Study of Cluster Fluctuations in Two-dimensional q-State Potts Model†

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Abstract The two-dimensional Potts Model with 2 to 10 states is studied using a cluster algorithm to calculate fluctuations in cluster size as well as commonly used quantities like equilibrium averages and the histograms for energy and the order parameter. Results provide information about the variation of cluster sizes depending on the temperature and the number of states. They also give evidence for first-order transition when energy and the order parameter related measurables are inconclusive on small size lattices.

Keywords: Phase transition, Potts model, clusters, Monte Carlo simulation

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1 Introduction

Identifying the phase structure of a statistical mechanical system has been one of the most challenging problems of contemporary physics. Second-order phase transitions are well understood in the contexts of renormalization group [1] and finite size scaling theories [2]. For the case of first-order phase transitions, (for a recent review, see [3]) the difficulty arises with the systems possessing finite, but very large correlation length. In such systems the transition can easily be confused with second-order phase transition when the measurements are done on a finite system. One of the commonly used methods to determine the order of a phase transition is due to Challa et al [4], which considers distributions of energy or order parameter and compares these distributions with a single or a double gaussian for second- or first-order phase transition cases, respectively. This method is based on the argument that for a first-order phase transition the barrier between the metastable states will be widened and hence distinct two gaussians will be apparent with increasing lattice size. Another method employed by Lee and Kosterlitz [5, 6] considers the minima in free energy, and similar arguments are also valid for distinguishing first-order phase transition from a second-order one. In both of these methods the main idea is that the system remains in metastable states for a considerable amount of time. Even if there exist metastable states, the size of the system may prevent the observation of the double-
peak behavior of the energy distribution. For the systems with finite but very large correlation length, where a first-order phase transition resembles second-order one, one needs to compare different size lattices in order to reach a conclusion on the order of the transition. The well-known examples of these systems are 5-state Potts model in 2-dimensions \[5, 7\] and 3-state Potts model in 3-dimensions \[6, 8\] as well as finite temperature SU(3) lattice gauge theory \[9\].

One of the major elements of a phase transition is the formation of clusters. Observing the clusters and their variations in size is expected to lead a better understanding of phase transitions occurring in the system. In the present work, the critical behaviour of the two-dimensional Potts model with 2 to 10 states is studied using cluster algorithm. Fluctuations in cluster size as well as the histograms for energy and the order parameter are obtained as a function of the temperature for different number of states.

Section II gives some information about the model and the algorithm. Results and discussions are given in section III, and the conclusions are presented in section IV.
2 Model and the method

The Hamiltonian of the two-dimensional Potts model \cite{10} is given by

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

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, ..., \( q \) for the \( q \)-state Potts model. The order parameter (\( OP \)) can be defined through the relation

\[ OP = \frac{q\rho^\alpha - 1}{q - 1} \]  

where \( \rho^\alpha = N^\alpha/L^D \), \( N^\alpha \) being the number of spins with \( \sigma = \alpha \), \( L \) the linear size and \( D \) the dimensionality of the system. The average cluster size (CS) is calculated by taking the average over the number of clusters \( (N_c) \),

\[ CS = \frac{1}{N_c} < \sum_{i=1}^{N_c} C_i > \]  

where \( C_i \) is the number of spins in the \( i^{th} \) cluster. The two-dimensional Potts model undergoes a second-order phase transition for 2, 3 and 4 states, while a first-order phase transition is known to occur for higher number of states\cite{7}. Reader can refer to the review article by Wu \cite{11} for detailed information about the model.

First-order transitions can be recognized by studying double-peak behaviour of the
energy probability distribution function $P(E)$ [4]. When the transition is first-order, order parameter probability distribution function $P(\text{OP})$ should also exhibit the same behaviour. If the energy distribution, measured on sufficiently large lattices, is a single gaussian at the critical point, this is a clear indication of a second-order phase transition, and having two gaussian distributions is an indication of a first-order transition as mentioned above. Even if the energy has a single gaussian distribution, the order parameter or the cluster size distribution may mimic a first-order transition. Larger lattices may lead to double gaussian shape of the energy distribution but measurements made on moderate size lattices may be inconclusive. Moreover, a double-peak behaviour in the distribution of the order parameter may be misleading [12].

Another observable which can provide information about critical behavior is the average cluster size (CS). The study of variations in cluster size for different $K$ and $q$ should give some indications about the nature of the transitions occurring in the system. By these considerations, identification of the order of phase transition is reduced to correct identification of the various size clusters which requires an extra computational effort when a usual local updating algorithm is used. The reduction of critical slowing down by a cluster flip algorithm was first introduced by Swendsen and Wang [13] and later modified by Wolff [14]. The cluster 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.

3 Results and discussions

After thermalization with $10^4 - 5 \times 10^4$ sweeps, $5 \times 10^5$ iterations are performed for
32 × 32 and 64 × 64 lattices of the 2 to 10-state models at different values of the
coupling $K$. Majority of the runs are started using a disordered initial configuration,
and the averages calculated for both ordered and disordered starting configurations
are observed to be equal within statistical errors. Longer runs with up to $10^6$
iterations are done near the finite-size critical value $K_c$ at each state $q$. As a result
of these runs, equilibrium averages for energy, cluster size and the order parameter
are obtained, specific heat and the Binder cumulant are calculated as a function of
$K$ for each value of $q$. These quantities are used as a test ground for the algorithm
used as well as for the thermalization and the accuracy, and they show expected
behavior for different lattice sizes and different number of states, therefore they will
not be reported here. $K_c$ values, which are estimated at the peak values of the
specific heat for the 64 × 64 lattice are close to $K_c^{\infty}$ values for the infinite lattice
within an error of about one percent. The errors calculated using jackknife analysis
are small (less than one percent for most of the quantities, within about 2 percent for the specific heat) and they can be decreased by increasing the number of Monte Carlo iterations.

The histograms for energy, order parameter, and the average cluster size as a function of the number of iterations are obtained for \( q = 2 \) to 10 near \( K_c \). The models with \( q = 2 \) and 3 have similar histograms with a single gaussian, and for the cases \( q \geq 5 \), all histograms have distinct double peaks, getting higher and sharper as \( q \) increases. In the histograms for energy, double peaks occur for \( q \geq 5 \) with almost equal maxima near the \( K_c \) values estimated using the specific heat data, as expected. Figure 1 shows the histograms for energy and the order parameter for \( q = 3, 4 \) and 5 on 64 × 64 lattice obtained at \( K_c \). Plots for \( q = 3 \) have single peaks for both energy and the order parameter. The histograms for \( q = 5 \) show indication of the first-order character, with the appearance of double peaks in both plots. The energy histogram for \( q = 4 \) is similar to the one for \( q = 3 \), but the order parameter histogram shows a variation which looks more similar to the plot for \( q = 5 \).

The fluctuations \( FCS \) (\( FCS = \langle (CS)^2 \rangle - \langle CS \rangle^2 \)) in the average cluster size \( CS \) are calculated for different values of \( q \) on 64 × 64 lattice as a function of \( K \). Figure 2 shows \( FCS \) for \( q \) varying from 3 to 7 and the CPU times for the corresponding Monte Carlo runs. As can be seen from these plots, \( FCS \) and the
CPU time give similar information about the formation of the clusters (1/FCS has a similar variation as the CPU time). When K is small (i.e. the temperature is high), the cluster sizes are small, hence FCS is small, and the algorithm spends a long time to search for the clusters small in size but large in number. As K increases, the cluster sizes are getting larger, so the CPU time decreases, but FCS increases due to the existence of the small-size clusters as well as the large ones. At the critical point, formation of the largest clusters results in the largest value of FCS, with the corresponding minimum value of the CPU time, since there are only a few clusters to be searched. One can make a similar discussion when the critical point is approached from above (in the region where \( K > K_c \)), with the exception that the CPU time is almost constant for large K, as mentioned in section II.

FCS plots also show that the maximum value of FCS increases as q increases. When q is getting larger, decreasing correlation length (due to increasing first-order character) results in breaking large clusters into smaller ones. Near the critical point, the tendency of forming large clusters together with the disintegration process causes FCS to increase with increasing q. In the second-order phase transitions, long range correlations keep the clusters as they are for a very long time or for large number of iterations (hence FCS is small for small q). The FCS and CPU plots show that the models with \( q > 4 \) behave differently at two sides of the critical point. The plots for
$q = 3$ are in the form of curves with a smooth variation, passing through a minimum near $K_c$. Plots for the other cases show different behaviour in two separate regions around the critical point, with a sharp variation near $K_c$ value. The CPU data for $q = 3$ can be fitted to a polynomial function around $K_c$ at both sides of the critical point, but no fit seems to be possible for $q > 4$. The only possibility is the fit of two distinct polynomials to two separate curves, for $K < K_c$ and $K > K_c$.

4 Conclusions

The two-dimensional Potts model with 2 to 10-states is studied using cluster algorithm for lattices with sizes $32 \times 32$ and $64 \times 64$. Energy, order parameter, cluster size, fluctuations in the cluster size, specific heat and the Binder cumulant are calculated, and the histograms for energy, order parameter and the cluster size are obtained as a function of the coupling $K$.

Studies in this work are focused on the cluster size related observables. One of these observables is the fluctuations in the cluster size (FCS) which measures the extent of the coexistence of different size clusters. This operator is very sensitive to the correlation length and exhibits sharp peak at the transition region if the transition
is first-order. The similar information can also be obtained from the CPU time spent to calculate the averages for a certain number of iterations. If there exist only small clusters, due to the modified algorithm used in this work, the CPU time is extremely large and growing cluster size reduces this time. In the first-order case, small clusters grow very fast near \( K_c \), while in the second-order case, the average cluster size grows smoothly. Both figures 2.a (FCS) and 2.b (CPU) indicate that on 64 × 64 lattice \( q = 3 \) and 4 have different character than \( q \geq 5 \) Potts models. From these two figures one can conclude that for the systems with varying correlation length, FCS and CPU are sensitive to the correlations even though the correlation length is much larger than the system size.

Further work is planned, using the same algorithm, to study cluster distributions in detail as well as random-field and random-bond Potts models.

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Figure captions

Figure 1. a) Energy, b) the order parameter histograms, as a function of the number of iterations for $q = 3, 4$ and $5$ on $64 \times 64$ lattice near $K_c$.

Figure 2. a) Fluctuations in the average cluster size, b) the CPU time, as a function of $K$ for $q$ varying from 3 to 7 on $64 \times 64$ lattice. Computations are done using IBM-RS/6000 workstations. The errorbars in $FCS$ plots are about the size of the data points and are visible only for large $q$. 
Figure 1:
Figure 2: