2D Ising Model

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I. INTRODUCTION

The Ising model was proposed by Ernst Ising in early 1920 to describe physical phase transition occurring under small parameter changes [1]. Originally developed to understand ferromagnetism, the Ising model has been extended to other fields to describe phase transitions; for example, microbiologists have employed the Ising model to determine lipid interaction in cell membranes [2]. The model of interest to us is a theoretical atomic model of a magnet. Consider a magnet consisting of a collection of atoms whose individual moments are represented by dipoles within a square lattice (in two dimensions). While physically there is no restriction on the spatial direction of the dipole moments of any given atom i, the Ising model makes the simplification that each dipole ("spin") is either up ($s_i = +1$) or down ($s_i = -1$). Individual spins may interact magnetically such that it is energetically favourable for them to line up in the same direction. However, they can also flip randomly since the system is thermodynamic [3]. In equilibrium at temperature T, the probability P of a lattice being in a state s with energy E is given by the Maxwell-Boltzmann distribution

$$P(s) = \frac{1}{Z} e^{-\beta E(s)} \tag{1}$$

where $Z = \sum_s e^{-\beta E(s)}$ is the partition function for normalization purposes and $\beta = \frac{1}{k_b T}$, where k_b is the Boltzmann constant and T is the temperature [4]. In the 2D Ising model, the total energy is calculated by summing over all interactions between a given particle in the lattice with its closest (non-diagonal) neighbors; note that periodic boundary conditions are employed such that particles on the edge of the visualization of the square lattice interact with the corresponding particle on the opposite boundary, thus every particle in fact has four neighbors in 2D. Each pair of atoms, indexed i and j, contributes to the total energy of the system as following

$$E = -J s_i s_j \tag{2}$$

where s is the spin of a single particle in the lattice and J is the interaction constant. In the case of a ferromagnetic, J is positive so spin-aligned pairs are energetically rewarded, while the opposite holds for an antiferromagnetic. The model seeks to find the equilibrium state of the lattice undergoing these random flips in atomic spins. The analytic form for magnetization of a system as a function of temperature can calculated as

$$M(T) = \begin{cases} 0 & T > T_c \\ \frac{(1+z^2)^{1/4}(1-6z^2+z^4)^{1/8}}{\sqrt{1-z^2}} & T < T_c \end{cases} \tag{3}$$

for $kT_c \approx 2..269185J$ and $z = e^{-\frac{2J}{kT}}$ [5] The asymptotic case of $M(T) = 0$ for $T >> T_c$ is to be expected; for sufficiently large temperature every state is approximately equally likely, driving the net magnetization towards zero.

The model can be extended to interact with an external magnetic field as well, in which the Hamiltonian includes a field coupling term

$$E = -J \sum_{<i,j>} s_i s_j - H \sum_i s_i \tag{4}$$

. With this term, states in which the net spin is aligned with the magnetic field are energetically favored. With a nonzero external field the analytic solution presented in Equation (3) no longer holds (in fact there is not a known analytic solution to the 2D Ising model with an external field).

Using Markov Chain Monte Carlo, we explore the zero-field Ising model first to compare results to the known theory, emphasizing the temperature dependence of the final distribution and both ferromagnetic ($J > 0$) and antiferromagnetic ($J < 0$) types of materials. We then examine the effect of external fields on the convergence of the magnetization and the response time of the lattice in a time-varying field.

II. COMPUTATIONAL METHODS

We employed Metropolis algorithm based on Monte Carlo Markov Chain method (MCMC). Monte Carlo simulation uses random numbers to simulate a random physical process in order to predict the deterministic output, and this method is mostly used in statistical mechanics. A Markov Chain is a sequence of events that the probability of each event depends solely on the previous event. For example, in Eq.1, we do not know the value of the partition function Z and it is not easy to calculate. We can instead utilize the Markov Chain to sample from probability distributions and generate states one after another [3].

A. Theory of Markov Chains

A Markov Chain is a sequence of events whose probability depends solely on the event before it. In simulating the Ising model, it is used to sample from the Boltzmann distribution (Equation (1)) without finding an explicit form for the partition function–this is an expensive computation for large system sizes. By initiating the Ising lattice in some state and taking Markov steps, it is possible to step through probability distributions, reach the Boltzmann distribution, and choose states within it after convergence provided the Markov steps are suitable [3].

More formally, a Markov chain is described by a matrix T_ij such that $\sum_j T_ij = 1$ to maintain the normalization of the prior and posterior distributions. For a particular T_{ij} constructed to sample a given distribution $P(E)$, a critical property of T_{ij} is that $\sum_i T_{ij} P(E_i) = P(E_j)$, or equivalently that $P(E)$ is a fixed point of the Markov process. This means once the desired distribution is attained, it can be sampled from without jumping to another distribution [3].

A natural pair of questions (one of which was posed in class) is whether the fixed point is unique, and whether given an arbitrary starting state the Markov chain will converge to its fixed point. For Markov matrices which are irreducible and ergodic, these are both true [3][6]. A complete proof is out of scope but it is worth summarizing. It hinges on the fact that the state space of the system is finite, and therefore the simplex formed by the state vectors is also finite; as a collection of points and lines in $\mathbb{R}^n$, it is closed and bounded (topologically compact). Sequences in a compact space admit convergent subsequences. It can be shown that the limit of a sequence of states in a Markov chain must be a fixed point. Moreover, it can be shown that for a large number of steps the Markov step T^n_{ij} is a contraction map (essentially, moves points in a vector space closer together in a uniform way) when the state simplex has the l^1 metric imposed on it. The result then follows immediately from the Banach fixed point theorem, which states that a contraction map on a compact (in particular complete) metric space has a unique fixed point [6].

With this, the utility of the Markov chain is apparent. With a properly selected updating step, it will enable us to sample from the Boltzmann distribution with the confidence that it will converge eventually.

B. Ising Model MCMC

For the Ising model, the states are updated by the Metropolis algorithm, which selects one point in the Ising model lattice and proposes a flip. The change is energy is evaluated and the state change can then be accepted or rejected. In particular, since lowering energy is favored a state which decreases energy is accepted with probability 1. If the change increase energy, it may still be accepted with probability $e^{-\frac{\Delta E}{kT}}$. Intuitively, this agrees with the asymptotic limit of equation (3) as $T \to \infty$; the exponent tends to zero, thus a flip will always occur no matter if the energy is increased or decreased. Essentially the lattice will be flipped randomly at high temperature, resulting in a zero average. More concretely, it can be shown that this update condition satisfies the properties laid out in the previous section, and that the Boltzmann distribution is the limit and fixed point of any sequence of steps [3].

To summarize the procedure, a square lattice of side length N is instantiated. At each timestep, a random point in the lattice is chosen. The energy associated with the initial and final states is computed based on the point's neighbors and its sign relative to the external field (Equation (4) but with no summation). If this difference is negative, the new state is accepted. If the difference is positive, choose a random number between 0 and 1; if it is less than $e^{-\beta_j \delta E}$, we accept the state, otherwise it is rejected. In this case β_j is a dimensionless description of the energy given by $\beta_j = J/kT$. This is repeated for 100,000 timesteps; to find the magnetization associated with a certain β_j, we average over the last 50,000.

To compute the total energy of the lattice in the case of zero external field (as the contribution to the energy by field coupling is a trivial summation over the spins), we slide a kernel over the lattice and use convolution to compute the energy between a point and its neighbors. This uses the "wrap" mode for periodic boundary conditions. The kernel is shown below.

False	True	False
True	False	True
False	True	False

FIG. 1. Designed kernel

For the case of no external field, we used the numba package to vectorize our python code and run it for more timesteps.

III. RESULTS

A. No External Field

As noted, with no external field Equation (3) provides a closed form solution for the magnetization of the lattice as a function of temperature in terms of k/J. The theoretical relationship between the magnetization and temperature is shown in Figure (2). These are to be compared to the magnetization resulting from direct simulation of the Ising model, starting from a state 50% spin up and 50% spin down. These are shown in Figure (3).

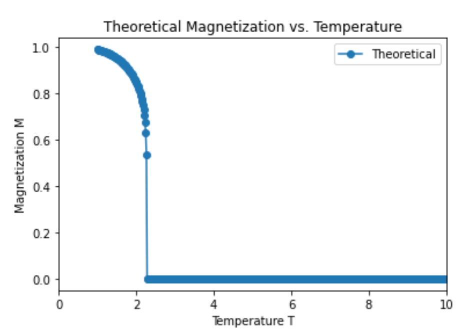

FIG. 2. Theoretical Magnetization for $T < T_c$

The simulated curves agree well qualitatively with the theoretical magnetization. As expected, at the critical temperature $kT_c = 2.269185J$, there is a sharp decline in the magnetization. For a lattice side length of 50, there is considerable noise where the curve would be expected to reach zero magnetization. Since the result is more stable for larger lattice size, this may be due to more pronounced edge effects and fewer timesteps. The $50x50$ lattice was run for $50,000$ timesteps and the $100x100$ for $200,000$ timesteps at each temperature; for each temperature, the starting lattice is the final lattice of the previous. The initial lattice ($T = 0$) is all spin up.

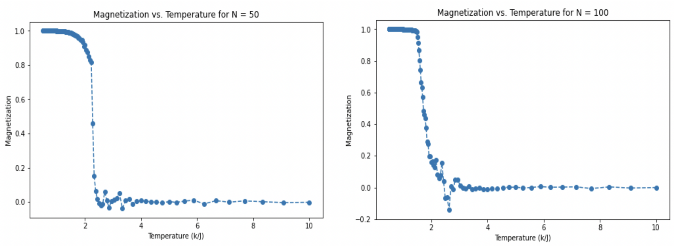

FIG. 3. Magnetic Vs. Temperature for lattice size N = 50 and 100

The slope of the plot corresponds to the work needed to raise the temperature of the Ising model by one unit of J/k. This is most intuitive when considering a cooling process; to cool the system from a high temperature is simple because the energy in the bonds is small compared to the thermal energy, while going lower than the critical temperature is difficult because it requires a shift from a disordered system where each state is equally likely to a highly ordered lattice.

If the temperature evolves in the opposite direction from a random lattice (50% spin up) as shown in the following figure, there is considerable noise in the result; the high temperature lattice still hovers about zero magnetization, however the low temperature regime seems comparatively unstable and the curve in Figure (1) cannot be perfectly recovered. Moreover, it depends highly on the random initial configuration; in the run shown the "steady state" for low temperature (excluding the irregularity around $T = 0$) is negative, while for other runs with the same parameters it was positive.

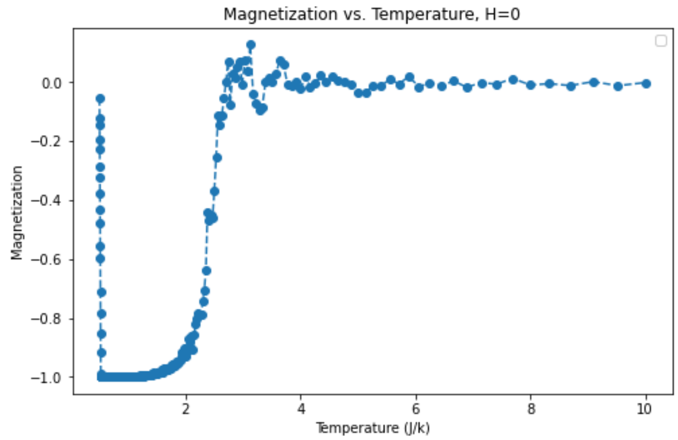

FIG. 4. Magnetic Vs. Temperature while cooling, random initial lattice. N=50

Finally, the Ising model can be visualized over its time steps. In each plot in Figure 5, the lattice is shown at a particular time and at a low temperature. Observe the aggregation of the spins.

As one might expect, the dipoles align in large clusters as this minimizes the local energy stored in bonds between neighbors. At higher temperatures or lower coupling factors, the lattice will stay in a disordered state reminiscent of the early time steps because the benefit to forming grains of aligned dipoles is minimal relative to the thermal energy scale.

B. External Field

1. *Constant Magnetic Field*

As explained in the Computational Methods section, the addition of a magnetic field causes the Ising model to favor alignment with the magnetic field. For field magnitudes comparable to the coupling coefficient J, this modifies the equilibrium state slightly; a converged Ising model with a temperature above the critical temperature will converge not to $M = 0$ but to some M whose sign agrees with that of the magnetic field. This is shown for a positive magnetic field in the following figure. Note the peculiar shape of the energy curve; this is likely due to the fact that the lattice begins fully aligned but the magnetic field points opposite the initial configuration, thus flips are still relatively likely to occur; each flip dramatically increases the energy of the system because the flipped dipole is antialigned with its neighbors, but over time the energy begins to decrease as the neighbors also align with the magnetic field and the coupling term in the energy becomes negative once again.

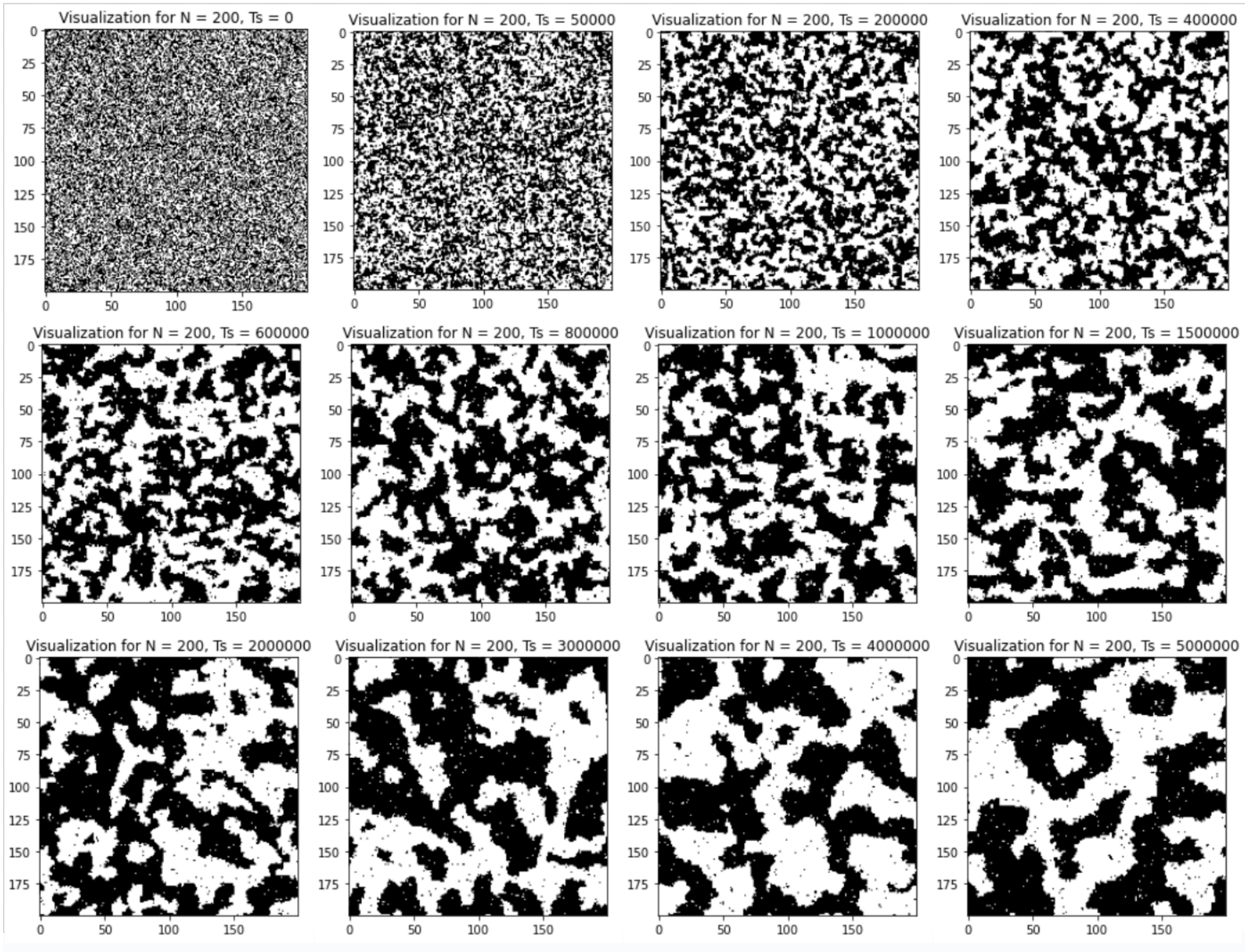

FIG. 5. Visualization of the Ising Model Over Time, no external field.

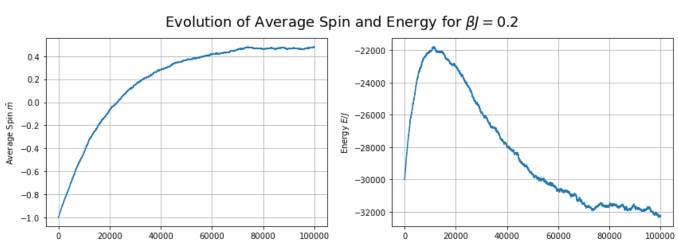

FIG. 6. Average Magnetization over time in a constant magnetic field of order 1

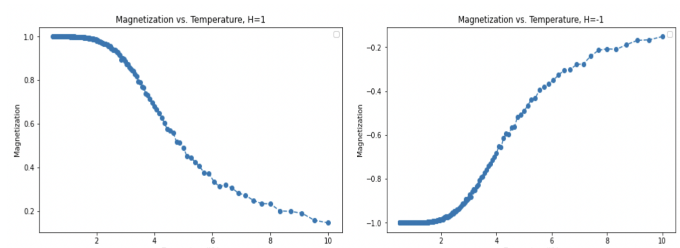

FIG. 7. Magnetic Vs. Temperature for lattice size N = 50 in a Magnetic Field

The magnetic field direction can be chosen to be positive or negative. Over a range of temperatures with lattice side length 50 and 50,000 timesteps per temperature, the evolution of magnetization with temperature under an external field can be observed.

The magnetic field increases the energy associated with any given point in the lattice, thus limiting the sharp drop off that occurs above T_c in the zero-field case. Nevertheless the magnetization still tends to zero with an increase in temperature as expected. Moreover, regardless of the fact that in each case the initial state of the lattice was perfectly aligned spin up, the end state for low temperature was to be aligned with the magnetic field.

When temperature is instead cooled, unlike the zero-field case the magnetic field seems to correct the noise present in the zero field. The curve agrees well with the analogous heating curve of Figure 7.

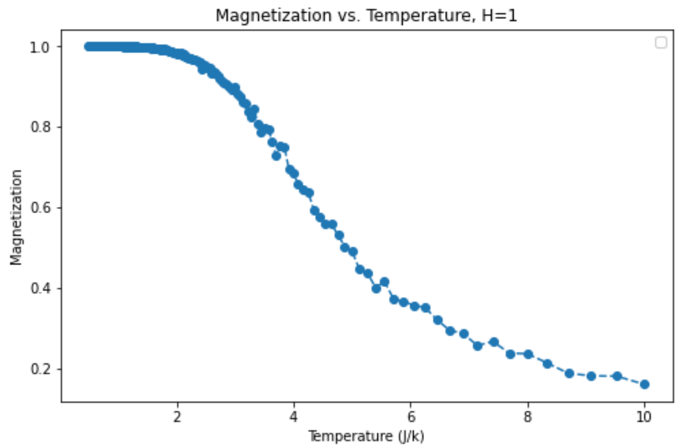

FIG. 8. Magnetic Vs. Temperature while being cooled down, $H = 1$, N=50.

2. Position Dependent Magnetic field

A position dependent, time constant magnetic field can be applied to the lattice to force the lattice into a certain configuration. In general this is not much different than the constant magnetic field as far as total magnetization, but for sufficiently large amplitudes the dipoles with strongly align to patterns in the external field. Inspired by David Grier's creation of the NYU logo with trapped particles, we created an Ising model whose steady state reads NYU. To accomplish this, the magnetic field outside of the lettering was negative and inside the lettering it was positive. The amplitude was $1J$, so even with a small coupling coefficient the system responded strongly to the external field.

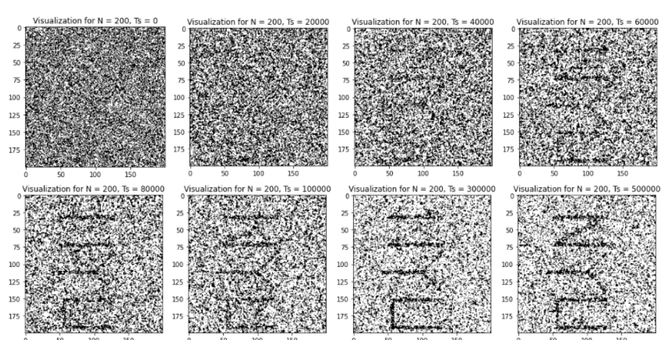

FIG. 9. Ising Model in a position dependent magnetic field which reads "NYU".

3. Time-Variable Magnetic Field

A time-variable magnetic field can be applied and at each time step, the contribution of the magnetic field will change. Of particular interest are oscillatory external fields of the form $A\sin(\omega t)$. For low temperatures (or any temperature provided the amplitude is large enough), one would expect a high frequency field to have little net effect because the effects are temporally local and average out over large timesteps. By contrast, a large amplitude, low frequency field would be expected to drive the shape of the magnetization curve at a frequency comparable to the field and with some lag as the Ising model catches up to the energy imposed by the field. Observe this in Figures 7 and 8. For high frequency the magnetization is forced towards zero, the average value of $sin(\omega t)$. For low frequency the individual periods can be made out and it can be observed that there is a lag between the peaks of the field and the spin.

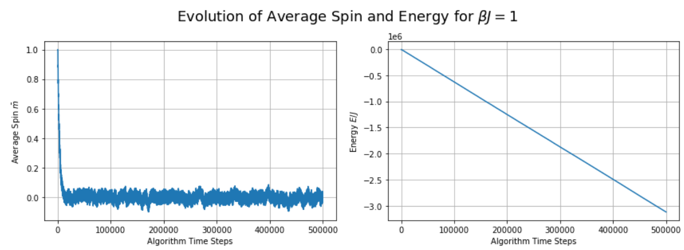

FIG. 10. Ising Model in a time dependent magnetic field with $A = 10, \omega = .005\pi$

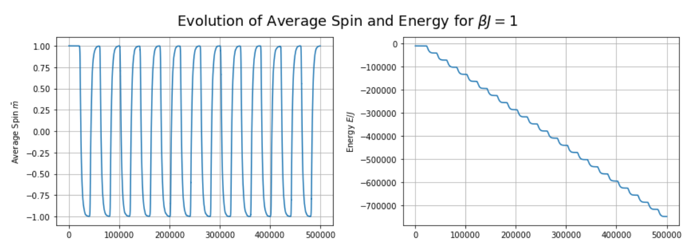

FIG. 11. Ising Model in a time dependent magnetic field with $A = 10, \omega = .00005\pi$

The response time of the system can be calculated by choosing some period of the sinusoid and finding the difference between the field peak and the spin peak within that period (this presupposes that the response time is relatively small). For the case of a cosine with frequency $.00005\pi$ against a fully positive starting lattice, this is comparable to 10000 timesteps. The plot of spin against this cosine is shown below; note the delay between the peaks, which is more obvious with fewer timesteps.

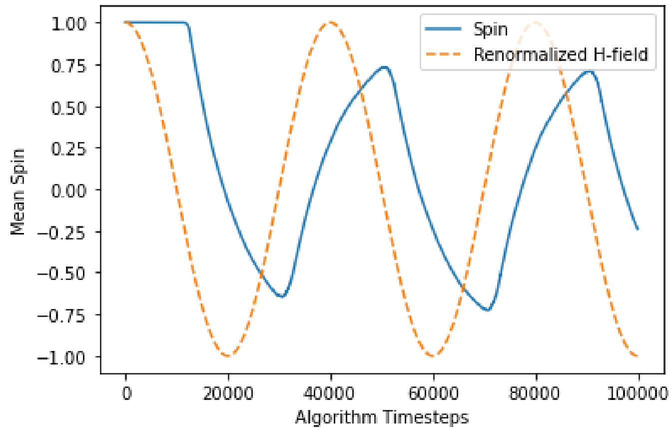

FIG. 12. Ising Model in a time dependent magnetic field $H = 10\cos(.0005\pi t)$

IV. SUMMARY

We employed Markov Chain Monte Carlo to sample from a Boltzmann distribution of Ising model lattice states, both with and without an external magnetic field. The theoretical solution to the 2D Ising model agrees well with the simulated results at both low and high temperature in the absence of a magnetic field, with the magnetization sharply falling off to zero around the critical temperature. When cooling the system instead of heating it and beginning from a random lattice instead of a fully aligned one, the final state around $T = 0$ was highly dependent on the initial configuration; it could converge either to an average spin of 1 or -1 without any parameter changes between runs. Applying a constant magnetic field biases the model towards certain states, and at high temperature the system converges not to zero spin but to something whose sign is shared with the magnetic field. When cooling the system, the field corrects the instabilities from initial conditions and recovers the expected plot without fail. We explored position-dependent and time-dependent fields of high amplitude to break local interactions in favor of external coupling and to examine the response time of the Ising model under a sinusoidal field.

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