A comparative study of 2d Ising model at different boundary conditions using non-deterministic Hexagonal Cellular Automata

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Abstract

The spin system of the 2d Ising model having a hexagonal-lattice is simulated using non-deterministic Cellular Automata. The method to implement this program is outlined and our results show a good approximation to the exact analytic solution. The phase transition in 2d Ising model is studied with a 40 × 40 hexagonal-lattice with five different boundary conditions (bcs) i.e., adiabatic, periodic, reflexive, fixed +1 and fixed −1 with random orientation of spins as initial conditions in the absence of an external applied magnetic field. The critical temperature below which the spontaneous magnetization appears as well as other physical quantities such as the magnetisation, energy, specific heat, susceptibility and entropy with each of the bcs are calculated. The phase transition occurs around $T_{c}^{H} = 1.5$ which approximates well with the result obtained from exact analytic solution by Wannier and Houtappel. We compare the behaviour of magnetisation per cell for five different types of bcs by calculating the number of points close to the line of zero magnetisation for $T > T_{c}^{H}$. We find that the periodic, adiabatic and reflexive bcs give closer approximation to the value of $T_{c}^{H}$ than fixed +1 and fixed −1 bcs with all three initial conditions for lattice size less than 50 × 50. However, for lattice size between 50 × 50 and 200 × 200, fixed +1 bc and fixed −1 bc give closer approximation to the $T_{c}^{H}$ with initial conditions in which all spins are in down configuration and all spins are in up configuration respectively.

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1 Introduction

The simple Hamiltonian for the Ising model and its variants are studied extensively for their ability to describe critical phenomena. This can be applied to understand magnetism, models for high-temperature superconductivity and phase diagrams, disordered and non-equilibrium systems. The model also provides means for testing algorithms. All the interesting phenomena of statistical mechanics and phase transitions are found to have counterparts in this model. It is an example of a lattice model for modeling simple interacting many-particle systems in statistical mechanics where a set of spins $s_i = \pm 1$ is assigned to each lattice site.

The spins interact with both their nearest neighbors and an external magnetic field via a Hamiltonian of the form

$$H(s) = -\sum_{<ij>} J_{ij} s_i s_j - \mu \sum_{k=1}^{N} h_k s_k$$

(1.1)

where $s$ is an arbitrary spin configuration, the notation $<ij>$ indicates a sum over nearest neighbor lattice points, $J_{ij}(>0)$ is a parameter describing inter-particle interactions, $\mu$ is the magnetic moment and $h_k$ is an external magnetic field at $k^{th}$ spin.

The model is best known for describing the emergence of ferromagnetism in crystals of atoms that interact via spin-spin coupling. The Ising model is useful even in cases for which it cannot be solved exactly. On both square-lattice and hexagonal-lattice geometries where the Ising model can be exactly solved and also for those where no exact solution has been found, numerical simulations can provide insight into critical behavior of these models. The most common method for simulating Ising systems is the Metropolis-Hastings algorithm, originally developed for use in molecular dynamics simulations.

The 1$\text{d}$ model introduced by Lenz was exactly solved by Ising, which showed that the one-dimensional case does not exhibit a phase transition [1]. This led to the general belief that the Ising model in higher dimensions would also be ineffective at describing systems with critical points. However, Onsager in 1944 exactly solved the Ising model for a two-dimensional square lattice configuration with periodic boundary condition by analytical method [2]. He demonstrated that, for an infinite square lattice, the ferromagnetic phase transition occurs at a critical temperature, $T_c^S$, of

$$T_c^S = \frac{2}{\ln (1 + \sqrt{2})} \approx 2.269$$

(1.2)

where $J = 1$, $k_B = 1$ and $S$ stands for square-lattice. The square and hexagonal lattices, both, have exactly computable critical temperatures. The hexagonal (honeycomb) lattice is the next simplest two dimensional lattice. The pure Ising model on the
honeycomb lattice has been studied by Wannier [3] and Houtappel [4] and have been exactly solved. The most straightforward way to find these critical temperatures is via duality between high-temperature and low-temperature behaviour. Duality is the hidden symmetry found by Kramers and Wannier that relates the partition function and the free energy of the Ising model at low and high temperatures for the two dimensional square-lattice [5, 6]. The system is mathematically modeled in two ways each of which is independent of the other and both of which are valid to describe the physical properties of the system. If one assumes that the free energy is singular at the critical temperature, and that this singularity is unique, then this leads to the determination of the critical temperature. For the two dimensional hexagon system the critical temperature \( T_{c}^{H} \) was found to be

\[
T_{c}^{H} = \frac{2}{\ln(2 + \sqrt{3})} \approx 1.519
\]

(1.3)

where \( J = 1 \), \( k_B = 1 \) and \( H \) stands for hexagonal-lattice. The above results are for lattice of infinite size with periodic boundary condition. Above this temperature the average magnetization is zero in the absence of external magnetic field. We performed the simulation taking lattices of finite size and in the absence of external magnetic field so as to compare the result obtained by the above analytic method as well as to those for our five different bcs.

A Cellular Automaton (CA) is a mathematical model, modeling a set of cells which interact with their neighbors. In this model, each cell have values known as states, all the cells update their states simultaneously at discrete time steps, and the new state of a cell is determined by current state of its neighbors according to a local function called rule of the CA. Hexagonal CA is a tessellation of the plane by regular hexagons which provide for higher packing density of cells and the unit cells of hexagonal grids are uniformly connected in the sense that the distance from a given cell to any adjacent cell is the same. To simulate the Ising model with Hexagonal CA, we can design a two states CA, for spin up state \((+1)\) and spin down state \((-1)\) and number of neighbors is six i.e, north, south, east, west, top and bottom. A definite rule is designed for which states of the cells are either all in up states or all in down states below \( T_{c}^{H} \) and above \( T_{c}^{H} \) on the average half in \(+1\) spin states and half in \(-1\) spin states. The 2d Ising model using non-deterministic hexagonal CA (HCA) has not been studied for five different boundary conditions. The CA used in this work differs from that of Metropolis-Hastings algorithm where the algorithm specifies that the transitions must be made for one site at a time whereas we consider transitions of many sites simultaneously. The work of Eltinge [7] uses Metropolis-Hastings algorithm to study numerically the case of periodic boundary condition.

Our computations will be on finite-size lattices with four different boundary con-
ditions, as well as, with the periodic boundary condition that effectively simulates accurately infinite-size lattice results in many respects. Apart from the Ising model, quantum spin models such as the Kitaev model [8] or Kitaev-Heisenberg model [9, 10] on the honeycomb lattice have recently received a lot of theoretical and experimental attention [11, 12, 13, 14, 15]. Hexagonal lattice has also been discussed in the context of high temperature and low temperature susceptibility series and extracting the scaling function [16]. Such a growing interest in the hexagonal-lattice systems motivates us to revisit the Ising model on the hexagonal lattice. Attempts have been made for mapping Ising models in different lattice geometry using CA. A deterministic CA (DCA) proposed by Domany and Kinzel [17], the Q2R CA [18, 19, 20, 21] and the Creutz CA [22, 23, 24, 25] are mostly used in analysing square-lattice Ising model. All these CA models are deterministic and the computation can be performed fast. It has been demonstrated that the probabilistic model of the CA like Metropolis algorithm [26] is more realistic for description of the Ising model even though the random number generation makes it slower. Probabilistic CA model under five different boundary conditions has been studied in the context of a square-lattice Ising model [27]. However, Ising model using two dimensional hexagonal CA (HCA) under different boundary conditions other than periodic boundary condition has not yet been studied.

The paper is organised as follows: in section 2, we discuss the basic theory to treat a 2d HCA and how to implement it in the Ising model with five different bcs. The results obtained out of the simulations are given and are analysed in section 3 and we have also compared Ising model with different boundary conditions by considering their converging points. Our conclusion and future perspective are discussed in section 4.

2 Implementation of Isotropic 2d Ising Model by Hexagonal CA

Two dimensional CA is described by finite states of cells ($s$), neighborhood cells ($n$) and its distance among neighbourhood ($r$), boundary conditions and transition functions or rules ($f$). In our 2d HCA model, $s = \{s_{i,j}, s_{i,j} \in -1/ +1\}$, number of nearest neighbour cells $n = 6$, $r = 1$ and we consider five different bcs.

Neighbourhoods of extreme cells are taken care of by boundary condition (bc). If the extreme cells are adjacent to each other then it is called periodic bc (pbc). In adiabatic bc (abc), the extreme cells replicate their state and in reflexive bc (rbc), mirror position states replace the extreme cells. In fixed bc, the extreme cells are connected to $+1$ or $-1$ state. If it is connected to $+1$ state, it is called fixed $+1$ bc ($f + 1bc$) and if it is connected to $-1$ state, then it is called fixed $-1$ bc ($f - 1bc$).
If the same rule is applied to all the elements of the matrix \((s)\), then it is called uniform CA and if different rules are applied to individual elements of the matrix or block of elements then it is called nonuniform CA. At different time intervals, if different rules are applied to the matrix then it is called varying CA e.g., probabilistic CA. With the application of these rules, elements (states) of the matrix change at successive intervals as shown in the following equation.

\[
s_{L \times L}^{t+1} = f_{L \times L}^t \times s_{L \times L}^t
\]  

where \(f\) is a time varying rule or transition matrix.

Consider an isotropic 2d Ising model in the form of hexagonal lattice \((s)\) with \(L\) rows and \(L\) columns. Here we consider each hexagonal cell as a lattice point as shown in figure 2. The lattice has then \(L^2 = N\) sites. The odd rows have different column positions i.e., 1, 3, 5, . . . etc. and even rows have different column positions i.e., 2, 4, 6, . . . etc. At each of the sites \(s_{i,j}\), \(i = 1, \ldots, L; j = 1, \ldots, 2L\), the spins are arranged in such a way that \(j\) increases as 1, 3, . . . , 2\(L - 1\) from left to right in case of odd rows, \(j\) increases as 2, 4, . . . , 2\(L\) from left to right in case of even rows and \(i\) increases from bottom to top, and has one of the \(\pm 1\) spin, which are the two states in CA. So, there are \(2L^2\) spin configurations. We consider only the nearest neighbor interactions, so the number of neighbor cells are 6. We include the five different bcs as follows.

For odd rows :

1. pbc : \(s_{i,2L+1} = s_{i,1}, s_{L+1,j+1} = s_{1,j},\) 
   \(s_{i,-1} = s_{i,2L-1}\) and \(s_{-1,j} = s_{L,j+1}\).

2. abc : \(s_{i,2L+1} = s_{i,2L-1}, s_{L+1,j+1} = s_{L,j},\) 
   \(s_{i,-1} = s_{i,1}\) and \(s_{-1,j} = s_{1,j-1}\).

3. rbc : \(s_{i,2L+1} = s_{i,2L-3}, s_{L+1,j+1} = s_{L-1,j+1},\) 
   \(s_{i,-1} = s_{i,3}\) and \(s_{-1,j} = s_{2,j}\).

4. f+1bc : \(s_{i,2L+1} = +1, s_{L+1,j+1} = +1,\) 
   \(s_{i,-1} = +1\) and \(s_{-1,j} = +1\).

5. f-1bc : \(s_{i,2L+1} = -1, s_{L+1,j+1} = -1,\) 
   \(s_{i,-1} = -1\) and \(s_{-1,j} = -1\).

For even rows :

1. pbc : \(s_{i,2L+2} = s_{i,2}, s_{L+1,j} = s_{1,j-1},\) 
   \(s_{i,0} = s_{i,2L}\) and \(s_{0,j} = s_{L,j+1}\).
2. abc: \( s_{i,2L+2} = s_{i,2L}, \ s_{L+1,j} = s_{L,j+1}, \)
\( s_{i,0} = s_{i,2} \) and \( s_{0,j} = s_{1,j-1}. \)

3. rbc: \( s_{i,2L+2} = s_{i,2L-2}, \ s_{L+1,j} = s_{L-1,j}, \)
\( s_{i,0} = s_{i,4} \) and \( s_{0,j} = s_{2,j}. \)

4. f+1bc: \( s_{i,2L+2} = +1, \ s_{L+1,j} = +1, \)
\( s_{i,0} = +1 \) and \( s_{0,j} = +1. \)

5. f-1bc: \( s_{i,2L+2} = -1, \ s_{L+1,j} = -1, \)
\( s_{i,0} = -1 \) and \( s_{0,j} = -1. \)

The average magnetization for the configuration is defined as,
\[
\langle M \rangle = \sum_{i=1}^{L} \sum_{j=1}^{2L} s_{i,j}
\tag{2.2}
\]
and the average magnetization per spin is given by
\[
\langle m \rangle = \frac{\langle M \rangle}{N}
\tag{2.3}
\]

Energy for the configuration \( s \) is defined as
\[
E(s) = \frac{-J}{6} \sum_{i=1}^{L} \sum_{j=1}^{2L} s_{i,j} \times \left( s_{i,j-2} + s_{i,j+2} + s_{i-1,j-1} + s_{i-1,j+1} + s_{i+1,j-1} + s_{i+1,j+1} \right)
\tag{2.4}
\]

Here, the factor of 1/6 has been put to remove the sextuple counting of energy, otherwise the interacting energy will be computed six times. \( J_{ij} = J \) (isotropic) for 6 neighbour cells, or else, \( J_{ij} = 0. \)

The configuration energy per spin is
\[
\langle e \rangle = \frac{E(s)}{N}
\tag{2.5}
\]

For updating the lattice in next iteration, we use the probabilistic approach by constructing a probabilistic CA. We use the following procedure.

We calculate the change in energy i.e., the energy difference at successive time intervals is \( \Delta E(s^t) = E(s^t) - E(s^{t-1}). \) Here, \( \Delta E \geq 0 \) or \( \Delta E < 0 \) but we have considered the case \( \Delta E \geq 0 \) i.e., \( E(s^t) \geq E(s^{t-1}). \) Next we calculate the probability of each site in the spin configuration \( s \) at time \( t \) (number of iterations) by using the Boltzmann factor
\[
p_t = \frac{p(E(s^t))}{p(E(s^{t-1}))} = e^{-\frac{\Delta E(s^t)}{k_BT}}
\tag{2.6}
\]
With the above probability for each site, we construct a probability weighted matrix (or transition matrix). This matrix leads to our probabilistic CA matrix \(PCA^t\) by comparing it with a random matrix and multiplying by a factor of 0.1 to normalise the \(PCA^t\).

Successive spin configurations are obtained from

\[
[s^{t+1}_{i,j}]_{L\times L} = [PCA^t_{i,j}]_{L\times L}[s^t_{i,j}]_{L\times L}.
\] (2.7)

Here, we consider \(s^{t+1}_{i,j}\) to be a new configuration. If in this new configuration the calculated energy is less than the initial configuration, then it is allowed to proceed forward; otherwise the new configuration is flipped backward. After a finite number of iterations we calculate the average energy of the system per cell \((e)\), magnetisation per cell \((m)\), and obtain the susceptibility per cell \((\chi)\), specific heat per cell \((C_v)\) and the entropy per cell \((S)\).

\[
\chi = \frac{N}{k_B T} (\langle m^2 \rangle - \langle m \rangle^2)
\] (2.8)

\[
C_v = \frac{N}{k_B T^2} (\langle E^2 \rangle - \langle E \rangle^2)
\] (2.9)

\[
S = -k_B (r_1 P_1 \log_2 P_1 - r_2 P_2 \log_2 P_2)
\] (2.10)

where \(r_1\) is the total number of spin up states, \(r_2\) is the total number of spin down states, \(P_1\) is the probability of spin up states and \(P_2\) is the probability of spin down states in the lattice \(s\). The Metropolis algorithm specifies that transitions must be made for one site at a time. But here we have considered transitions of many sites simultaneously for which we go to a regime of oscillating behavior. For instance, nearly every site that is flipped in the direction of higher energy becomes unflipped on the next iteration. CA is desirable to perform transitions on every lattice site simultaneously. For instance such simultaneous transitions take advantage of matrix operations for increased computational efficiency. This algorithm checks the time complexity better than the Metropolis algorithm [26].

3 Simulation, results and discussions

In this work, we have considered hexagonal-lattice of size \(40 \times 40\) for the determination of critical temperature at which a phase transition occurs. Here we have considered lattice size of \(40 \times 40\) for our convenience in computation. In this simulation we take \(J = 1\), \(k_B = 1\) and the external magnetic field to be zero i.e., \(h = 0\). We have considered the temperature range from 0.1 to 4.0 with increment of 0.05 unit in each
step. At each temperature, we have considered $10^5$ runs. Each of the simulation starts with random spin configurations. We have considered five different bcs i.e., periodic, adiabatic, reflexive, fixed +1 and fixed −1.

The magnetisation per cell ($m$) versus temperature results are shown for all five bcs in figure 3. One can observe that in the case of fixed ±1 bcs, the curves obtained provide better result than either of the other boundary conditions, i.e., pbc, abc or rbc at low temperature regions ($T < T^H_c$).

3.1 Phase transition with pbc, abc, rbc, f1bc and f-1bc

To study the phase transition we have calculated energy per cell ($e$), magnetisation per cell ($m$), susceptibility per cell ($\chi$), specific heat per cell ($C_v$) and entropy of the configuration ($S$) by considering average of ten simulation. Here each simulation starts with random spin configuration in hexagonal-lattice of size $40 \times 40$ and we take temperature range from 1.0 to 4.0 with increment of 0.05 unit since we have to find the phase transition corresponding to all five different bcs and hence the $T^H_c$.

In figure 4, we have plotted $e$ vs $T$; $m$ vs $T$; $m$ vs $e$; $\chi$ vs $T$; $C_v$ vs $T$ and $S$ vs $T$ with initial random spin configuration with pbc, abc, rbc, f+1bc and f-1bc respectively. One finds that around temperature $T^H_c = 1.5$, the magnetisation approaches the value zero, the energy gradually increases, as well as the entropy gradually increases, as shown in figures 4(a), 4(b) and 4(f). The susceptibility and specific heat also change, initially they increase with a sudden rise at $T = 1.5$ and then start decreasing as shown in figures 4(d) and 4(e) respectively. So, a phase transition is clearly visible around $T^H_c = 1.5$ as the second order derivative of energy and magnetisation is extremely large with all five bcs.

In the $m$ vs $e$ graphs shown in figure 4(c), the regions with higher density of points indicate three states. We find three states, two of them are low temperature ground states around ($m = \pm 1, e = -6$) with random initial conditions in the cases of abc, pbc and rbc, and the third one is the high temperature phase which is centered at ($m = 0, e = 0$). But in the case of f+1bc there is one low temperature ground state around ($m = 1, e = -6$) and one high temperature phase is centered at ($m = 0, e = 0$). Also in the case of f-1bc there is one low temperature ground state around ($m = -1, e = -6$) and one high temperature phase is centered at ($m = 0, e = 0$).
4 Comparison of 2d Ising model simulation among boundary conditions

In figure 3, one can observe that the magnetization approach the zero line after $T > T^H_c$ in different manner depending on the bcs. The analytic solution gives a zero magnetization above $T^H_c$ and our simulation for different bcs also show that it converge toward the zero value at increased temperatures. With one simulation for all bcs, it is not possible to predict which bc is closer to $T^H_c$. So, we analyze the points for magnetization in the range $-0.01 \leq m \leq +0.01$, $-0.1 \leq m \leq +0.1$ and $-0.2 \leq m \leq +0.2$ which are close to the zero line of magnetization after $T > T^H_c$. We call such points as converging points.

In this simulation, we have taken various lattice sizes ranging from $5 \times 5$ to $200 \times 200$ in this manner. We consider an increment of lattice size 5 in each step while going from lattice size from $5 \times 5$ to $60 \times 60$ and subsequently for $60 \times 60$ to $100 \times 100$ an increment of 10 for each step and from $100 \times 100$ to $200 \times 200$ with increment of 50 for each step. The temperature ranges from 1.0 to 4.0 with small increments of 0.05 units. We have iterated 1000 times for each simulation for lattice sizes $\leq 10 \times 10$, 10000 times for lattice sizes in between $10 \times 10$ and $40 \times 40$ and 100000 times for lattice sizes above $40 \times 40$. Figure 5 shows the converging points in the above mentioned range of magnetization. We have counted the number of converging points as defined above by taking average result of ten simulations for each bc with three different initial conditions. We carry out all the simulation with three initial conditions and with all five bcs. Here, three initial conditions are (i) all up (or most of spins up), (ii) all down (or most of the spins down) and (iii) random (or randomly oriented spins up/down).

For lattice sizes $\leq 50 \times 50$ with pbc, abc and rbc, one finds more convergent points in both cases $-0.1 \leq m \leq +0.1$ and $-0.2 \leq m \leq +0.2$ than that for f+1bc and f-1bc for all up and all down spin initial conditions.

With lattice sizes in between $50 \times 50$ and $200 \times 200$ with f-1bc, one finds more convergent points in both the cases corresponding to $-0.1 \leq m \leq +0.1$ and $-0.2 \leq m \leq +0.2$ with initial condition of all up spins. For f+1bc, one finds more convergent points in both the cases with initial condition of all spins down.

In the case of lattice sizes $\leq 30 \times 30$ with pbc and lattice size $> 30 \times 30$ with abc, one finds more convergent points both cases $-0.1 \leq m \leq +0.1$ and $-0.2 \leq m \leq +0.2$ among all bcs with random spin initial conditions. For all initial cases with $-0.01 \leq m \leq +0.01$, the result is better for pbc, abc and rbc and converging points increase as lattice sizes are increased.

It is observed that lattice size $= 200 \times 200$ with all five bcs, one can observes same convergent points in both cases $-0.1 \leq m \leq +0.1$ and $-0.2 \leq m \leq +0.2$ but pbc, abc
and rbc show more convergent points in $-0.01 \leq m \leq +0.01$ than f+1bc and f-1bc.

## 5 Conclusion

In the present work, we have studied 2d Ising model in hexagonal-lattice with five different boundary conditions using non-deterministic Cellular Automata algorithm in which transitions of many sites takes place simultaneously in contrast to transitions being made for one site at a time. We have observed a phase transition that occurs at the critical temperature $T_c^H \approx 1.5$ for each of the five bcs. The result of $T_c^H \approx 1.5$ agrees with the exact solution presented in equation 1.3. The findings for fixed $+1/−1$ bcs also show a smoother curve at low temperatures than pbc, abc and rbc with random initial condition. This implies that with the different initial conditions on different lattice sizes $\leq 50 \times 50$, one can take care of boundary spins by not only pbc but also by abc and rbc. Further in our analysis, abc shows more converging points than pbc and rbc for lattice size $> 30 \times 30$ with random initial condition. For lattice size greater than $50 \times 50$, f+1bc and f-1bc are better suited to use than other bcs in case of initial spin configuration with all down or all up spins respectively. It is also observed that for lattice size $= 200 \times 200$, in all cases of initial spin configuration, in all bcs give almost same converging points. From the simulation point of view, our algorithm flipped most of the spins at a single iteration. It is computationally more efficient than Metropolis algorithm [26] which flips single spins at a single iteration. The analysis done in this paper will help us in finding the values of critical exponents more accurately for hexagonal-lattice, which we plan to study next. The present work is expected to facilitate the use of non-deterministic CA in the study of phase transition in case of anti-ferromagnetic materials, binary alloys and spin glasses etc with different boundary conditions.

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Figure 1: Hexagonal-lattice with row and column vectors.

Figure 2: $4 \times 4$ hexagonal-lattice.

Figure 3: $m$ versus $T$ for all five bcs with random initial spin configuration in $25 \times 25$ hexagonal-lattice.
Figure 4: Random initial spin configuration in $40 \times 40$ hexagonal-lattice with five different bcs.
Figure 5: Converging points of bcs for 50×50 lattice size after $T > T_c^H$. Red lines are for magnetization $|m| \leq 0.2$, blue lines are for magnetization $|m| \leq 0.1$ and yellow lines are for magnetization $|m| \leq 0.01$ with the initial condition of random spin configuration. Magenta line represents a parallel line to magnetization per cell at $T = T_c^H$. 