Numerical Ising Model Simulations on Exactly Solvable and Randomized Lattices

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(Dated: May 17, 2015)

The Ising model is enormously useful in statistical mechanics, both as a model system for concepts such as the lattice renormalization group method and lattice duality, and as a tool for describing physical phenomena such as ferromagnetism. Its simplicity and built-in symmetries allow for exact calculations of quantities such as the critical temperature and critical exponents. Additionally, numerical methods such as the Metropolis-Hastings algorithm complement exact solutions and allow for insight in cases which cannot be exactly solved. This paper describes an implementation of the Metropolis-Hastings algorithm for several geometries with exact solutions, as well as an implementation on a random lattice. The critical behavior of each system is examined and compared to theoretical predictions.

I. INTRODUCTION

The Ising model is one of the most commonly used tools in statistical mechanics for modeling simple interacting many-particle systems. It consists of a set of spins $\sigma_i = \pm 1$ on a lattice. The spins interact with both their nearest neighbors and an external magnetic field via a Hamiltonian of the form

$$\beta\mathcal{H} = -K\sum_{\langle i,j\rangle}\sigma_i\sigma_j - h\sum_{i=1}^{N}\sigma_i, \tag{1}$$

where the notation $\langle i,j\rangle$ indicates a sum over nearest neighbor lattice points, $K > 0$ is a parameter describing inter-particle interactions, and h is a nondimensionalized external magnetic field.[1] We see that is energetically favorable both for spins to locally align with one another, as well as for spins to align with an external magnetic field. The parameters K and h are generally regarded as being inversely proportional to temperature—$K = \hat{K}/k_BT$, $h = \hat{h}/k_BT$—but as they are purely phenomenological parameters, they do not necessarily have this form.

The Ising model is best known for describing the emergence of ferromagnetism in crystals of atoms that interact via spin-spin coupling. However, many other systems that experience second-order phase transitions, such as water near its critical point, exhibit the same critical behavior as the Ising model. This phenomenon of universality further increases the utility of the Ising model. Ising, who was first introduced to the model by his thesis supervisor, W. Lenz, in 1920, solved the model exactly in the one-dimensional case. However, the one-dimensional case does not exhibit a phase transition, so the general model was initially assumed to be ineffective at describing systems with critical points. Bragg and Williams tried to approach the model with a mean-field theory, but their approach predicts a phase transition in any number of dimensions, which is at odds with the exact one-dimensional result.[2]

In 1944, Onsager exactly solved the Ising model for a two-dimensional square lattice. He demonstrated that, for an infinite lattice, the ferromagnetic phase transition occurs at critical temperature of

$$T_c = \frac{2}{\ln(1+\sqrt{2})}\frac{\hat{K}}{k_B} \approx 2.269\,\hat{K}/k_B, \tag{2}$$

where k_B is Boltzmann's constant. Onsager's derivation, which is long and involved, takes advantage of a symmetry in the model to develop an infinite-dimensional Lie algebra that makes the solution simpler.[3][4] One writer, in order to illustrate the complexity of Onsager's approach, notes that the famously laconic Landau and Lifshitz take eight pages to recreate the solution.[5] Since the publication of Onsager's solution, many physicists have employed simpler or more direct techniques to reproduce his solution in a more accessible way;[6] other writers have used intuitive or physical reasoning to arrive at the same answer with minimal computation.[5]

The Ising model is useful even in cases for which it cannot be solved exactly. For example, it has been used on random graphs to study the spread of diseases in complex networks.[7] Other variants that have been studied include models introducing time dependent statistics[8] and Monte Carlo algorithms on randomized nonlinear σ models.[9]

On both geometries where the Ising model can be exactly solve and those where it cannot, numerical simulations can also provide insight into critical behavior. The most common model for simulating Ising systems is the Metropolis-Hastings algorithm, originally developed for use in molecular dynamics simulations.[10] In this paper, we describe an implementation of the Metropolis-Hastings algorithm in Mathematica on four lattices: a square lattice, a triangular lattice, a hexagonal lattice, and a randomized lattice constructed via a Delaunay triangulation. We investigate the critical behavior of the systems and find generally good agreement with theoretical predictions.

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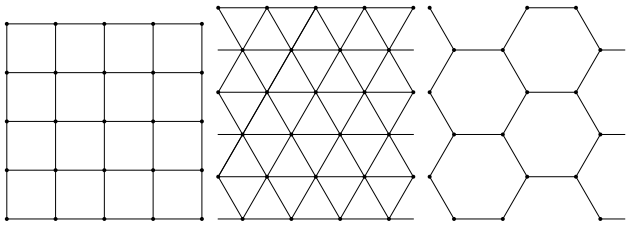

FIG. 1: The square, triangular, and hexagonal lattices.

II. DESCRIPTION OF THE LATTICES

In this section, we present the lattices to be studied and review some theoretical predictions about each lattice.

A. Exactly solvable lattices

The square, triangular, and hexagonal lattices, shown in Figure 1, all have exactly computable critical temperatures. The most straightforward way to find these critical temperatures is via *duality*. The partition function for the square lattice admits both high- and low-temperature series expansions. One can identify a one-to-one correspondence between terms in the two expansions, with corresponding values of the coupling constant related by the duality relation

$$e^{-2\widetilde{K}} = \tanh K,$$

where $\widetilde{K}$ is the low-temperature parameter and K is the high-temperature parameter. The square Ising model is therefore referred to as *self-dual*—high-temperature configurations of the system can be mapped onto low-temperature configurations, and vice versa. The partition function is expected to be analytic everywhere except at a unique phase transition, which must therefore occur when $\widetilde{K} = K \equiv K_c$—otherwise, the duality would give another divergent point for the partition function. Solving for K_c yields

$$K_c^{\square} = \frac{\ln(1+\sqrt{2})}{2}, \tag{3}$$

$$T_c^{\square} = \frac{2}{\ln(1+\sqrt{2})}\frac{\hat{K}}{k_B} \approx 2.269\,\hat{K}/k_B, \tag{4}$$

as promised in the introduction.

The triangular lattice is not self-dual, but it is the dual of the hexagonal lattice—and vice versa. The critical temperatures for both systems can therefore be found by composing the two dualities in both orders, yielding

$$T_c^{\triangle} = \frac{4}{\ln 3}\frac{\hat{K}}{k_B} \approx 3.641\,\hat{K}/k_B, \tag{5}$$

$$T_c^{\hexagon} = \frac{2}{\ln(2+\sqrt{3})}\frac{\hat{K}}{k_B} \approx 1.519\,\hat{K}/k_B. \tag{6}$$

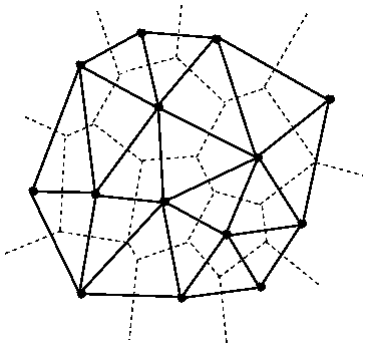

FIG. 2: An example of a Delaunay triangulation (solid lines). The dual figure, in dashed lines, is known as a Voronoi diagram. (Kristof Van Laehoven, `http://www.comp.lancs.ac.uk/~kristof`)

The above results are for lattices of infinite size. Our computations will be on finite-size lattices with periodic boundary conditions, which accurately recreate infinite-size results in many respects.

B. Randomized 2D lattice

To generate the random lattice, we select 400 points from a random distribution on the unit square. We then perform a Delaunay triangulation on the points in order to generate a plausible set of nearest neighbors. The Delaunay triangulation finds a set of triangles covering the lattice such that the circumcircle through the vertices of each triangle encloses no other points in the lattice.[11] Figure 2 shows an example of a Delaunay triangulation. However, we would prefer for the lattice to have periodic boundary conditions, and by default the Delaunay triangulation cannot wrap around the edges. In order to rectify this, we construct a second lattice by shifting each point (x, y) to $(x + 0.5, y + 0.5) \bmod 1$, essentially swapping the roles of the center and the corners of the lattice. We then construct a second Delaunay triangulation on this other lattice—this one connects the points lying on the edges of the first diagram, while leaving gaps in the center. Since the Delaunay triangulation is a local construction, points not near the edges or the center of the grid had the same connections in both triangulations. Taking the union of the two triangulations, then, yields a periodic triangulation. This construction is analogous to the idea of stitching together multiple charts to create a continuous atlas on a manifold in differential geometry.

Table I compares the number of nearest neighbors in the various regular lattices the average number of nearest neighbors in the Delaunay triangulation. The Delaunay connectivity is closer to that on the triangular lattice than the square or hexagonal lattices. As a first estimate, then, we expect to observe behavior on the 2D lattice that more closely recreates the triangular-lattice behavior than any of the other systems. Dorogovtsev,

Lattice	(Avg.) Connectivity
Hexagonal lattice	3
Square lattice	4
Triangular lattice	6
Random 2D lattice	6.64

TABLE I: Exact number of nearest neighbors on the hexagonal, square and triangular lattice; and average number of Delaunay-triangulated nearest neighbors on the random lattice.

Goltsev, and Mendes give a formula for the critical temperature on random networks with a power-law connectivity distribution that predicts a critical temperature of $T_c = 6.15\,\hat{K}/k_B$ for our system. However, the connectivity on our lattice does not follow a power law, so this prediction may not turn out to be accurate.

III. METROPOLIS-HASTINGS ALGORITHM

The Metroplis-Hastings algorithm is a common algorithm for performing Monte Carlo computations on statistical mechanical ensembles. We have implemented the algorithm in Mathematica, extending earlier work by Gaylord and Nishidate.[12] The goal of the Metropolis-Hastings algorithm is to explore the state space of a system ergodically, and hence not only locate thermally stable configurations but also generate an ensemble of states from which thermodynamic variables can be computed. There are three steps to the algorithm:

1. Generate an initial configuration with spins randomly selected to be up or down. In each model, we used 400 points with periodic boundary conditions, a scale at which real phase transitions could be observed but whose computations could still be feasibly performed on a laptop computer.

2. Select a random spin and compute the change in the system's total energy ΔE that would arise due to flipping it.

   (a) If $\Delta E < 0$, flip the spin with probability 1.

   (b) If $\Delta E > 0$, flip the spin with probability $e^{-\Delta E/k_B T}$, where T is the temperature of the system.

   This approach is intended to mimic the physical result that an excitation of energy ε in a canonical ensemble will occur with relative probability $e^{-\varepsilon/k_B T}$. This step is repeated until the system thermalizes—*i.e.*, the mean magnetization relaxes to its equilibrium value.

3. Repeat the spin-flip procedure many times and collect statistical data from the resulting ensemble of microstates. For a lattice with 400 points, we did this on the order of 10^5-10^6 times.

By performing this procedure at different temperatures, a profile of the system's thermal behavior can be constructed.

IV. RESULTS

For each geometry, we randomly selected 400-800 values for the nondimensionalized temperature between $T = 0.0$ and $T = 5.0$ ($T = 0.0$ to $T = 8.0$ for the random lattice). At each temperature, we ran the Metropolis-Hastings algorithm in the zero-field limit, with $B = h = 0$. We computed the average magnetization of each run after it had thermalized; the results are plotted in Figure 3.

For a system with N particles, $N_\uparrow$ of which are spin-up and $N_\downarrow = N - N_\uparrow$ of which are spin-down, the magnetization is defined as

$$M \equiv \frac{N_\uparrow}{N} - \frac{N_\downarrow}{N}.$$

It ranges in value from -1 to $+1$ and provides a rough picture of how well-aligned the overall system is. Above the critical temperature, we expect to observe a magnetization close to zero. Below the critical temperature T_c, the magnetization relaxes to $M = \pm 1$, with the relaxation governed by a critical exponent β:

$$|M| \propto |T_c - T|^\beta. \tag{7}$$

Since we are working in the zero-field limit, neither the spin-up nor the spin-down direction is preferred; the occurrence of one or the other is an example of spontaneous symmetry breaking.

The key test of the Metropolis-Hastings algorithm is its ability to successfully reproduce a ferromagnetic phase transition at the Ising critical temperature, as well as the proper critical exponents governing the system's behavior near that point. We performed a nonlinear fit to the data to extract the parameters T_c and β for each lattice. Our results are quoted in Figure 3 and Table II; our method for computing them is outlined below.

A. Critical curve-fitting

The critical temperature T_c and critical exponent β were computed by performing a nonlinear fit to the data of the form

$$|M(T)| = A|T_c - T|^\beta, \tag{8}$$

where A is an additional undetermined constant. We performed this fit using Mathematica's `FindFit[]` command.

A brief examination of Figure 3 will reveal that the data did not follow a clean power law, as might be expected from (8). Finite magnetization persisted above the critical temperature in all four geometries, making the plot look more like a logistic plot than a power law

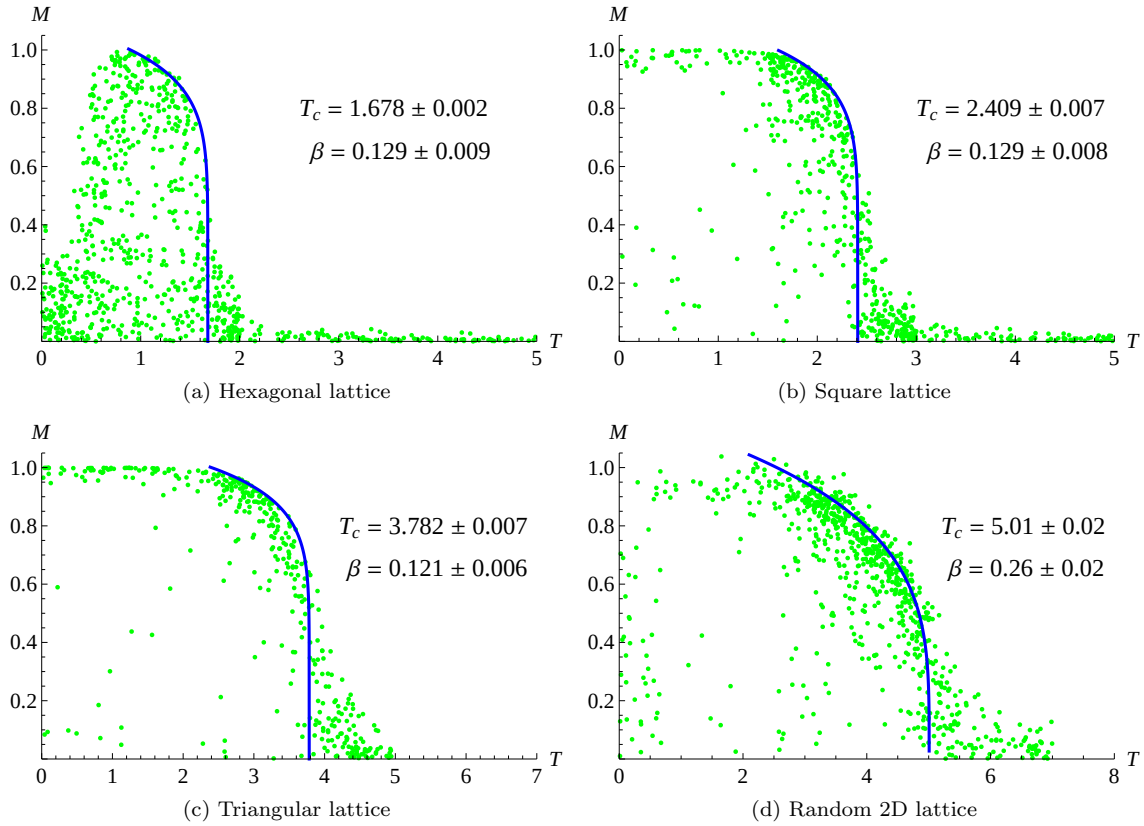

FIG. 3: Absolute magnetization as a function of temperature, with critical exponent fit, on (a) the hexagonal lattice, (b) the square lattice, (c) the triangular lattice, and (d) the random 2D lattice. Note the softer transition to the magnetized phase in the random lattice.

distribution. This was likely due to the finite size of the system—even above the critical temperature, correlations across the scale of the system do not vanish, and hence a finite magnetization may be thermally favorable.

Furthermore, many iterations of the model exhibited low magnetizations even below the critical temperature. This was due to our finite computational resources: at low temperatures, it is possible for the Ising model to become frozen into locally optimal energy configuration that nonetheless has a low net magnetization, because it lacks the thermal energy to escape this nonoptimal configuration. In principle, given infinite time such a system should eventually equilibriate to a high-M configuration, but it would take prohibitively long to actually simulate this entire thermalization process. This freezing-in is especially prevalent in the hexagonal lattice (see Figure 3(a)), which has the lowest connectivity of the three systems—with fewer links for fluctuations to move through the system, it is more likely for a nonoptimal configuration to become frozen in. In fact, at the very lowest temperatures the hexagonal lattice *never* reached the fully magnetized state.

The part which *could* be fitted well by (8) was the upper edge of the magnetization distribution for $T < T_c$. For each of the regular lattices in Figs. 3(a-c), this edge curved smoothly away from the critical point in a manner consistent with a power-law model. In order to fit the model to this edge, we computed the convex hull of the data in the (T, M) plane, extracting the outermost points along the edge. We then fit the model to those data points. For the random lattice, the upper edge was somewhat less sharply defined, so we computed the fit on a thin strip of data points near the outer edge. The uncertainties were computed by incrementing the number of points in the convex hull that were used to compute the fit and examining how much the fitted parameters changed under this perturbation.

V. DISCUSSION

Table II collects both the computed critical parameters and the theoretical values for the exactly solvable lattices. The critical temperatures for the exactly solvable systems were discussed in Section II.A above. The measured critical temperatures are all somewhat higher than the theoretical values. This is likely due again to the finite size of the system—as long as correlations on the scale of the system do not completely vanish, an ordered state can survive at a higher temperature than in an infinite system. Notice also that the critical temperature increases

Lattice	z	$T_{c,\text{exact}}$	$T_{c,\text{measured}}$	β_{exact}	β_{measured}
Hexagonal lattice	3	1.519	1.678 ± 0.002	0.125	0.129 ± 0.009
Square lattice	4	2.269	2.409 ± 0.007	0.125	0.129 ± 0.008
Triangular lattice	6	3.641	3.782 ± 0.007	0.125	0.121 ± 0.006
Random 2D lattice	6.64		5.01 ± 0.02		0.26 ± 0.02
Power-law random lattice	6.64	6.15			

TABLE II: Theoretical and measured critical temperatures and critical exponents for hexagonal, square, triangular, and random lattices. The measured critical exponents are in good agreement with theory, while the critical temperatures vary with the number of nearest neighbors z, as is expected. The critical exponent for the random lattice is substantially larger than the ones for the ordered lattices.

as the number of nearest neighbors increases. Unsurprisingly, then, the random 2D lattice, with $\langle z \rangle = 6.64$, had the highest measured critical temperature. It still fell short of the prediction by Dorogovtsev et al. of $T_c = 6.15$, but as mentioned previously, this is not surprising.[7]

The critical exponent β is known to be exactly 1/8 for all three regular planar lattices.[1] The computed values for β for the hexagonal, square, and triangular lattices are all consistent with this prediction, while the value for the random 2D lattice is somewhat higher. This suggests that it is harder for spin-spin correlations to carry information over a random network, as the magnetization sets in more slowly below the critical temperature.

In this paper, we have given an overview of the history of the Ising model, described an implementation of the model via the Metropolis-Hastings algorithm, and examined Metropolis-Hastings calculations on four different geometries. We have found good agreement with theory for the systems that are exactly solvable, and have demonstrated plausible results for the non-exact system.

Acknowledgments

Prof. Mehran Kardar introduced the author to many of the formal concepts presented in this paper, including the theories of criticality and duality. Dr. John Dell of the Thomas Jefferson High School for Science and Technology provided the author's original introduction to the Ising model, the Metropolis-Hastings algorithm, and computational implementations thereof. Andre Kessler collaborated with the author on early versions of the code later repurposed into this project.

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