Phase-Shifts in 2D Potts Model by Means of Markov Chain Monte Carlo Simulations

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We consider a generalized Ising model where each discrete site can take q different spins. We purely consider $q = 3$ as it has been studied analytically. We report that as the temperature reaches below the critical temperature, the system will break symmetry and converge to a single spin. Temperatures slightly above this critical value will resemble an amorphous glass, and temperatures greatly above resemble a random noise.

I. INTRODUCTION

The Ising model is one of the most exhausted statistical models in physics. It has become a right of passage for aspiring computational physicists to solve it numerically. The Ising model describes ferromagnetism. It does this by randomly constructing a mesh of discrete variables. These variables can only have the values 1 or -1. This limitation is set due to the fact that each discrete site either has spin up or spin down. We can express the Hamiltonian of such a model as:

$$H_I = J \sum_{<i,j>} s_i s_j + B \sum_i s_i, \tag{1}$$

where J is a ferromagnetic coupling constant, s_i is a discrete spin, and B is an external magnetic field. In the 40s-50s, Cyril Domb wanted to generalize such a model. His initial prescription was to chop the unit circle into equidistant angles such as:

$$\theta_s = \frac{2\pi s}{q}, \tag{2}$$

where q is the number of slices, and $s \in \{0, 1, 2, ..., q-1\}$. As $q \to \infty$, any angle spin is applicable and the model becomes the XY-model. Domb defined a Hamiltonian for only the ferromagnetic contribution as:

$$H_c = J_c \sum_{<i,j>} \cos(\theta_i - \theta_j) \tag{3}$$

His Ph.D student, Renfrey Potts, made some alterations. He considered a simpler model whose Hamiltonian is given as:

$$H_P = -J_P \sum_{<i,j>} \delta_{s_i, s_j}, \tag{4}$$

where δ is the Kronecker delta. In this model, s_i is still an element of the same set as in Domb's original formulation. For the Potts model, a continuous phase transformation exists for $1 \leq q \leq 4$. [1] The critical point for such a transition is modeled as:

$$\frac{J}{k_B T} = \log(1 + \sqrt{q}) \tag{5}$$

II. METHODOLOGY

The Hamiltonian in eq. (4) is simulated by means of Markov Chain Monte Carlo. Initially, the system is in an entirely random configuration where at each site $s_i \in [0, q-1]$. For each step, a random site is chosen. The site is then assigned a random available spin. From this spin, the change in eq. (4) is recorded. If the change is less than zero, the move is accepted. If it is higher than zero, it is accepted with a certain probability. This probability being:

$$P(\text{accept}) = e^{-\beta \Delta H}, \tag{6}$$

where $\beta = k_B T$. This is then repeated for N steps. For each simulation, J is set to be 1. For this consideration, this gives the critical point at $k_B T = 0.436$ Due to computational constraints, the system size considered is 100×100. To help alleviate issues due to such a small system size, we employ periodic boundary conditions (PBCs). We also consider only $q = 3$.

III. RESULTS

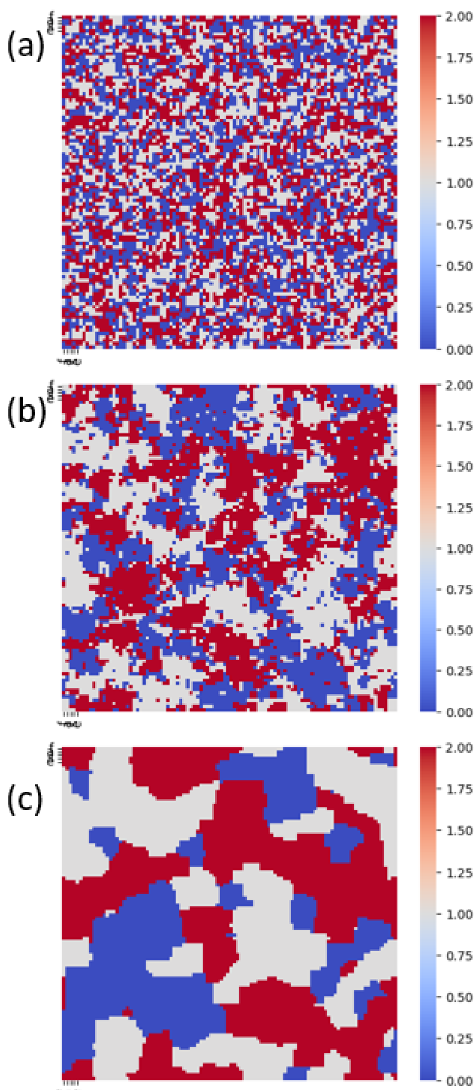

FIG. 1. System after 1000000 Monte Carlo steps for varying temperatures: (a) $k_BT = 2$, (a) $k_BT = 1$, and (c) $k_BT = 0.4$

In fig. 1, each simulation ran for 1000000 steps. Although this is not enough for the system to truly reach equilibrium, it provides a nice qualitative view into how quickly each system begins to clump together. For $k_BT = 2$, the system still seems to represent the initial uniform random distribution it was initialized to with very slight aggregation. In part (b) of fig. 1, the system appears to be in some sort of amorphous glass configuration. The highest order system is that of part (c) in fig. 1. This system is in fact under the critical temperature and should eventually break symmetry and converge to one of the available spins.

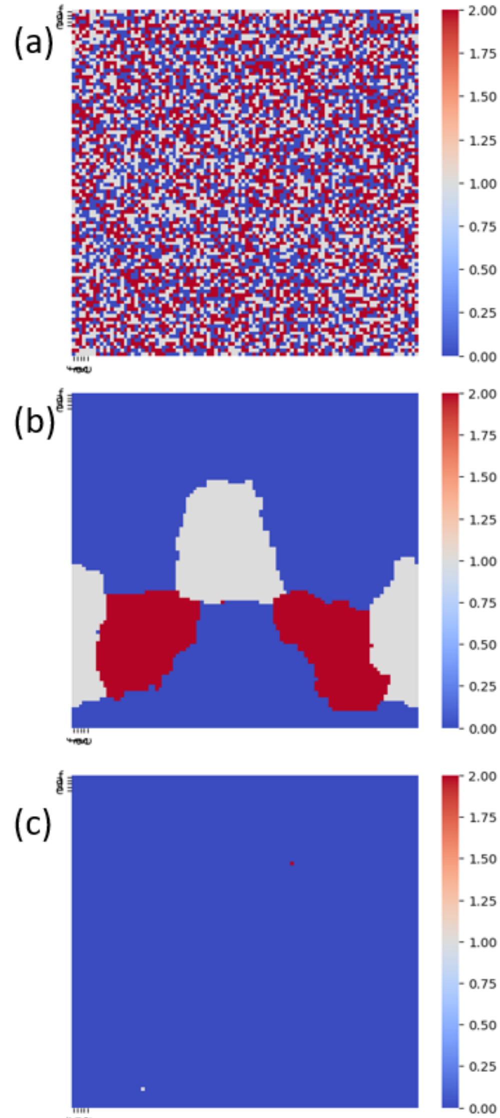

FIG. 2. Snapshots of a system with $k_BT = 0.4$ evolved through time: (a) 0 Steps, (b) 12500000 Steps, and (c) 75000000 Steps

In fig. 2, we provide snapshots of a system evolved through time. In part (c), The prediction of the critical temperature is confirmed. As in after enough time, the system breaks symmetry and converges onto a single spin. Any spin can be converged to as there is not an external magnetic field considered. Part (b) show a features of striking symmetry, but this is probably due to the PBCs.

IV. SUMMARY AND CONCLUSION

Our findings of a phase transition are in line with the analytical results for a Potts model with $q = 3$. We report that, at high temperatures, the system remains entirely noisy. As temperature begins to approach the critical temperature, the system does not break symmetry, but it appears to become an amorphous glass. Once the temperature is lower than the critical temperature, the system will converge to only one of the available spins. For the system to equilibrate to this, it took around 75000000 Monte Carlo steps. It has no preferred spin as we do not consider any external magnetic field coupled to our system. Overall, our findings agree with the predictions for $q = 3$ and even phenomena seen in $q = 2$ (the Ising model).

[1] H. Duminil-Copin, V. Sidoravicius, and V. Tassion, Communications in Mathematical Physics **349**, 47 (2016).