Measuring Critical Exponents using Numerical Simulations for the 2-D Ising Model

S. Nicholls[1] and T. Foldy-Porto[1]
[1] *Department of Physics, Yale University*

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In this experiment we used numerical methods to simulate the two-dimensional Ising Model in a 100 by 100 spin lattice. Using the *Metropolis* algorithm to select a sample of microstates from the system, we estimated the thermodynamic averages of energy, magnetism and spin correlation at a range of temperatures. Measuring these quantities and the derived quantities heat capacity, magnetic susceptibility and correlation length, we were able to observe the phase-transition-like behaviour of this finite system, estimating the critical temperature (T_c) and the critical exponents. While our estimates for T_c were in close agreement with the theoretical value for an infinite lattice, our estimates of the critical exponents and demonstration of power-law behaviour near the critical temperature were less accurate. Effects from the finite-size of our lattice as well as biases introduced by our sampling method may be able to account for these discrepancies.

I. INTRODUCTION

A. Background

The Ising Model is a simplified statistical mechanical model of ferromagnetism. It involves a d-dimensional (where d can be arbitrarily high) lattice of particles which each have a spin of ± 1. The model was invented in 1920 by the German physicist Wilhelm Lenz. The one-dimensional version, which consists of an infinite line of adjacent spins, was solved analytically in 1925 by Ernst Ising[1]. It is much more difficult to find an analytic solution for the thermodynamic properties of a two-dimensional Ising lattice, but in 1944 Lars Onsager solved this case analytically, and also showed the existence of a phase transition[2]. While Onsager's equations, which are referred to later on in this paper, are true for an infinite-size lattice, we can only perform a numerical simulation on a finite-size lattice. Theoretically, we don't expect a finite-size system to show any phase transition, so a large part of this experiment is to verify how well the Onsager equations apply to a large but finite two-dimensional Ising Model.

B. The Ising Model

For our two-dimensional lattice of spins, the Hamiltonian of the system depends on the coupling of each individual particle's spin with nearby particle spins (we will assume it interacts only with its nearest neighbours), as well as coupling with an externally applied magnetic field. Specifically, the Hamiltonian can be written as

$$H = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j - B \sum_i \sigma_i \tag{1}$$

where J represents the strength of nearest neighbour interactions, $\langle i, j \rangle$ denotes a sum over all neighbour pairs in the lattice, $\sigma_i = \pm 1$ is the spin of the particle at the i^{th} lattice position, and B is the strength of the applied magnetic field. In this experiment, we are looking at the case where there is no external magnetic field, so the Hamiltonian reduces to the first term in 1.

If we specify that the spin lattice is to be kept at thermal equilibrium (in contact with a thermal reservoir), then we can use the canonical ensemble to model the statistical behaviour of the system. In the canonical ensemble, the probability that the system occupies a microstate s_i with energy per unit site E_i is given by

$$P(s_i) = \frac{e^{-\frac{E_i}{k_B T}}}{Z} \tag{2}$$

where

$$Z = \sum_i e^{-\frac{E_i}{k_B T}} \tag{3}$$

is the sum of all Boltzmann factors over every possible microstate. Z is called the canonical partition function. Since Z tells us the relative likelihoods of individual microstates occurring, if we determine Z we can use it to calculate the expected values of many thermodynamic variables. We can express the thermodynamic average of the energy of the system at a particular temperature as

$$\langle E \rangle_T = \frac{\sum_i E_i e^{-\frac{E_i}{k_B T}}}{Z} \tag{4}$$

and the expected magnetization is

$$\langle M \rangle_T = \frac{\sum_i M_i e^{-\frac{E_i}{k_B T}}}{Z} \tag{5}$$

Here, M_i is the magnetization per unit site of the microstate s_i. Moreover, manipulating Z also allows us to calculate the heat capacity (c_v) and the magnetic susceptibility (χ) from the variance of the expectations of E and M respectively:

$$c_v = \frac{1}{(k_B T^2)} (\langle E \rangle_T{}^2 - \langle E^2 \rangle_T) \tag{6}$$

$$\chi = \frac{1}{(k_B T^2)}(\langle M \rangle_T{}^2 - \langle M^2 \rangle_T) \tag{7}$$

However, apart from trivially small lattice sizes, it is impractical to calculate the full partition function, because the number of microstates is so large. Therefore, it is necessary to take a representative sample of the possible microstates of a system. From a representative sample, we can estimate the thermodynamic averages of energy and magnetization at a particular temperature, and then use the relationships in eq. 6 and eq. 7 to estimate c_v and χ. To do this, we will use a form of Monte Carlo sampling method. Before discussing this, we will introduce the phenomenon of primary interest to this experiment: phase transitions.

C. Phase Transitions and the Critical Temperature

In thermodynamics, the term phase transition denotes a sudden change in the physical properties of a system. In the absence of an external magnetic field, we expect that the spins in our lattice will try to align themselves with their neighbours, as 1 tells us that when the nearest neighbours are all aligned, the energy of the system is minimized. At very high temperatures, however, where the size of the thermal fluctuations is much greater than the strength of the nearest neighbour interactions, we expect the spins will be arranged randomly (meaning M is 0). It is only at low temperatures where the nearest neighbour interactions between spins will dominate that we expect to see the alignment of all spins in the system. Here, M will be either $\pm N^2$. Somewhere in between these two extremes, as we decrease the temperature of the system, we expect to see $|M|$ rise sharply above 0 and start moving toward N^2. This is a phase transition, and the temperature at which this occurs is known as T_c, the critical (or Curie) temperature.

At T_c we expect there to be a sharp rise in M and E of our system. Since χ and c_v represent the first derivatives of M and E with respect to temperature, we expect to see a divergence in the behaviour of these quantities at T_c. Since the derivative of E is showing a divergence at T_c, this is known as a second-order phase transition. By graphing these four quantities against temperature and observing the temperature at which there is a sharp rise (for M and E), or the temperature at which there is a discontinuity (for χ and c_v), we can estimate T_c for our system.

II. METHODS

A. Monte Carlo Sampling with the Metropolis Algorithm

Theoretically, it possible to obtain all relevant thermodynamic variables about an $N \times N$ Ising lattice (for finite N) by simulating every possible microstate of the system and calculating the relevant variables for that state. However, even for relatively small N this is computationally impossible. For a 100×100 lattice, for example, there are on the order of $2^{100^2} \approx 10^{3010}$ distinct microstates. Therefore, we need some way to to take a representative sample of a manageable size of the microstates of our system.

In this experiment, we used the *Metropolis* algorithm, a type of Markov Chain Monte Carlo sampling method. The *Metropolis* algorithm uses the fact that microstates with a higher total energy are less likely to occur than microstates with a lower total energy. The algorithm takes a modified random walk through the space of microstates of our system. From any given microstate during the random walk (call the current state s_c), the next microstate is chosen either as a repeat of the current microstate (s_c) or as a new microstate. From each microstate s_c, a possible next microstate $s_{c'}$ is created by flipping a given ratio of the spins in the whole system. The spins to be flipped are chosen randomly, and the system decides to move to state $s_{c'}$ if and only if $s_{c'}$ has a higher occurrence probability than s_c. From the Boltzmann probabilities for the canonical ensemble we know that the probability of the system occupying a microstate s is proportional to

$$P(s) \propto e^{-\frac{E_s}{k_B T}} \tag{8}$$

The algorithm decides whether or not to transition to $s_{c'}$ based on the ratio of the probabilities of the two states occurring:

$$a = \frac{P(s_{c'})}{P(s_c)} = \frac{e^{-\frac{E_{c'}}{k_B T}}}{e^{-\frac{E_c}{k_B T}}} \tag{9}$$

If this ratio is greater than 1 (meaning $s_{c'}$ has a lower energy than s_c), then the system will always transition. If this ratio is smaller than 1, the system will transition to $s_{c'}$ with probability a, and will remain at s_c with probability $1 - a$.

Using these selection rules, the *Metropolis* algorithm is able to sample a wide range of randomly-generated microstates, among which the proportion of times that certain microstates are selected is proportional to the probability of those microstates occurring. In this way, the algorithm produces a set of microstates that is representative of all possible microstates; this set is called the *typical set*.

B. Simulation Paradigm

The aim of this experiment is to simulate the behaviour of a phase transition at T_c. Therefore we need to make many simulations of a spin lattice kept in thermal equilibrium at temperatures near the predicted T_c value. We ran the simulation at 281 different temperatures (between 1.20 and 4.00, at increments of 0.01). We used

a 100 by 100 grid of spins, which wraps around itself in both the vertical and horizontal directions (so that the first and the hundredth spins are neighbours). In effect, therefore, our lattice of spins is laid out on the surface of a torus. Before beginning the *Metropolis* sampling where we actually collect data on the energy, magnetization and spin correlation coefficient, it is necessary to undergo a process of "annealing". This involves starting the simulation at a temperature much higher than T_c and gradually reducing the temperature to T_{min}. While the temperature is being reduced, we cycle through a large number of microstates (we chose 60,000), before arriving at T_0. The purpose of annealing is to make sure the system is in a thermodynamically probable region of the space of all microstates. After annealing, but before taking measurements, the simulation also cycled through 40,000 microstates at T_0. This is called burning-in, and the goal is to prevent the system from becoming stuck in a region which is a local minimum of energy of the system, but not a global minimum and therefore not representative of the typical set of microstates we would expect to occur. Finally, at each temperature we took a sample of 10,000 microstates at which the Energy and Magnetization were measured, and 100 microstates at which $\langle\sigma(0)\sigma(x)\rangle$ (the spin correlation coefficient) was measured. Refer to the appendix for a summary of the parameters used in the simulation.

III. RESULTS

A. Determination of T_c

The data we procured from our implementation of the *Metropolis* algorithm, as described in the **methods** section, is shown in figures 1 through 6. Our first aim was to calculate the critical temperature, T_c, since that would inform our later calculations of the critical exponents. To do this, we plotted four quantities as a function of temperature: the magnetization per site M, the specific heat capacity c_v, the magnetic susceptibility χ, and the correlation length ξ.

The magnetization plot (figure 1) indicates a phase transition at T_c, where the system experiences a rapid change in properties. For the magnetization per site, specific heat capacity, and energy per site, shown in figures 1, 2, and 3 respectively, we were able to plot our experimental results alongside Lars Onsager's theoretical predictions of these quantities. Onsager's solution for the 2D Ising model predicts a magnetization per site of

$$M(T) = \left(1 - [\sinh(2/T)]^{-4}\right)^{1/8} \tag{10}$$

The specific heat capacity is given by

$$c_v = \frac{\partial E}{\partial T} \tag{11}$$

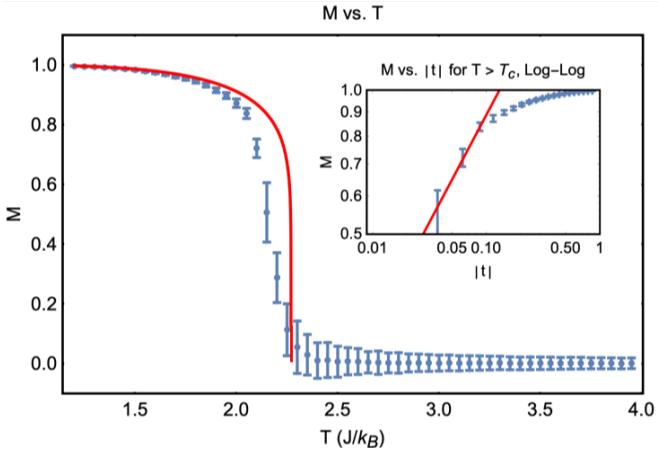

FIG. 1. Magnetization per site M vs. temperature T (J/k_B) simulated on an $N = 100$ lattice. Onsager's exact solution for $M(T)$ is plotted in red alongside our data. Critical behavior in the experimental data occurs at $T_c = 2.2 \pm 0.1$. **Inset:** magnetization per site vs. reduced temperature plotted on a log-log scale with a line of best fit plotted in red.

where,

$$E(T) = -2\tanh(\frac{2}{T}) - \frac{\sinh^2(2/T) - 1}{\sinh(2/T)\cosh(2/T)}\left[\frac{2}{\pi}K_1(\kappa) - 1\right] \tag{12}$$

$$\kappa = 2\frac{\sinh(2/T)}{\cosh^2(2/T)} \tag{13}$$

$$K_1(\kappa) = \int_0^{\pi/2} \frac{\mathrm{d}\phi}{\sqrt{1 - \kappa^2\sin^2\phi}} \tag{14}$$

Our experimental data (in blue) did not align entirely with the theoretical values (in red), which can be attributed to the fact that we are working with a lattice of finite size. This can be seen in all three plots that included both experimental and theoretical results: $M(T)$, $c_v(T)$, and $E(T)$. The finite-ness of our lattice also affects the critical temperature: Onsager's equations predict a critical temperature of $T_c \approx 2.269$, which is where the red lines experience second-order discontinuities in figures 1 through 3. Our data exhibits such behavior slightly below that temperature. In the plots of χ and ξ, this can be observed as a left-shift (with respect to $T = 2.269$) of the peak. In M, a left-shift of the rapid decline in magnetization, and in E, a left-shift of the inversion point, where the curve switches from convex to concave.

Through a visual inspection of each plot, we noted the location of the extremal behavior (rapid decline for M, maxima for c_v, χ, and ξ) and the corresponding uncertainty. This data is presented in the table below:

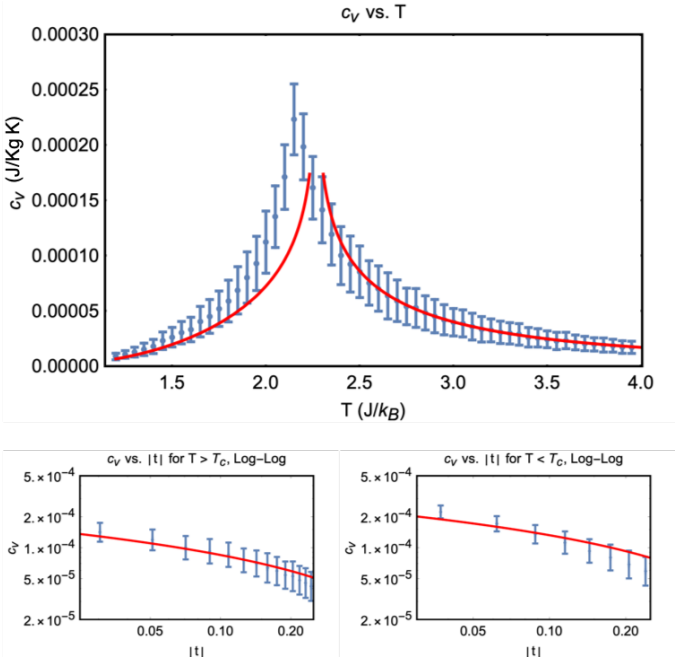

FIG. 2. Specific heat capacity c_v vs. temperature T (J/k_B) simulated on an $N = 100$ lattice. Onsager's exact solution for $c_v(T)$ is plotted in red alongside our data. A maximum occurs at $T_c = 2.2 \pm 0.1$. **Inset left:** specific heat capacity vs. reduced temperature plotted for $T > T_c$ on a log-log scale. Line of best fit plotted in red. **Inset right:** specific heat capacity vs. reduced temperature plotted for $T < T_c$ on a log-log scale. Line of best fit plotted in red.

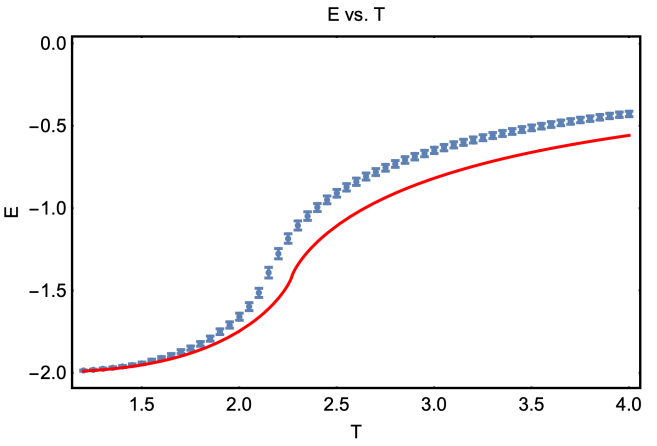

FIG. 3. Energy per site E vs. temperature $T(J/k_B)$ simulated on an $N = 100$ lattice. Onsager's theoretical prediction (equation 15) is plotted in red.

Location of critical behavior		
Quantity	T_c	δT_c
M	2.2	0.1
c_v	2.2	0.1
χ	2.3	0.1
ξ	2.22	0.02

Averaging the T_c for each of these four plots, we determined the critical temperature for our 100 × 100 lattice to be:

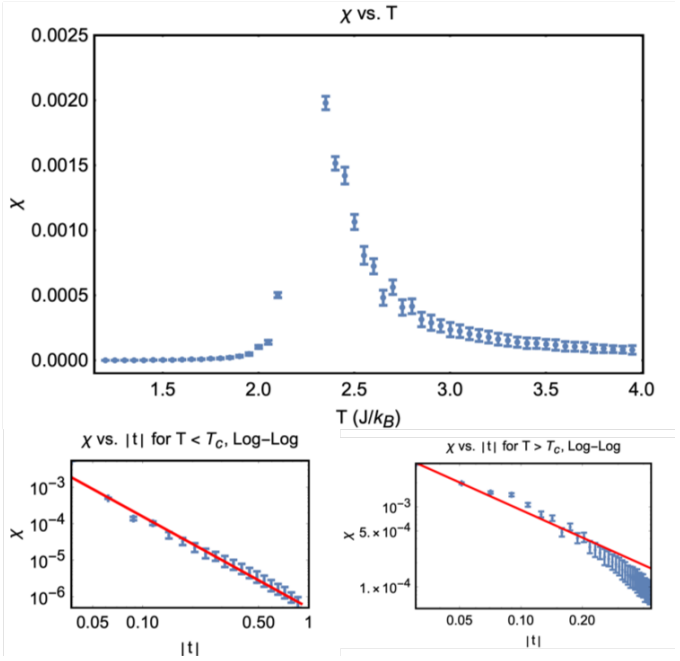

FIG. 4. Magnetic susceptibility χ vs. temperature T (J/k_B) simulated on an $N = 100$ lattice. A maximum occurs at $T_c = 2.3 \pm 0.1$. **Inset left:** magnetic susceptibility vs. reduced temperature plotted for $T < T_c$ on a log-log scale. Line of best fit plotted in red. **Inset right:** magnetic susceptibility vs. reduced temperature plotted for $T > T_c$ on a log-log scale. Line of best fit plotted in red.

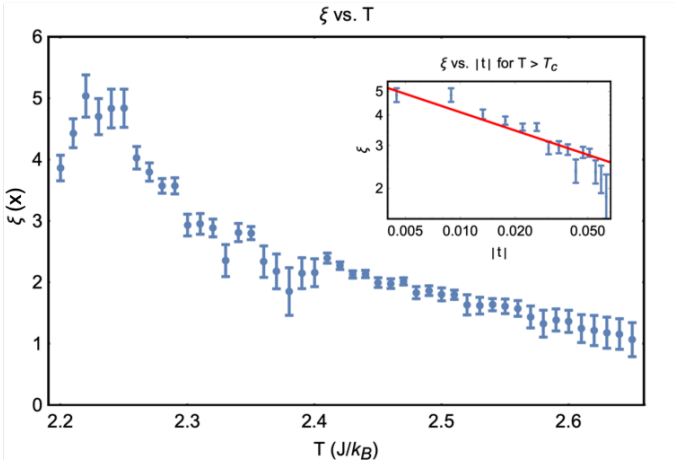

FIG. 5. Correlation length ξ (measured in units of x, the lattice site index) vs. temperature T (J/k_B) simulated on an $N = 100$ lattice. A maximum occurs at $T_c \approx 2.22 \pm 0.02$. **Inset:** correlation length vs. reduced temperature plotted for $T > T_c$ on a log-log scale. Line of best fit plotted in red.

$$T_c = 2.23 \pm 0.08 \tag{15}$$

Note that the theoretical value of $T_c = 2.269$ falls

within the error of the T_c that we calculated.

Two other quantities we measured in this simulation were the correlation function $R(x)$ (figure 6) and the correlation length ξ (figure 5). The correlation function is defined as

$$R(x) = \langle \sigma(0)\sigma(x) \rangle \tag{16}$$

meaning it is the expected value (the average over the whole lattice) of the product of a particle's spin and the spin of a particle x lattice grid units away. We expect the correlation function to follow an inverse exponential distribution:

$$R(x) \propto e^{-\frac{x}{\xi}} \tag{17}$$

From this we can see that ξ is a measure of how quickly the correlation between spins dies off as a function of distance. We expect that ξ will vary as a function of temperature, however since it is not a first derivative of a quantity with respect to temperature, we don't expect to see a divergence at T_c.

B. Determination of critical exponents

In analyzing the behaviour of various thermodynamic quantities near the critical temperature it is useful to introduce the reduced temperature t:

$$t = \frac{T - T_c}{T} \tag{18}$$

The reduced temperature is useful because the theory of critical phenomena tells us that near T_c heat capacity, magnetic susceptibility, correlation length and magnetization all follow power law distributions as a function of $|t|$.

Using our estimate for T_c we plotted our thermodynamic variables against the reduced temperature. For c_v and χ, we plotted the behavior above and below T_c on separate log-log plots (figures 2 and 4, respectively). For M and ξ, the critical exponents were only valid for temperatures above T_c, so only one plot was necessary (figures 1 and 5, respectively). We plotted our data on a log-log scale to demonstrate the power-law behavior of the variables.

For each variable, we found a line of best fit (along with the corresponding χ^2 value), from which we extracted our critical exponents. To obtain an uncertainty for our critical exponents, we varied them until the χ^2 value doubled, and then marked that variation as our uncertainty. The critical exponents we obtained are presented in table 1.

Critical Behaviour near T_c		
Relationship	**Theoretical Value**	**Our result**
$c_v \propto \lvert t \rvert^{-\alpha}$	$\alpha = 0$	0 ± 0.1
$\chi \propto \lvert t \rvert^{-\gamma}$	$\gamma = 7/4$	1.8 ± 0.2
$\xi \propto \lvert t \rvert^{-\nu}$	$\nu = 1$	0.27 ± 0.03
$\lvert M \rvert \propto \lvert t \rvert^{\beta}$	$\beta = 1/8$	0.4 ± 0.2

TABLE I. Showing the expected critical behaviour of thermodynamic quantities near T_c alongside our experimental results. The fact that $\alpha = 0$ indicates that c_v has logarithmic scaling rather than power-law scaling. Note that the relations for c_v, χ and ξ are expected to hold both above and below T_c, while the relationship for $|M|$ is relevant only below T_c. Above T_c we expect the magnetization to be 0 as the spins are randomly aligned.[3]

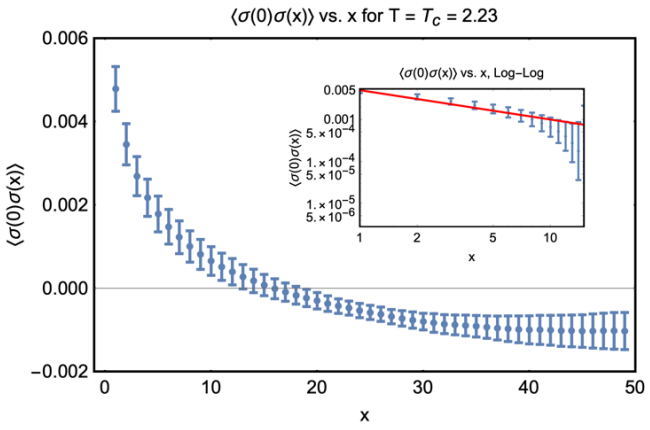

FIG. 6. Correlation strength $\langle \sigma(0)\sigma(x) \rangle$ vs. distance x (measured in discrete lattice indices) simulated on an $N = 100$ lattice. **Inset:** correlation strength vs. distance plotted on log-log scale with a line of best fit (for $x < 20$) plotted in red.

C. Calculation of Uncertainties

The uncertainties in E, M and $R(x)$, at a specific temperature, are calculated simply as the standard deviation of all of the measurements of these quantities taken for each lattice configuration sampled. Equation 6 tells us that c_v is proportional to the variance of E. Therefore, to calculate an uncertainty for c_v we had to estimate an uncertainty in the variance of E. This was done by dividing the 10,000 measurements of E taken at each temperature into 200 separate bins of 50 measurements. If we define the random variable $BinVar(E)$ as the variance of a particular 50-member bin of Energy values, then we calculate the uncertainty of our variance of E from the variance of the 200 measurements of BinVar(E) that are made. Thus, the uncertainty in c_v is

$$\delta(c_v) = \frac{1}{k_B T^2} \sqrt{Var(BinVar(E))} \tag{19}$$

An identical method was used to calculate σ_χ from the mean values and variances of M at each temperature.

Finally, ξ was estimated from the slope of the graph of

$\log R(x)$ vs. x. If we call the slope of this regression line k, which has a standard deviation δk, then by 17

$$\xi = \frac{-1}{k} \tag{20}$$

$$\delta(\xi) = \xi^2 \delta k \tag{21}$$

IV. CONCLUSION

The data presented here demonstrate the success of numerical methods in producing data that agree with theoretical predictions. We observed critical behavior, indicating a phase transition, at a temperature of $T = 2.23 \pm 0.08$. Our calculation of the critical exponents differed slightly from the theoretical predictions of Onsager. The exponents for M, c_v, and χ were reasonably close to predicted values (within error bars even, for χ and c_v); we attributed that deviation to the fact that our lattice was of finite size while the theoretical values are for a lattice of infinite size.

The critical exponent we calculated for ξ was not near the predicted value. This is not totally surprising, since the raw data for spin correlation output by the simulation showed that at almost every temperature the correlation coefficient went and stayed below 0 at a certain distance x (this can be seen for T = 2.23 in 6). Not only is this indicative that the spin correlation is behaving not entirely as expected (we would expect the correlation to go to zero at far distances, not that particle spins would be anti-correlated), but it also introduced greater error in the calculation of ξ, as it meant there were fewer positive data points at each temperature for which $\log R(x)$ could be calculated. The cause of this phenomenon is not clear, but it may be worth testing with a larger lattice size to see if it may be a finite-size effect. Furthermore, as it is computationally demanding to calculate $R(x)$, we only did so for 100 microstates sampled. It is quite possible that this is not large enough to attain a representative sample of the typical set of microstates, which could explain some degree of the unexpected behavior observed for ξ.

V. REFERENCES

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[2]L. Onsager, "Crystal statistics. i. a two-dimensional model with an order-disorder transition," Physical Review **65**, 117 (1944).
[3]D. Stewart, "Physics 381/382/504 lab handout," (2019).

VI. APPENDIX

Simulation Parameters	
N	100
$T_{min}(J/k_B)$	1.20
$T_{max}(J/k_B)$	4.00
$T_{step}(J/k_B)$	0.01
T_0(anneal) (J/k_B)	5.0
steps (anneal)	60 000
steps (burn in)	40 000
steps (for E, M)	10 000
steps (for $\langle\sigma(0)\sigma(x)\rangle$)	100
flip ratio	0.2

TABLE II. Showing the values of various parameters used in our simulation. The meaning of these parameters is described in the **methods** section, part **b** "Simulation Paradigm."