

The Ising Model in Two Dimensions: Theory and Simulation

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Abstract: The Ising model has been one of the most well-studied physical systems to exhibit a phase transition (in two dimensions or higher). Historically developed as a toy model for ferromagnetism, the Ising model has proved to be a host for various interesting physical phenomena, some (or more aptly, most) of which remain popular research questions till date. This paper serves as supporting documentation for a Monte Carlo simulation of the 2D Ising model. We present a brief review of the theoretical and computational framework behind simulations of Ising models. We then discuss our simulation in particular, providing the algorithm employed, and commenting on sections of the code. We also discuss how to interpret the results obtained from the simulation. These details put together will hopefully serve as an illustration for the plethora of exotic phenomena displayed by the Ising model, and ferromagnetic materials in general.

Keywords: Ising model, Monte Carlo, Glauber algorithm, critical phenomena, ferromagnetism.

I. INTRODUCTION

The Ising model was historically developed as a simple physical system (a spin lattice, to be precise) that could display ferromagnetic behavior. Physicists soon observed that in certain dimensions, the Ising model exhibits a phase transition between two phases of magnetic behavior observed in nature: ferromagnetism and paramagnetism. Initially the behavior of the one-dimensional (1D) model was posed as a question by W. Lenz to E. Ising, then a graduate student of his, who provided an exact solution in his doctoral thesis (whence the name “Ising model”) [1]. In his thesis, Ising provided exact descriptions of the free energy and the spin correlations in the system, but he observed no phase transition in the system (in more precise language, there was no phase transition in the system). The 2D model however proved to be more subtle, and was only exactly described 19 years later by L. Onsager [2], who provided an exact form for the free energy of the system (in the absence of an external magnetic field), and showed that the 2D Ising model exhibits a transition between ferromagnetic and paramagnetic phases as the temperature reaches a prescribed critical value. Critical phenomena of the 2D Ising model, encoded in the observables of the system like magnetization and specific heat, have been greatly studied since Onsager’s solution using both theory and computation. The 3D Ising model proves to be much more difficult to solve, and there is no known solution to this date (even in the absence of an external field) that describes the full behavior of the system. To summarize the historical context, the Ising model in D dimensions is an extremely simple system to write down that demonstrates ferromagnetic behavior (and more interestingly, phase transitions between ferro- and paramagnetic regimes) that hosts a plethora of

interesting physical and statistical phenomena that has kept physicists, mathematicians, biologists, computer scientists, and chemists on the edges of their seats for about a century now.

This paper serves as supporting documentation for a simulation of the 2D Ising model using Monte Carlo methods. In II we setup the 2D Ising model and relevant notation. We also present the necessary theoretical background to understand the mechanics of the simulation, and to appreciate the results gained from the Monte Carlo methods employed. We do not go over Onsager’s exact solution since it is not relevant here, although we provide results due to his exact solution for illustrative purposes (more details can however be found in [2]). In III we review the computational methods used to simulate Ising models, and particularly those used in our simulation. In III A, we present the Metropolis, Glauber, and Wolff spin-flipping algorithms, briefly arguing why they work, and in III B we review brief snippets of the code accompanying this document to illustrate important steps. In IV, we conclude by discussing the results obtained from our simulations which include snapshots of the spin lattice, instructions on how to construct plots of observables of the system, and instances of critical phenomena observed.

We hope that this document, alongside our simulation, will serve as a fascinating visualization for the myriads of exotic phenomena observed in a simple model for ferromagnetism.

II. THEORY

This material has been adapted from sections of [3] and [4]. While we only provide a brief review of the setup and related observables of the system, for more details about solving the Ising model we refer the reader

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(i.e. the covariance of σ_i, σ_j)? What is the average magnetization of the system? What is the specific heat of the system? More generally, how does one quickly compute the average values of various observables associated to the system?

We address some of these questions briefly before moving on, beginning with 1. For $D = 1$, the free energy has been obtained exactly by Ising in [1], and is in fact a simple computation to conduct (although we omit it here for relevance). For $D = 2$, in the absence of an external magnetic field, Onsager derived an exact expression for the free energy of the system in terms of a double integral (seen in [2]). Both of these computations were done using the method of transfer matrices constructed so that $\mathcal{Z} = \text{Tr}(T^N)$ for some $N \in \mathbb{N}$ (once such matrices have been constructed, the problem resolves to diagonalizing T). These methods have been extensively discussed in [4]. Newer methods using quantum field theory and renormalization groups can also be used to analyze the partition function of the system. For $D > 3$, physicists have employed methods from mean-field theory to approximate the free energy of the system. For $D = 3$, we are not aware of any known exact result.

Moving onto 2, there is no phase transition in the 1D Ising model. In fact, the spin correlation in 1D is given by [1]:

$$\langle \sigma_i \sigma_j \rangle - \langle \sigma_i \rangle \langle \sigma_j \rangle = C(\beta) \exp(-c(\beta)|i - j|), \quad (\text{II.4})$$

where $C(\beta), c(\beta) > 0$. We see that this decays exponentially with separation between the sites for all β (here we assume that the sites are placed at $0, 1, 2, \dots, L$ on the real line), as perhaps one would expect. For $D \geq 2$, an argument now known as the Peierls argument establishes that there is a phase transition, and that the average magnetization defines an order parameter for this transition. This argument relies on the fact that it is not statistically possible, at very low β to switch from a state with all spins down, to a state with most spins up – and that there are spin regimes which cannot be linked by a finite number of statistical fluctuations in the system. The argument shows that one always obtains a phase transition from a disordered phase (for small β , the paramagnetic regime), to an ordered phase (for large β , the ferromagnetic regime) with positive spin correlation. For $D = 2$, this transition is known to be continuous, and it occurs at $\beta_c = \frac{\log(1+\sqrt{2})}{2} \frac{1}{J}$ (in the absence of an external field). In sum, for $D \geq 2$, we obtain a phase transition between a disordered and an ordered phase – and the key to identify these transitions is to look at the average magnetization, and the spin correlation.

Finally for 3, the result in one-dimension has been expressed in (II.4). For $D = 2$, such exact solutions have been harder to obtain, and are not of such a simple form,

although there exist approximations in various regimes. We refrain from commenting more on this aspect of the theory, but refer the reader to more contemporary work in the area. The average magnetization of the system m is defined as $\frac{1}{N} \sum_i \langle \sigma_i \rangle$, is the order parameter of the Ising model phase transition (as discussed in light of 2), and is one of the most important observables of the system as it characterizes the transition. We do not comment on exact forms for the magnetization, but we note that Onsager conjectured a formula for the spontaneous magnetization of the 2D Ising model in 1948, $M = (1 - (\sinh(2\beta J))^{-4})^{\frac{1}{8}}$, and this conjecture was later proven by Yang in [5]. We also define the specific heat of the system as $C = \frac{\langle \mathcal{H}^2 \rangle - \langle \mathcal{H} \rangle^2}{N k_B T^2}$. To compute the average values of these observables, and many others efficiently, we would need to sum over all spin configurations. Particularly, for any observable \mathcal{O} , we have:

$$\langle \mathcal{O} \rangle = \sum_{\sigma} \mathcal{O}(\sigma) \exp \left[\beta \left(J \sum_{\langle ij \rangle} \sigma_i \sigma_j + h \sum_i \sigma_i \right) \right] \quad (\text{II.5})$$

In III, we discuss how to efficiently compute this sum using Monte Carlo methods, without having to touch each point in configuration space.

III. COMPUTATIONAL METHODS

This material has been adapted from sections of [3], [6], [7]. Although we only briefly go over some of the computational methods used to simulate Ising models, we refer the reader to [6] and [7] for a more detailed exposition, the latter of which is entirely devoted to Monte Carlo methods and the Ising model.

As discussed in II, computing the average values of observables in the Ising model becomes extremely cumbersome due to exponentially many terms appearing in the sum (for large lattice sizes, and for $D > 1$). Monte Carlo methods give us a way out of having to sample every point in configuration space, by allowing us to sample ‘virtually all’ configurations. This is done by only computing the terms that contribute the most to the value of the sum. We make this more concrete as follows. A Monte Carlo simulation starts the system at a random configuration. At each step (called a *Monte Carlo move*), we propose a small random change to the configuration, resulting in a *trial configuration*. This change is accepted with a certain acceptance probability, or rejected. Let $P_A(t)$ denote the probability that the system is in a configuration A at a given time t . Let $C(A \rightarrow B)$ denote the probability of proposing a trial change from configuration A to B , and $A(A \rightarrow B)$ the probability that this change is accepted. This defines a *transition probability* $T(A \rightarrow B) = C(A \rightarrow B) \cdot A(A \rightarrow B)$. In principle,

these definitions only make sense if B is accessible from A using a Monte Carlo move, but as we will see, using ergodicity one may extend these definitions to any two distinct states A, B . We now define constraints on this setup that allows us to consistently simulate the system, *ergodicity* and *detailed balance*.

Ergodicity requires that starting at a possible configuration of the system, it is always possible to reach any other configuration of the system in a finite number of Monte Carlo moves. This allows us to ensure that we will never miss out on a region in configuration space that has nonzero net contribution to the partition function. Detailed balance requires that at the limiting distribution (i.e. the distribution after a long time) we have $P_A T(A \rightarrow B) = P_B T(B \rightarrow A)$ for any two distinct configurations A and B . This is called the *stationary distribution* for the following reasons. The rate of change of P_A is given by:

$$\frac{dP_A}{dt} = \sum_{B \neq A} (P_B(t)T(B \rightarrow A) - P_A(t)T(A \rightarrow B)), \quad (\text{III.1})$$

so that at the limiting distribution, we have $dP_A/dt = 0$ for any state A . This ensures that we never eventually trap the Monte Carlo process in a cycle. Ergodicity and detailed balance put together allow us to sample all important regions of configuration space eventually. For consistency purposes, we also require that P_A (which we define as $P_A(t)$ at thermal equilibrium) is equal to its Boltzmann weight $\frac{e^{-\beta E_A}}{\mathcal{Z}}$ for the corresponding partition function \mathcal{Z} and energy of the state E_A .

A. Algorithm

Now we review the Metropolis and Glauber algorithms to simulate the Ising model, before briefly mentioning the cluster-flipping Wolff algorithm. The Metropolis algorithm on the Ising model is defined in 1.

Algorithm 1 The Metropolis Algorithm

```

Initialize all spins to a random configuration  $A$ .
 $n \leftarrow 1$ .
while  $n \leq N$  do
    Pick a random site  $i \in \Gamma$ .
    Compute  $\Delta E = \beta(E_{A'} - E_A)$ , where  $A'$  is the state with
    the spin of  $i$  flipped.
    Let  $r$  be a pseudorandom number chosen uniformly from
     $[0, 1]$ .
    if  $\Delta E \leq 0$  or  $r < \exp(-\Delta E)$  then
        Flip the spin ( $A \leftarrow A'$ ).
    end if
     $n \leftarrow n + 1$ .
end while

```

If we wish to compute the average value of an observable, we may simply take the mean value of the

observable over the $\#\Gamma$ moves listed in 1, or sample it at the end of the procedure. Notice that 1 corresponds to the probabilities: $T(B \rightarrow B') = \frac{1}{\#\Gamma}$ and $A(B \rightarrow B') = \min(1, \exp(-\beta(E_B - E_A)))$. It is easy to see that the Metropolis algorithm then satisfies the ergodicity, detailed balance, and the Boltzmann weight constraints introduced above. In summary, each move in the Metropolis algorithm is a flip of a singular site. This flip is accepted without question if it doesn't increase the energy of the system. If the flip increases the energy of the system, it is accepted with probability corresponding to the Boltzmann weight of the energy gap between the two states. We now provide the Glauber algorithm which corresponds to a different acceptance probability.

Algorithm 2 The Glauber Algorithm

```

Initialize all spins to a random configuration  $A$ .
 $n \leftarrow 1$ .
while  $n \leq N$  do
    Pick a random site  $i \in \Gamma$ .
    Compute  $\Delta E = \beta(E_{A'} - E_A)$ , where  $A'$  is the state with
    the spin of  $i$  flipped.
    Let  $r$  be a pseudorandom number chosen uniformly from
     $[0, 1]$ .
    if  $r < \exp(-\Delta E)/(1 + \exp(-\Delta E))$  then
        Flip the spin ( $A \leftarrow A'$ ).
    end if
     $n \leftarrow n + 1$ .
end while

```

It is easy to see once again that the new acceptance probability still satisfies the detailed balance and the Boltzmann weight conditions. Algorithm 2 is the one we employ in our simulation, and hence is of much import to this study.

The algorithms seen above are local algorithms, particularly their action is focussed on a chosen site. We now sketch an example of a non-local flipping algorithm known as the Wolff algorithm [8]. The idea here is once again to first pick a random site i in a given configuration. Then we form a cluster of sites by the following iterative process. We add the sites adjacent to i whose spins are aligned with that of i , with probability $P_{\text{add}} = 1 - e^{-2\beta J}$. We repeat this adding procedure on each site added to the cluster, until we can add no more sites. Once we can no longer add sites to the cluster, we flip the spins of the cluster all at once. The simulation is then provided by iteratively performing these cluster-flipping moves.

B. Mathematica Code

In this section, we discuss snippets of the mathematica code accompanying this document. The source code written in mathematica employs the Glauber algorithm to simulate the 2D Ising model in the presence of an

external magnetic field. The material in this section, and the source code, were inspired by [9] and [10].

In this section, we discuss the `flippity` function in the `IsingGlau` module of the code accompanying this document. Throughout the code, we work in $\beta = 1$ units. Up until this point of the code, we have established the Ising model Hamiltonian, the magnetization of a lattice, and a module `IsingGlau` that takes in the length of the lattice, number of steps, external field strength, interaction strength, and temperature as parameters. We have also, at this point, computed the energy associated to flipping spins. The `flippity` function begins as follows.

```
flippity =
(
  s = #[[1]]; mag = #[[2]]; energy = #[[3]];
  {i, j} = {RandomInteger[{1, L}], RandomInteger
    [{1, L}]};
  ns = 0;
  If[1 < i < L && 1 < j < L,
    ns = s[[i - 1, j]] + s[[i, j - 1]] + s[[i + 1, j]]
      + s[[i, j + 1]], ns];
  If[i == 1 && 1 < j < L,
    ns = s[[2, j]] + s[[1, j - 1]] + s[[1, j + 1]],
    ns];
  If[1 < i < L && j == 1,
    ns = s[[i - 1, 1]] + s[[i + 1, 1]] + s[[i, 2]],
    ns];
  If[i == L && 1 < j < L,
    ns = s[[L, j - 1]] + s[[L, j + 1]] + s[[L - 1, j]]
      ns];
  If[1 < i < L && j == L, ns = s[[i - 1, L]] + s[[i
    + 1, L]] + s[[i, L - 1]], ns];
  If[i == 1 && j == 1, ns = s[[2, 1]] + s[[1, 2]],
    ns];
  If[i == 1 && j == L, ns = s[[1, L - 1]] + s[[2, L
    ]], ns];
  If[i == L && j == L, ns = s[[L, L - 1]] + s[[L -
    1, L]], ns];

  If[RandomReal[] < Exp[-dE[s[[i, j]], ns]]/(1 + Exp
    [-dE[s[[i, j]], ns]]), mag = mag - 2 s[[i, j]],
    energy = energy + dE[s[[i, j]], ns];
  s[[i, j]] = -s[[i, j]]; s, s];
  {s, mag, energy}
) &;
```

In the above snippet, we have chosen a random site in the lattice, and added up the neighboring spins (the series of `if` statements allows us to do this based on whether or not the chosen site is on the edge of the lattice).

```
If[RandomReal[] < Exp[-dE[s[[i, j]], ns]]/(1 + Exp
  [-dE[s[[i, j]], ns]]), mag = mag - 2 s[[i, j]],
  energy = energy + dE[s[[i, j]], ns];
s[[i, j]] = -s[[i, j]]; s, s];
{s, mag, energy}
) &;
```

This is where the Glauber flip happens. `RandomReal[]` generates a pseudorandom number in $[0, 1]$, which we then use to enforce the probabilistic Glauber flip. We also update the magnetization and the energy of the system after the flip. Overall, `flippity` completes the Glauber flip and returns the new spin configuration, magnetization, and energy. We can now apply `flippity` iteratively on a random initial configuration we call `initLat`. This is encoded in the nested list `flippitedList`. We note that the Metropolis algorithm is enforced the same way, with the appropriate change in acceptance probability.

IV. RESULTS

Now we present the results obtained using the methods discussed in III with brief comments. We run the code discussed in IIIB for an 80×80 lattice with $J = 2$, $h = 0.1$, and temperature $2K$ (for 250000 steps). The system is initialized to the following random configuration.

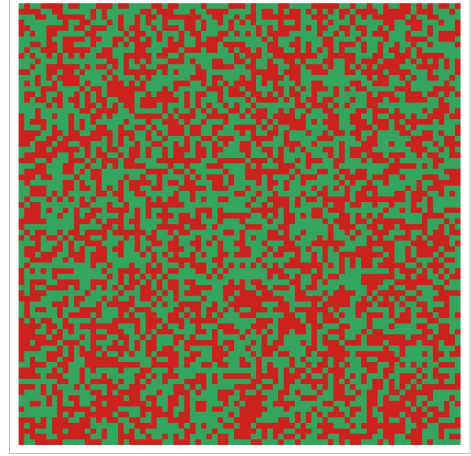


FIG. 2: Initial configuration for a trial on an 80×80 lattice with $J = 2$, $h = 0.1$, and $T = 2$ (here red indicates a spin of $+1$, and green a spin of -1).

Figures 3, 4, and 5 show snapshots of the system at 62500, 125000, and 250000 iterations of `flippity`. Apart from being pretty pictures, these snapshots tell us about the impact of temperature, external field, and interaction strength toward the stable state of the system.

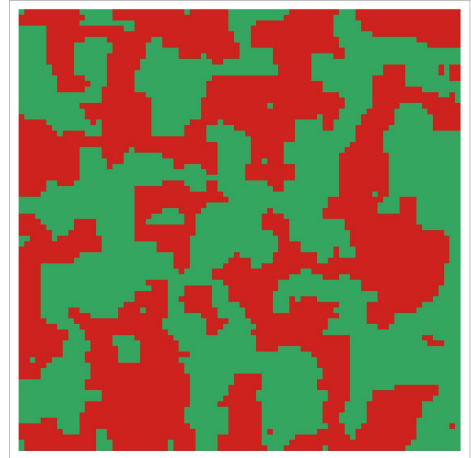


FIG. 3: The configuration in 2 after 65000 steps, for $J = 2$, $h = 0.1$, and $T = 2$.

We already see the system thermalizing steadily at 65000 steps. Since the temperature is fairly low, the thermal fluctuations are minimal, and we see clusters of aligned spins. Since the strength of h is quite low, the

system isn't flooded red. Also, since $J > 0$ we only see ferromagnetic behavior as opposed to anti-ferromagnetic checkered patterns.



FIG. 4: The configuration in 2 at 125000 steps, for $J = 2$, $h = 0.1$, and $T = 2$.

Figures 4 and 5 show the system's steady approach toward the system's 'stable state.' It is also illustrative to see an example at higher temperature (and we leave it to the reader to run the code at around $4.54K$, the expected transition temperature in the absence of an external field).



FIG. 5: The configuration in 2 at 250000 steps, for $J = 2$, $h = 0.1$, and $T = 2$.

We run the code now for an 80×80 lattice with $J = 2$, $h = 0.1$, and temperature $20K$ (for 250000 steps). The system is initialized to the following random configuration.

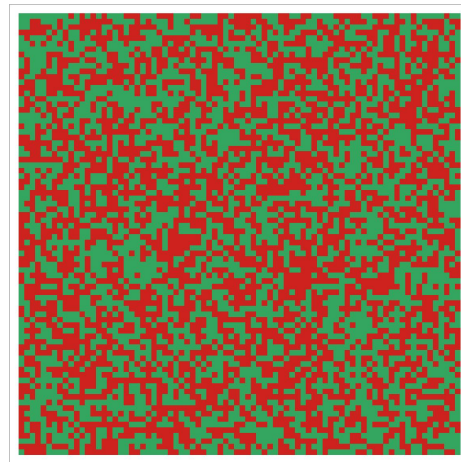


FIG. 6: Initial configuration for a trial on an 80×80 lattice with $J = 2$, $h = 0.1$, and $T = 20$.

Figures 7, 8 show snapshots of the system at 125000 and 250000 iterations of `flippity`. They show the thermal fluctuations that are prevalent at higher temperatures in the system.

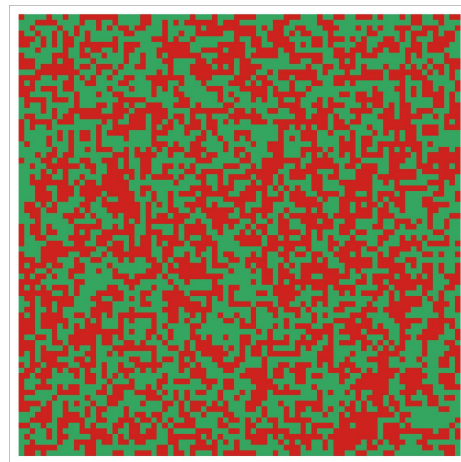


FIG. 7: The configuration in 6 at 125000 steps, for $J = 2$, $h = 0.1$, and $T = 20$.

We see that there is no noticeable steady approach to a stable state with clusters of aligned spins as seen at lower temperatures. This is because at higher temperatures, the acceptance probability (as a function of ΔE) approaches a step function, leading to thermal fluctuations.

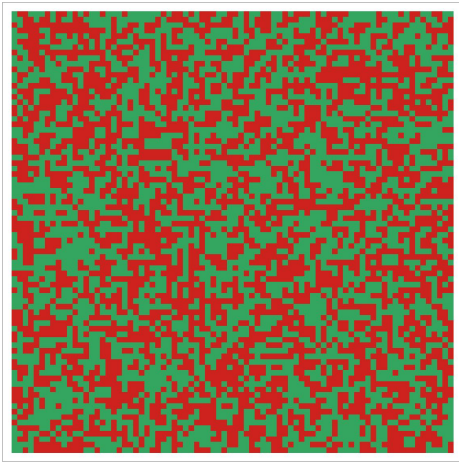


FIG. 8: The configuration in 6 at 250000 steps, for $J = 2$, $h = 0.1$, and $T = 20$.

The fluctuations in the system continue to persist around 8.

Finally we run the simulation on an 80×80 lattice for $h = 0$, $J = 1$ and temperature $2.27K$ (for 250000 steps). This is particularly illustrative since $2.27K$ is the predicted transition temperature for the 2D Ising model in the absence of an external field! We start with the following random initial configuration.

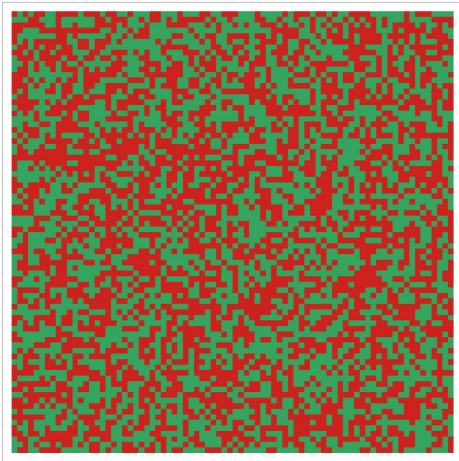


FIG. 9: Initial configuration for a trial on an 80×80 lattice with $J = 1$, $h = 0$, and $T = 2.27$.

Figures 10 and 11 show snapshots of the spin configuration at 125000 and 250000 iterations of flippity.

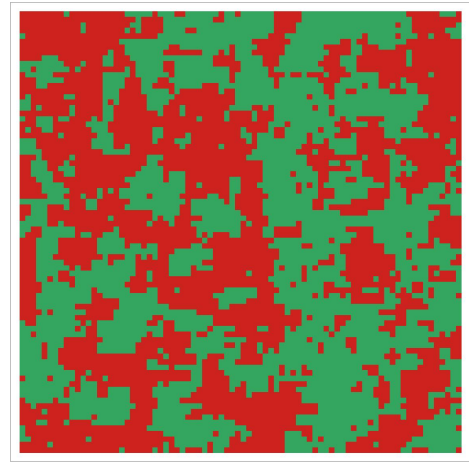


FIG. 10: The configuration in 9 at 125000 steps, for $J = 1$, $h = 0$, and $T = 2.27$.

In 10 we notice visual features from both the low-temperature and high-temperature regimes here, characteristic of the behavior of the system around the phase transition. We see clusters of aligned spin characteristic for low temperatures, as well as the characteristic noise seen in higher temperatures.

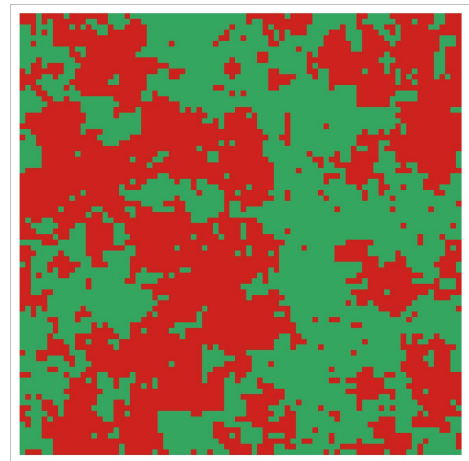


FIG. 11: The configuration in 9 at 250000 steps, for $J = 1$, $h = 0$, and $T = 2.27$.

The features seen in 11 persist after 250000 iterations as well. We don't see a steady approach toward a stable state, but we observe a more chaotic behavior of the system. However, we also don't see an abundance of thermal noise seen at higher temperatures and some of the spin clusters persist. This qualitative analysis confirms that the 2D Ising model experiences a phase transition from a characteristically disordered phase at low β to an ordered phase at large β (and that there is a critical β value about which this transition takes place)

While the discussion in this section so far has been completely qualitative, the infrastructure of the source

code allows us to quantify the critical phenomena seen in the 2D Ising model. We noted in IIIB that we kept track of the energy and magnetization of the system throughout the many iterations of `flippity`. This data can be extracted after the last iteration to obtain the average energy and magnetization of the system at a given temperature. Having obtained the average magnetization and energy at a sample of temperatures, we may then produce a scatter plot of this data (average value of the observable vs. time). For example, one will be able to confirm that magnetization is an order parameter of the 2D Ising model phase transition (particularly, you will note that the magnetization is approximately 0 in the disordered phase at high temperatures, and is non-zero in the ordered phase at lower temperatures). Other observables like specific

heat C can also be easily computed either by updating the observable through each `flippity` iteration or by using thermodynamic relations (for example, one might compute $\langle \mathcal{H}^2 \rangle$ and use the definition of C in II to compute C). These plots will confirm the qualitative analysis conducted previously in this section.

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- [1] E. Ising, Beitrag zur theorie des ferromagnetismus, Zeitschrift für Physik **31**, 253 (1925).
 - [2] L. Onsager, Crystal statistics. i. a two-dimensional model with an order-disorder transition, Phys. Rev. **65**, 117 (1944).
 - [3] J. Binney, N. Dowrick, A. Fisher, and M. Newman, *The Theory of Critical Phenomena: An Introduction to the Renormalization Group* (Clarendon Press, 1992).
 - [4] S. Sachdev, *Quantum Phase Transitions*, 2nd ed. (Cambridge University Press, 2011).
 - [5] C. N. Yang, The Spontaneous Magnetization of a Two-Dimensional Ising Model, Phys. Rev. **85**, 808 (1952).
 - [6] T. Pang, *An Introduction to Computational Physics*, 2nd ed. (Cambridge University Press, 2006).
 - [7] J.-C. Walter and G. Barkema, An introduction to Monte Carlo methods, Physica A: Statistical Mechanics and its Applications **418**, 78 (2015).
 - [8] U. Wolff, Collective Monte Carlo Updating for Spin Systems, Phys. Rev. Lett. **62**, 361 (1989).
 - [9] R. Singh, Ising model, <https://rajeshrinet.github.io/blog/2014/ising-model/> (2014).
 - [10] P. Coleman, Simulation of the 2D Ising Model, https://www.physics.rutgers.edu/~coleman/611/Resources/ising_snippets_class_project.pdf (2017).