Dynamics of Clusters in Two-dimensional Potts Model *

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Abstract

Dynamical behavior of the clusters during relaxation is studied in two-dimensional Potts model using cluster algorithm. Average cluster size and cluster formation velocity are calculated on two different lattice sizes for different number of states during initial stages of the Monte Carlo simulation. Dependence of these quantities on the order of the transition provides an efficient method to study nature of the phase transitions occurring in similar models.

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1 Introduction

Recent interest in models possessing weak first-order phase transition has increased the importance of distinguishing first- and second-order phase transitions for the simulation type of studies. One of the most successful methods to determine the order of the transition is introduced by Challa et. al. [1]. This method is based on comparing the shape of the energy probability distribution of the system with a single or double Gaussian for first- and second-order transitions respectively. Similarly, observing a double minima or single minimum in free energy may lead to conclusive evidence on the order of the transition [2]. However, for a finite lattice with large correlation length, it is very difficult to determine the order of the phase transition even if one uses a series of lattices with increasing sizes.

The information during a Monte Carlo run propagates with the relaxation time which is proportional to a power of the correlation length. During first few iterations, this finite propagation speed reveals physics of different time scales. This approach has successfully used to investigate perturbative and non-perturbative effects in 2-dimensional $O(3)$ sigma and $CP^{(N-1)}$ models [3], as well as $SU(2)$ and $SU(3)$ lattice gauge theories [4]. The same idea is also applied to $(2 + 1)$- dimensional scalar field theories to study the dynamics of first-order phase transitions [5]. In this work similar ideas will be used to devise tools of distinguishing first- and
second-order phase transitions in spin systems by simply studying the evolution of some observables in the first couple of hundred Monte Carlo iterations. In this approach the major concern is the choice of observables; since the global quantities are most sensitive to the correlations in the system, their effects can be seen clearly by use of such observables. Two of the possible candidates of these observables may be the cluster size and the cluster formation velocity. These quantities show different behaviour depending on the magnitude of the correlation length. Large correlation length results in faster initial thermalization, while in the case of short range correlations the convergence is very slow; hence initial iterations in a Monte Carlo simulation possess vital information on the phase structure of the system. The aim in this work is to extract information about the phase transition by observing cluster (growth) dynamics in two-dimensional \( q \)-state Potts model during early stages of a Monte Carlo simulation.

The Hamiltonian of the two-dimensional Potts model is given by

\[
H = K \sum_{\langle i,j \rangle} \delta_{\sigma_i, \sigma_j}.
\]  

Here \( K = J/kT \), where \( k \) and \( T \) are the Boltzmann constant and the temperature respectively, and \( J \) is the magnetic interaction between spins \( \sigma_i \) and \( \sigma_j \), which can take values \( 1, 2, \ldots, q \) for the \( q \)-state Potts model. In a Monte Carlo simulation the average cluster size (CS) can be calculated by taking the average of \( N_c \) clusters per
iteration,

\[ CS = \frac{1}{N_c} < \sum_{i=1}^{N_c} C_i > \]  \hspace{1cm} (2)

where \( C_i \) is the number of spins in the \( i \)th cluster. Being a function of the largest cluster, the order parameter (\( OP \)) is also a global observable and it can be calculated through the relation

\[ OP = \frac{q \rho^\alpha - 1}{q - 1}, \]  \hspace{1cm} (3)

where \( \rho^\alpha = N^\alpha / L^D \), \( N^\alpha \) is the number of spins in state \( \sigma = \alpha \), \( L \) and \( D \) are the linear size and the dimensionality of the system respectively.

The two-dimensional, \( q = 2, 3 \) and 4 state Potts model exhibits second-order phase transition, while for \( q \geq 5 \) the transition is known to be first-order \[7, 8\]. For \( q = 5 \) the correlation length is finite but very large and it decreases with increasing \( q \). In this work the two-dimensional \( q \)-state Potts model (\( q = 2, 3, \ldots, 8 \)) is chosen as the test ground for the above mentioned ideas. It is believed that comparisons of the behavior of the cluster growth or the change in the order parameter (per Monte Carlo iteration) for different \( q \) can give some information about the degree of the phase transition.

In the present work, the two-dimensional \( q \)-state Potts model for \( q = 2 \) to 8 has been simulated during thermalization, using a cluster update algorithm. Dynamical
information about the cluster formation is to be extracted through the calculation of the cluster size. Commonly used quantities like energy, order parameter and the relaxation time are also obtained. The organization of the article is as follows: Section 2 gives general information about the cluster dynamics during relaxation. Results and discussions are given in section 3, and the conclusions are presented in section 4.

2 Dynamics of clusters in a spin system

When a spin system is set to relax at a given temperature, spins tend to form clusters with different sizes and shapes, depending on the temperature and the strength of the interaction between the spins. This formation occurs either by integration (forming large clusters) or by disintegration (breaking into smaller clusters). If the system is ordered initially, first few Monte Carlo iterations immediately break the configurations and small clusters start to appear. This process gradually slows down as the system relaxes and reaches the “equilibrium”. For a disordered start, the system remains as it is for the first couple of iterations, while the information still has not been propagated to the distances long enough to form clusters. After a few iterations, clusters at reasonable sizes start to appear and their average size increases as the system relaxes towards equilibrium.
To check how the thermodynamic quantities approach the equilibrium values or more precisely how the cluster size changes with increasing number of iterations, one can start Monte Carlo runs from different starting configurations. The average of a quantity like the cluster size over all different starting configurations at every iteration gives the time dependent ensemble average of that quantity. If the correlation length is very large, sizable clusters immediately grow and the cluster size, after initial few tens of iterations, fluctuates around an average value. On the contrary, for the systems with correlation length smaller than the lattice size, this thermalization requires very long Monte Carlo runs and a distinguishing aspect is that fluctuations around the iteration-dependent average value are very large. The formed large clusters can not maintain their sizes around an average value for many iterations; they break into smaller clusters contributing the fluctuations in the system. For a given $q$, average cluster size reaches a different equilibrium value for different temperatures and the number of Monte Carlo iterations to reach the equilibrium depends on the temperature at which the simulation is performed. To avoid ambiguities, all simulations in this work are performed at the temperature $T = T_c$ where the specific heat peaks are observed.

A possible function for the relaxation process may be

$$f(t) = f_0 [1 - \exp \left( -t / \tau \right) \theta]$$

(4)
where $f_0$ is the final value of the function, $\tau$ is the relaxation time which is related to the inverse of the correlation length, $\theta$ is some exponent and $t$ indicates the number of iterations (Monte Carlo time). By fitting the time dependent average cluster size data to equation (4), one can obtain quantities $f_0$, $\tau$ and $\theta$. The change in the average cluster size per iteration, which may be called the “cluster formation velocity” ($CFV$), gives another important information of the same type. This quantity can be calculated through the relation

$$CFV = \frac{\partial f(t)}{\partial t}$$

which is simply the derivative of the function $f(t)$ which represents the mean cluster size and is given in equation (4), or the derivative of the fitted polynomial function, with respect to Monte Carlo time. Cluster formation velocity gives a clear indication of how fast the clusters are formed and how many iterations can be used for the initial thermalization of the system. Hence it is related to the dynamics of the spins and to the correlation length in the system.

3 Results and discussions

Averages of energy, order parameter and cluster size during relaxation of the system are obtained in the two-dimensional Potts model with number of states $q$ varying from 2 to 8, using the cluster flip algorithm which was first introduced by Swendsen and Wang [10] and later modified by Wolff [11]. The algorithm used in this
work is the same as Wolff’s algorithm with the exception that before calculating
the observables, searching the clusters is continued until the total number of sites
in all searched clusters is equal to or exceeds the total number of sites in the lattice.
The averages are calculated about 5000 replicas of the system starting from differ-
ent disordered initial configurations and errors are calculated using jackknife error
analysis. All the computations are performed at the finite size critical value $K_c$ of
the coupling $K$ on $32 \times 32$ and $64 \times 64$ lattices. $K_c$ values are obtained as the values
corresponding to the maxima of specific heat calculated at a previous work, where
the cluster size related measurables are studied at equilibrium [9].

Figure 1 shows plots of average cluster size ($CS$) calculated dynamically during the
thermalization for $q = 2$ to 8 on $64 \times 64$ lattice. Results for the $32 \times 32$ lattice give
basically the same information with higher slopes for early iterations or with faster
thermalizations. These plots show that the slope of the curves at early iterations
decreases as $q$ increases, which is consistent with the discussion given in Section 2.
Large slopes in $CS$ data for $q < 5$ (i.e. when the transition is second-order) indicate
fast formation of the clusters. For $q \geq 5$, phase transition is first-order and the
correlation length decreases as $q$ increases, therefore the cluster formation is rather
slow.

Dynamical data for energy, order parameter and average cluster size calculated on
small and large lattices with different $q$ are fitted to both exponential (equation(4)) and the polynomial functions. These functions are used to calculate cluster formation velocity ($CFV$). $CFV$ shows variation in $CS$ as a function of the number of iterations, so it is simply calculated by taking derivative of the fitted function (equation(5)) with respect to Monte Carlo time. Figure 2 shows $CFV$ for the large lattice for $q$ values varying from 2 to 8. For small $q$, clusters form very quickly, so maximum of $CFV$ occurs at a higher value than that of large $q$. As these plots show, $CFV$ has a distinct maximum for $q < 5$ and it is in the form of a curve with a broad maximum for $q = 5$ and 6. It is observed that starting from $q = 7$, it is difficult to find a maximum for $CFV$ data. For $q = 8$ the maximum is at about the first or second iteration, and after a few iterations, $CFV$ values are almost constant. The runs performed for $q = 9$ and 10 show the same behaviour. As it is seen from figure 2, number of iterations where the maximum of $CFV$ occurs increases as $q$ increases. This information is consistent with the observation that cluster formation is slow for large $q$. $CFV$ plots for the $32 \times 32$ lattice show similar variations, the only difference being that the maximum points of $CFV$ occur at higher values than that for the large lattice for each $q$ value.

Relaxation time $\tau$ and the exponent $\theta$ for each $q$ are calculated through exponential fit by use of equation(4). $\theta$ values are related to initial behaviour of the relaxation process. It is observed (both for $32 \times 32$ and $64 \times 64$ lattices) that $\theta$ is around a value
of about 2.0 for \( q = 2 \) and decreases monotonically as \( q \) increases, reaching a value of about 1.0 for \( q = 7 \) (and lower for \( q = 8 \)). To see the variation of \( \tau \) for different \( q \) on small and the large lattice, its ratio to \( \tau \) for \( q = 2 \) is plotted on a logarithmic scale. Plots of \( \tau(q = 2)/\tau(q) \) versus \( q \), for small and large lattices are shown in figure 3. One can see from this figure that the slope of \( \tau(q = 2)/\tau(q) \) remains almost constant for the smaller lattice, while the slope of the ratio calculated on the larger lattice continuously changes with increasing \( q \) for \( q \geq 5 \), as an indication of the sensitivity of \( \tau \) to decreasing correlation length. In other words, the \( \tau \) values for different size lattices are parallel within error limits for small \( q \) \((q = 2, 3 \text{ and } 4)\), and starting from \( q = 5 \), the discrepancy between two curves increases as \( q \) increases. \( \tau \) values calculated using the order parameter \((OP)\) data is also shown in figure 3. As it is clear from figure 3, their behaviour as a function of \( q \) is very similar. For comparison, \( CFV^{\text{max}}(q)/CFV^{\text{max}}(q = 2) \) versus \( q \) for small and the large lattice is plotted on a logarithmic scale as well (figure 4), and it gives similar information about the \( q \) dependence of the cluster size and the order parameter data given in figure 3. Since the definition of the order parameter involves all spins in the same orientation (throughout the lattice rather than individual clusters) the order parameter can not be used to calculate a quantity similar to \( CFV \). Hence in figure 4 the information comes from the cluster size data only.

If the phase transition is second-order (i.e. the correlation length is infinite), on
a finite lattice, the lattice size sets the limits of the correlation length. Hence for
$q = 2, 3$ and $4$ $\tau$ ratios for different sizes exhibit this limit and this ratio is about
2.0. If the correlation length is larger than the lattice size, the measurements of any
quantity which is proportional to correlation length will lead to a value proportional
to the lattice size. For $q \geq 5$, since the correlation length is finite, the discrepancy
starts to appear. The behaviour of a local operator such as energy is very different
and one can not observe the above discussed changes as $q$ varies.

4 Conclusions

Dynamical behaviour of clusters is studied in two-dimensional Potts model for the
number of states $q$ varying from 2 to 8 on $32 \times 32$ and $64 \times 64$ lattices. Dynamical data
for energy, order parameter and the cluster size ($CS$) are obtained during relaxation
of the system at the finite size critical coupling value $K_c$ and this data is fitted
to both exponential and the polynomial functions for each value of $q$. Relaxation
time $\tau$ (from the exponential fit) and the cluster formation velocity $CFV$ (from the
exponential and polynomial fits) are obtained for small and large lattices. $CFV$
curves given in figure 2 have distinct maxima for $q = 2, 3$ and $4$, while they have
a broad maximum for larger $q$ (and almost constant for $q = 7$ and $8$). This is
consistent with the information given by dynamical data shown in figure 1. It is
also observed in figure 1 that the slope of the dynamical data decreases as $q$ increases.
This observation, together with the information from the exponential fit ($\tau$ versus $q$), enhances the idea that the clusters form quite slowly for large $q$ starting from $q = 5$, for which case the transition is first-order.

On a finite lattice, if the transition is second-order ($q = 2, 3, 4$), the correlation length is infinite and the size of the system sets the limit on the correlation length. This is consistent with the information obtained when $\tau$ and $CFV$ measurements on different sizes are compared. It is observed that their ratios for different sizes are about to be the same for small $q$ ($q = 2, 3, 4$); close to the ratio of the linear sizes when calculated directly. For $q \geq 5$, although the correlation length is larger than both lattice sizes (especially for $q = 5$ and 6), the size ratios start to deviate from 2.0 significantly, corresponding to the discrepancy between two curves in figures 3 and 4. This behaviour is indicative of the sensitivity of the measured quantities to changes in the correlation length (hence to changes in the order of the transition).

This means that cluster size related measurables like $CFV$ can give some relevant information about the nature of the transition in the Potts model and in similar models (using only a first few hundreds of the Monte Carlo iteration).

It should be stressed here that the $\tau$ values calculated from autocorrelations obtained as a result of the runs of $1 - 2 \times 10^6$ iterations (after thermalization) at $K_c$ are the same as the ones obtained from dynamical data, within the error limits. This shows that the results of cluster formation dynamics are reliable, and the
quantities like $CS$, $\tau$ and $CFV$ obtained during early iterations can give reliable information about the critical behaviour of the system. When computing times to calculate autocorrelations and the dynamical data are compared, it is easy to see that critical behaviour of similar systems can be studied using this new method, and the computational effort is much less than that for the standard and commonly used methods.

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FIGURE CAPTIONS

Figure 1. The average cluster size calculated dynamically ($CS$) for $q = 2, 3, ... 8$ on $64 \times 64$ lattice.

Figure 2. Cluster formation velocity ($CFV$) for $q = 2, 3, ... 8$ calculated on $64 \times 64$ lattice.

Figure 3. $\frac{\tau(q = 2)}{\tau(q)}$ versus $q (q = 2, 3, ... 8)$ for cluster size ($CS$) and the order parameter ($OP$) calculated on $32 \times 32$ and $64 \times 64$ lattices.

Figure 4. $\frac{CFV^{max}(q)}{CFV^{max}(q = 2)}$ versus $q (q = 2, 3, ... 8)$ for cluster formation velocity ($CFV$) calculated on $32 \times 32$ and $64 \times 64$ lattices.
Figure 1:

Figure 2:
Figure 3:

Figure 4: