

Cluster size distribution to characterize the first-order phase transitions of equilibrium systems

Abstract

Through Monte Carlo simulations we study cluster size distribution (CSD) of equilibrium systems. The system is simulated by applying the Wolff algorithm or single cluster Monte Carlo update algorithm. Our results show that CSD is a good tool in the identification of first-order transitions.

Keywords: phase transition, potts model, clusters, wolff

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Lima FWS

Department of Physics, Federal University of Piauí, Brazil

Correspondence: Francisco Wellington De Sousa Lima, Department of Physics, Dietrich Stauffer Computational Physics Lab, Federal University of Piauí, 64049-550, Teresina-PI, Brazil, Tel +5586 3237 1424, Email fwslima@gmail.com

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Introduction

Equilibrium systems such as the Potts model with q -states in two-dimension presents two types of phase transition. Continuous or second order and one explosive or first order.^{1,2} To identify the type of phase transition we have some useful tools such as examining the minimum free energy^{3,4} by considering the probability distribution of energy,⁵ the distribution function of the system order parameter PDF,^{6,7} fourth-order Binder cumulant^{8,9} and CSD.¹⁰⁻¹²

In systems that exhibit first-order phase transition the most common feature is the coexistence of ordered and disordered states in the phase transition region. In the region of ordered phase the large clusters are dominant and in the disordered phase, small clusters are dominant. The existence of both small and large clusters in a first-order phase transition region gives rise to double-peak energy behavior and PDFs. Studying the Potts model in two dimensions Aydin et al.,¹⁰ and Gündüç et al.,¹¹ observed that global operators related to cluster size are more sensitive to structural changes in a phase transition than energy-related local operators and the order parameter of the system. Notably, the CSD may give a better indication of the order of phase transition for small networks than the distribution of energy.

In this work, we investigate the CSD to study the phase structure of the 8-state Potts model on Voronoi-Delaunay random lattices (VDRL)¹³ concerning quenched randomness on the links in a range of alpha values $a=0$ to 0.5

Model and simulations

We consider the Potts model with $q=8$ states on VDRL by a set of spin variables taking the values situated on every site i of a VDRL with N sites. In this random lattice, we start from a two-dimensional random lattice consisting of sites linked to their k (where $3 < k < 20$) and different for each site of network nearest neighbors by both outgoing and incoming links.

The Hamiltonian of the Potts model with $q=8$ states can be written as

$$-KH = \sum_{ij} J_{ij} \delta_{\sigma_i \sigma_j} \quad (1)$$

where $K=1/k_B T$, T is the temperature, $\delta_{\sigma_i \sigma_j}$ is the delta of Kronecker, k_B is the Boltzmann constant, the sum goes over all nearest-neighbors pairs of sites. Here, we assume that the coupling factor J_{ij} depends on the relative distance r_{ij} between sites i and j and is given by

$$J_{ij} = J_0 e^{-ar_{ij}}, \quad (2)$$

where J_0 is a constant and $a \geq 0$ a model parameter. In the simulations, we apply the Wolff update algorithm¹⁴⁻¹⁷ on different VDRL to generate different sizes of the cluster and perform simulations comprising a number $N=4000$ of sites of random lattices. For each system quenched averages over the connectivity disorder are approximated by averaging over $R=100$ independent realizations. For each simulation, we have started with a uniform configuration of spins. We ran 3×10^5 Monte Carlo steps (MCS) per spin with 2×10^5 configurations discarded to reach steady state.

Results and discussions

From CSD we calculate the average cluster size defined by

$$ACSD = \frac{1}{N_c} \left\langle \sum_{i=1}^{N_c} C_i \right\rangle \quad (3)$$

where N_c and C_i are the number and sizes of clusters generated by the Wolff algorithm, respectively. In the above equations $\langle \dots \rangle$ stands for thermodynamic averages.

In Figure 1 we show the histogram of the energy for the values $a=0.1, 0.15, 0.29, 0.23, 0.25, 0.27, 0.50$ and for $N=4000$ sites. From $a=0.0$ to 0.20 we have a double peak structure indicating that a first order phase transition to the Potts model with $q=8$ states, while for $a=0.5$ we have a single Gaussian peak structure that represents an indication for a second order phase transition. To further clarify this behavior we use the mean distribution of clusters as seen in Figure 2.

As shown in Figure 2 the peaks in the region of small clusters indicate the presence of first-order transition.

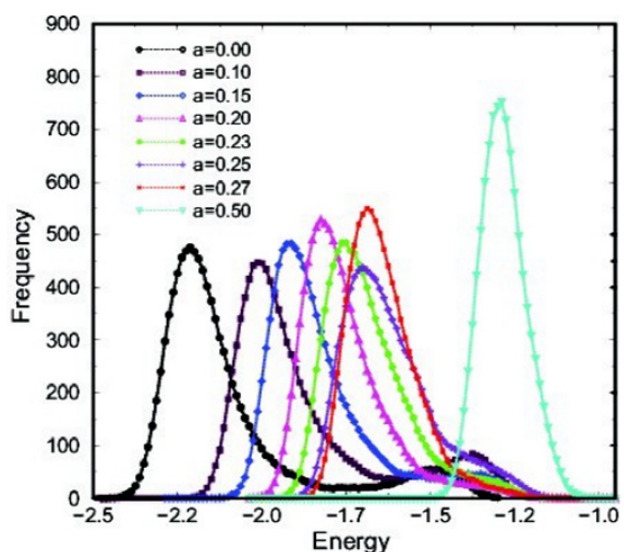


Figure 1 Histogram of the energy for some values of $a = 0.1, 0.15, 0.29, 0.23, 0.25, 0.27, 0.50$ and $N = 4000$ sites.

Conclusion

In summary, the energy histogram is very useful in identifying a first-order phase transition as long as the systems structures are regular as the square lattice, triangular, and other two-dimensional archimedean lattices. In the case here, that is, on VDRL or others random lattices where the Wolff algorithm can be used we have seen that the ASCD is more appropriate for the identification of first-order phase transitions.

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Conflict of interest

The author states that there is no conflict of interest.

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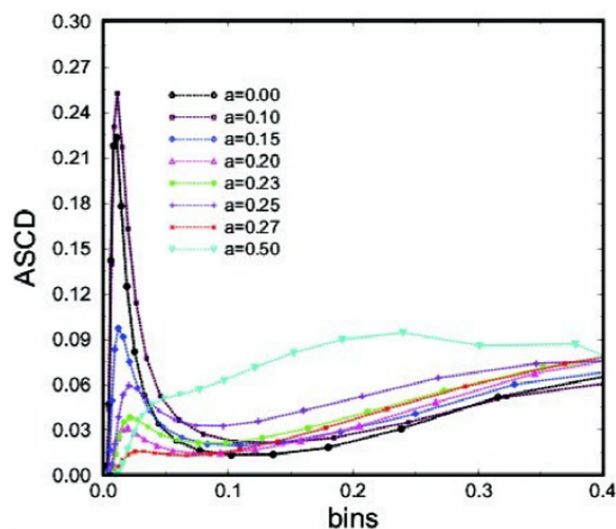


Figure 2 Distribution of the average sizes of clusters to several values of a on a VDRL of $N = 4000$ sites and with $q = 8$.

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