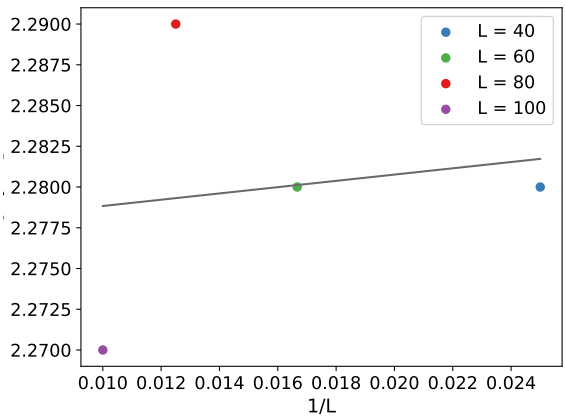


FIG. 4. Linear regression based on the critical temperatures inferred from the heat capacity results from Figure 3. Data points are not ordered in a straight line as we would expect from background theory. Resulting critical temperature for $L = \infty$ is $T_c(L = \infty) = 2.28 J/k_{\mathrm{B}}$. This agrees well with our analytical result.

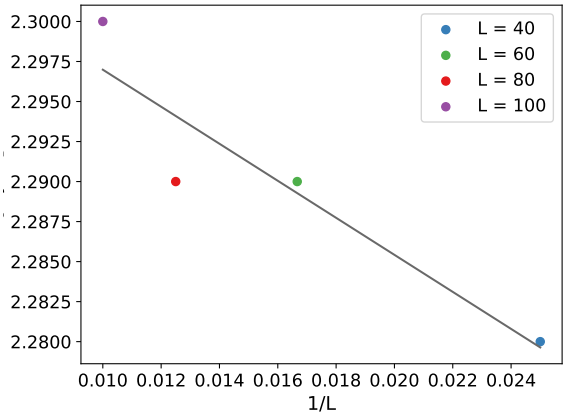


FIG. 5. Linear regression based on the critical temperatures inferred from the susceptibility results from Figure 3. Resulting critical temperature for $L = \infty$ is $T_c(L = \infty) = 2.31 J/k_{\mathrm{B}}$. This somewhat agrees with our analytical result, but only to the 1st decimal.

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Appendix A: Analytical solution for 2×2 lattice

For a square lattice of size $L = 2$, there exists $2^4 = 16$ microstates. They are summarized in Table III along with corresponding total energy, total magnetization and degeneracy.

↑	↓	Energy	Total magnetization	Degeneracy
4	0	-8J	4	1
3	1	0J	2	4
2	2	0J	0	4
2	2	8J	0	2
1	3	0J	-2	4
0	4	-8J	-4	1

TABLE III. Summary of possible microstates in $L = 2$ Lenz-Ising model. The number of degeneracies adds up to 16 microstates. ↑ and ↓ denote spin up and down, respectively.

Using the Boltzmann distribution (Equation 7) and energy function (Equation 3), the partition function of this system is given by

$$\begin{aligned} Z &= 12 \cdot e^{-0J\beta} + 2 \cdot e^{-8J\beta} + 2 \cdot e^{-(-8J)\beta} \\ &= 12 + 2(\underbrace{e^{-8J\beta} + e^{8J\beta}}_{=2\cosh(8J\beta)}) \\ &= 12 + 4\cosh(8J\beta), \end{aligned} \tag{A1}$$

The total energy, normalized by number of spin is

$$\begin{aligned} \langle \epsilon \rangle &= \sum_{\mathbf{s}} \epsilon(\mathbf{s}) p(\mathbf{s}) \\ &= \frac{1}{N} \sum_{\mathbf{s}} E(\mathbf{s}) p(\mathbf{s}) \\ &= \frac{1}{N} \frac{1}{Z} \sum_{\mathbf{s}} E(\mathbf{s}) e^{-\beta E(\mathbf{s})} \\ &= \frac{1}{N} \frac{1}{Z} ((-8J)e^{8J\beta} + 2 \cdot (8J)e^{-8J\beta} + (-8J)e^{8J\beta}) \\ &= -\frac{16}{N \cdot Z} (\underbrace{e^{8J\beta} - e^{-8J\beta}}_{=2\sinh(8J\beta)}) \\ &= \frac{-32J}{4 \cdot Z} \sinh(8J\beta) \\ &= \frac{-8J}{Z} \sinh(8J\beta) \end{aligned} \tag{A2}$$

and $\langle \epsilon^2 \rangle$

$$\begin{aligned} \langle \epsilon^2 \rangle &= \frac{1}{N^2} \frac{1}{Z} \sum_{\mathbf{s}} E^2(\mathbf{s}) e^{-\beta E(\mathbf{s})} \\ &= \frac{1}{N^2} \frac{1}{Z} ((-8J)^2 e^{8J\beta} + 2 \cdot (8J)^2 e^{-8J\beta} + (-8J)^2 e^{8J\beta}) \\ &= \frac{128J^2}{N^2 \cdot Z} \frac{1}{Z} (\underbrace{e^{8J\beta} + e^{-8J\beta}}_{=2\cosh(8J\beta)}) \\ &= \frac{256J^2}{4^2 \cdot Z} \cosh(8J\beta) \\ &= \frac{16J^2}{Z} \cosh(8J\beta). \end{aligned} \tag{A3}$$

Total magnetization normalized by number of spins is

$$\begin{aligned}\langle|m|\rangle &= \frac{1}{N}\frac{1}{Z}\sum_{\mathbf{s}}|M|(\mathbf{s})e^{-\beta E(\mathbf{s})} \\ &= \frac{1}{N\cdot Z}(4e^{8J\beta}+4\cdot 2e^{0}+4\cdot|-2|e^{0}+|-4|e^{8J\beta}) \\ &= \frac{1}{N\cdot Z}(16+8e^{8J\beta}) \\ &= \frac{4+2e^{8J\beta}}{Z}\end{aligned} \tag{A4}$$

and $\langle m^2\rangle$

$$\begin{aligned}\langle m^2\rangle &= \frac{1}{N}\frac{1}{Z}\sum_{\mathbf{s}}M^2(\mathbf{s})e^{-\beta E(\mathbf{s})} \\ &= \frac{1}{N^2\cdot Z}(4^2\cdot e^{8J\beta}+4\cdot 2^2\cdot e^{0}+4\cdot(-2)^2\cdot e^{0}+(-4)^2\cdot e^{8J\beta}) \\ &= \frac{1}{N^2\cdot Z}(32+32e^{8J\beta}) \\ &= \frac{2}{Z}(1+e^{8J\beta})\end{aligned} \tag{A5}$$

The heat capacity of the system is

$$\begin{aligned}\frac{C_{\mathrm{V}}(T)}{N} &= \frac{1}{N}\frac{1}{k_BT^2}\mathrm{Var}(E) \\ &= \frac{1}{N}\frac{1}{k_BT^2}[\langle E^2\rangle-\langle E\rangle^2] \\ &= N\frac{1}{k_BT^2}[\langle\epsilon^2\rangle-\langle\epsilon\rangle^2] \\ &= N\frac{1}{k_BT^2}\left[\frac{16J^2}{Z}\cosh(8J\beta)-\left(\frac{-8J}{Z}\sinh(8J\beta)\right)^2\right]\end{aligned} \tag{A6}$$

and susceptibility

$$\begin{aligned}\frac{\chi(T)}{N} &= \frac{1}{N}\frac{1}{k_BT}\mathrm{Var}(M) \\ &= \frac{1}{N}\frac{1}{k_BT}[\langle M^2\rangle-\langle|M|\rangle^2] \\ &= N\frac{1}{k_BT}[\langle m^2\rangle-\langle|m|\rangle^2] \\ &= N\frac{1}{k_BT}\left[\frac{2}{Z}(1+e^{8J\beta})-\left(\frac{4+2e^{8J\beta}}{Z}\right)^2\right].\end{aligned} \tag{A7}$$