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Monte Carlo Simulations of Conformal Theory Predictions for the Three-State Potts Model

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The critical properties of the three-state Potts model are investigated using Monte Carlo simulations. Special interest is given to the measurement of three-point correlation functions and associated universal objects, i.e., structure constants. The results agree well with predictions coming from conformal field theory, confirming, for this example, the correctness of the Coulomb gas formalism and the bootstrap method.

KEY WORDS: Conformal field theory; Monte Carlo; two-dimensional Ising model; two-dimensional three-state Potts model; structure constants; correlation functions.

1. INTRODUCTION

Conformal field theory[1] has produced many precise predictions for two-dimensional (2D) equilibrium critical systems. They fall into two large classes: critical exponents[2] and operator-product structure constants.[3] Theoretical calculations of these quantities are based on very special properties of the representations of the conformal group that are believed to be relevant to 2D critical statistical systems (see ref. 4 for review) —degenerate Verma modules[5] and modular invariance.[6] For many models, these properties have led to the only available theoretical calculations of the structure constants.

Further efforts to measure the structure constants are justified on two grounds. First, they define the scattering amplitudes of 2D conformal field

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theories. Second, the conformal calculation of the structure constants exploits indirect techniques of constructing correlation functions—the bootstrap equation[5] and the Coulomb gas formalism.[3] These methods were not involved in conformal predictions of critical exponents and fusion rules. Their use requires new assumptions—that the Coulomb gas formalism gives a complete basis of conformal blocks and that nontrivial analytic continuations in the variables defining the blocks are unique. While there is widespread belief that these assumptions are correct, they merit experimental tests.

Though many structure constants have been theoretically calculated,[3] few have been measured. Finite-size effects on the spectrum of 1D spin chains are determined by them. These effects have been used to find the ratio of two structure constants and to verify two fusion rules in the three-state Potts model.[7] Further studies of finite-size effects could enable the measurement of all structure constants.[7]

Experiments to determine the structure constants are difficult and do not presently exist. They require measuring both two-point and three-point correlation functions at the critical point. Such measurements are much simpler in Monte Carlo simulations. The purpose of this article is to report on Monte Carlo experiments for the three-state Potts model. The results will give measured values for structure constants that will be compared to predictions of conformal field theory[9] (also see last Appendix of ref. 4 and, for a review, ref. 8). They will provide us with both an "experimental" test of conformal field theory and an insight into the methods necessary to "directly" measure the new "universal" quantities that it predicts in 2D critical systems.

We will briefly summarize some facts about the Potts models that will be important to our analysis. A review of the statistical properties of these models can be found in refs. 10–12. Their identifications with conformal field theories are discussed in refs. 4, 5, 8, and 9. Since the theoretical tools necessary to perform the simulations are minimal, we refer to refs. 5 and 9 for explanations of the theoretical calculation of structure constants.

Our simulations will be for models on square lattices with periodic boundary conditions generated by two primitive vectors $\mathbf{n}$. The Hamiltonian of these models has the following form:

$$H = \sum_{\mathbf{x}} E(\mathbf{x}) = (-J)/2 \sum_{\mathbf{x},\,\mathbf{n}} [S(\mathbf{x}+\mathbf{n}) + S(\mathbf{x}-\mathbf{n})]\, S^*(\mathbf{x}) \tag{1}$$

where $\mathbf{x}$ is a vector on the lattice. The spin density $S(\mathbf{x})$ and the energy density $E(\mathbf{x})$ are operators that describe the coupling of the physical system to magnetic and temperature perturbations, respectively. They are

fundamental conformal operators (primary fields) having simple local definitions on the lattice. The field $S(\mathbf{x})$ takes the discrete values ± 1 for the Ising model (two-state Potts) and 1, $\exp(2\pi i/3)$, and $\exp(-2\pi i/3)$ for the three-state Potts model. The energy density operator is defined locally by the value of $S(\mathbf{x})$ on five neighboring lattice sites, i.e.,

$$E(\mathbf{x}) = -J \sum_{\mathbf{x}} \tfrac{1}{2}[S(\mathbf{x}+\mathbf{n}) + S(\mathbf{x}-\mathbf{n})]\, S^*(\mathbf{x}) \tag{2}$$

Both of these operators exhibit scaling behavior at the critical point.

Traditionally, the Hamiltonian for the Potts model is written in a slightly different form, i.e.,

$$H = -J \sum_{\mathbf{x},\,\mathbf{n}} \delta(S(\mathbf{x}), S(\mathbf{x}+\mathbf{n})) \tag{3}$$

The Hamiltonians (1) and (3) of the three-state model are equivalent, up to an overall additive constant of $-J/2$ per bond and a scaling factor of 2/3: a pair of aligned neighboring spins contributes 1 to the summation in both cases, but a pair of nonaligned neighboring spins contributes $-1/2$ in (1) and 0 in (3).

The scaling behavior of two-point correlations at a critical point defines the conformal dimensional Δ_i of a scaling field $\phi_i(\mathbf{x})$. For spinless fields like $S(\mathbf{x})$ and $E(\mathbf{x})$, it is given by

$$\langle \phi_i(\mathbf{x})\, \phi_j^*(\mathbf{0}) \rangle = \frac{\delta_{ij} N_i^2}{|\mathbf{x}|^{4\Delta_i}} \tag{4}$$

True scaling fields (thus also conformal primary fields) have vanishing statistical averages at a critical point,[5] e.g., $\langle \phi_i(\mathbf{x}) \rangle = 0$. To obtain such fields, one must subtract the thermal averages from lattice fields with nonzero averages, like $E(\mathbf{x})$. Only the subtracted operators obey the scaling law of (4). The subtraction constants are not universal and are not described by conformal theory. This subtraction procedure must be explicitly done in any simulation.

Finally, we mention that (4) and all other equations for critical correlation functions manifestly respect the discrete symmetries of (1). The spin field $S(\mathbf{x})$ transforms under the discrete symmetry Z_3 for the three-state Potts model. Its correlation functions will obey superselection rules, at the critical point, associated with these symmetries.

The conformal dimensions of $S(\mathbf{x})$ and $E(\mathbf{x})$ have been known for the Potts models for some time.[4, 5, 9, 10] Their explicit values are given in Table I.

Table I. Scaling Dimensions of the Spin and Energy Density Fields in the Three-State Potts Model

Field	Scaling dimension
$S(\mathbf{x})$	1/15
$E(\mathbf{x})$	2/5

Our main interest concerns the predictions from conformal field theory for the three-point correlation functions. It is well known that the three-point correlations of conformally invariant theories have the following special form:[1]

$$\langle \phi_i(\mathbf{x}_i)\, \phi_j(\mathbf{x}_j)\, \phi_k(\mathbf{x}_k) \rangle = \frac{C_{ijk} N_i N_j N_k}{|\mathbf{x}_{ij}|^{2\Delta_i + 2\Delta_j - 2\Delta_k} \times \text{cyclic perms.}} \tag{5}$$

The quantities C_{ijk} are the structure constants. Much of the revival of interest in conformal theories during the 1980s was associated with the realization that, in 2D, the C_{ijk} were new universal quantities different from critical exponents. More importantly, they were shown to be calculable from symmetry considerations alone.[5] The N_i define the normalizations of the two-point functions. They are not universal and must be measured in our simulations of two-point correlations before extracting the universal constants C_{ijk} from (5).

The calculation of the structure constants has been achieved for a large variety of minimal conformal models by using their special mathematical properties—the existence of null vectors.[3,5] These models are believed to describe the critical behavior of many of the important statistical systems. The critical point of the Ising model has been identified with the A_3 conformal minimal model.[5] The critical point of the three-state Potts model has been identified with a Z_3 symmetric version of the D_5 conformal minimal model.[4,9] The values of the structure constants resulting from theoretical calculations based on these identifications are summarized in Table II; the detailed calculations are found in refs. 8 and 9.

Table II. Predicted Structure Constants of the Three-State Potts Model

Structure constant	Value
C_{SES^*}	0.546
$C_{SSS}\,(= C_{S^*S^*S^*})$	1.092

The structure constants not shown in Table II vanish due to the discrete symmetries. The vanishing of C_{EEE} results from a fusion rule ($\Phi_{21} \times \Phi_{21} = 1$). Its discovery stimulated the revival of interest in 2D conformal symmetry[5] in 1984. This particular fusion rule is also related to the duality symmetry of the critical point, i.e., the dual transformation on E is $E \to -E$. The fusion rules are fundamental predictions of conformal field theory. Nevertheless, they only state when structure constants are nonzero. The actual values for nonzero C_{ijk} of Table II have been calculated by using two other tools of 2D conformal theory—the screened Coulomb gas formalism[3] and the so-called "bootstrap" equations.[5] The values of the nonzero C_{ijk} are a second fundamental prediction of conformal field theory. Experimental confirmation of their explicit values supports the validity of these latter two tools of 2D conformal theory.

While the structure constants of the Ising model were known before the arrival of conformal field theories,[13] those for the three-state Potts model have not been found by other methods.[9] Thus, the latter model allows a real test of the methods of conformal field theory.

2. ANALYSIS

Our simulations utilize the following procedure. First, the infinite-lattice critical temperature is found from duality considerations $T_c = T_D$. Next, the exact value of T_c for our finite lattice is determined by calculating the two-point correlations of $S(\mathbf{x})$ near T_D: below T_c, the correlations approach a constant value at large distances; above T_c, the correlations fall off exponentially; and exactly at T_c the correlations show power-law scaling behavior. After constructing the two-point correlation of $S(\mathbf{x})$ at T_c, we can measure the scaling dimension of $S(\mathbf{x})$ and the normalization constant N_S in (4). Next, the thermal average of $E(\mathbf{x})$, $\langle E \rangle$, is measured at the critical temperature. Then, the critical two-point correlation of $E(\mathbf{x})$ is simulated. The nonscaling contribution $\langle E \rangle^2$ is subtracted, and the scaling dimension of $E(\mathbf{x})$ and N_E are determined. Finally, the three-point correlations are simulated. The scaling exponents can be extracted. The structure constants are found with the help of (5) and the values of N_S and N_E. The last step is to compare our "simulated" scaling dimensions and structure constants with the conformal field theory predictions of Tables I and II.

The Monte Carlo methods for the three-state Potts model were carried out on a 500×500 lattice with periodic boundary conditions. The algorithm used to generate sample configurations is a cluster algorithm, as outlined by Wolff.[14] In one such cluster move, the time scale was incremented by the fraction of spins included in the cluster. In the work presented here, this time scale is only relevant for defining the thermalization time and time

between samples. In our Potts simulations, we thermalized over 300 such time units and took 21,000 samples separated by 20 time units. To obtain statistical error bars, these samples were blocked in groups of 150 samples, and their standard deviation was obtained.

By finding the temperature at which the two-spin correlation $\langle S(\mathbf{x})\, S^*(\mathbf{0})\rangle$ shows power-law scaling, we found that, for our system size, $T_c/T_D = 1.0005 \pm 0.0003$. All data reported for the Potts model are obtained with this lattice size and at the above value of T_c.

Figure 1 shows the two-point correlations for the Potts model. The vacuum expectation value $\langle E\rangle^2$ has already been subtracted in graphs of correlation functions of $E(\mathbf{x})$. The simulations of the two-point functions give $N_S^2 = 0.54 \pm 0.03$ and $N_E^2 = 0.125 \pm 0.005$ (Fig. 1). The power-law dependence of these correlations gives an $\eta_{SS^*} = 0.26 \pm 0.02$ in agreement with Table I, i.e., four times the dimension of the field $\eta_{SS} = 4/15$. The measured value for η_{EE} is 1.66 ± 0.04. This disagrees slightly with the

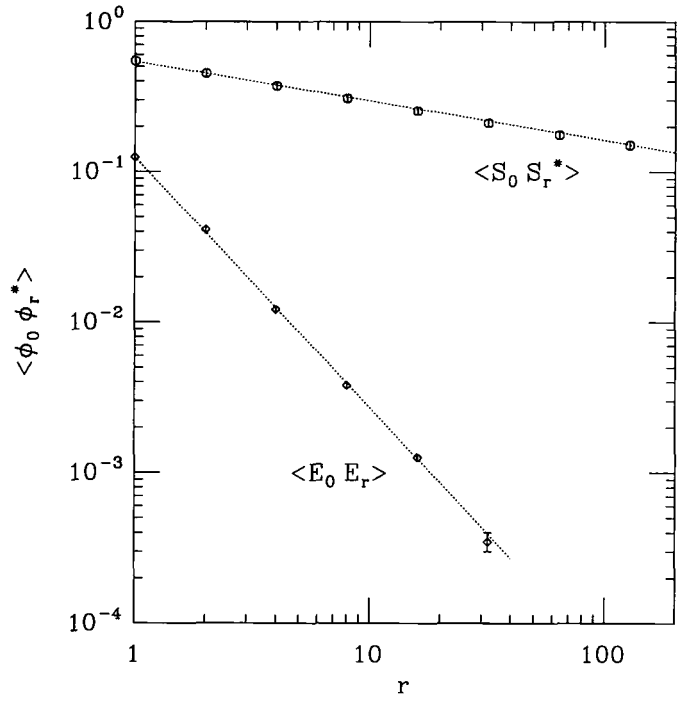

Fig. 1. Two-spin correlations (top) and energy density two-point correlations (bottom) in the three-states Potts model on a 500×500 lattices at $T = T_c$. The dashed lines are our fit to the power-law behavior, given by $\langle S_0 S_r^* \rangle = k_{SS^*} r^{-\eta_{SS^*}}$, where $k_{SS^*} = 0.54 \pm 0.03$ and $\eta_{SS^*} = 0.26 \pm 0.02$, and $\langle E_0 E_r \rangle = k_{EE} r^{-\eta_{EE}}$, where $k_{EE} = 0.125 \pm 0.005$ and $\eta_{EE} = 1.66 \pm 0.04$.

prediction of Table I ($\eta_{EE} = 8/5$). These results are reasonable from the statistical nature of our errors.

The three-point correlations were measured by placing one operator at $\mathbf{0} = (0,0)$ (the center of the lattice) and the other two at $\mathbf{r}_1 = (r, 0)$ and $\mathbf{r}_2 = (0, r)$, i.e., two vectors along the two perpendicular lattice directions at a distance r. Figure 2 shows this correlation for the Potts model as a function of r. Conformal field theory, Eq. (5) and Table I, predicts for the Potts model that

$$\langle S_{r_1} S_0 S_{r_2} \rangle = 2^{-1/15} N_S^3 C_{SSS} r^{-2/5} \tag{6}$$

and

$$\langle S_{r_1} E_0 S_{r_2}^* \rangle = 2^{4/15} N_S^2 N_E C_{SES^*} r^{-16/15} \tag{7}$$

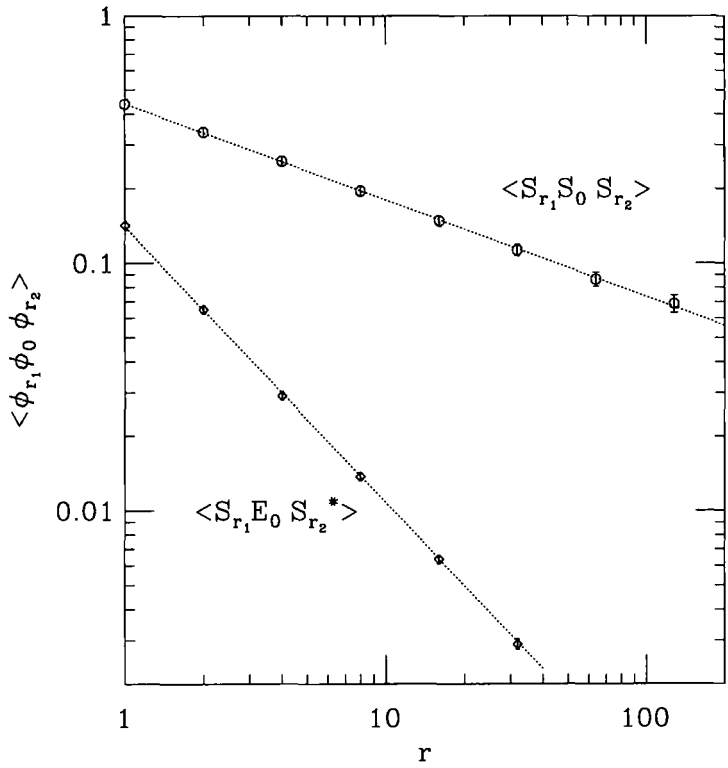

Fig. 2. Three-spin correlations (top) and mixed three-point correlations (bottom) in the Potts model on a 500×500 lattice at $T = T_c$. The dashed lines are our fit to the power-law behavior, given by $\langle S_{r_1} S_0 S_{r_2} \rangle = k_{SSS} r^{-\eta_{SSS}}$, where $k_{SSS} = 0.44 \pm 0.04$ and $\eta_{SSS} = 0.39 \pm 0.02$, and $\langle S_{r_1} E_0 S_{r_2}^* \rangle = k_{SES^*} r^{-\eta_{SES^*}}$, where $k_{SES^*} = 0.14 \pm 0.01$ and $\eta_{SES^*} = 1.11 \pm 0.04$.

The measurements shown in Fig. 2 fit the form

$$\langle S_{r_1} S_0 S_{r_2} \rangle = k_{SSS} r^{-\eta_{SSS}}$$

with $k_{SSS} = 0.44 \pm 0.04$ and $\eta_{SSS} = 0.39 \pm 0.02$, and

$$\langle S_{r_1} E_0 S^*_{r_2} \rangle = k_{SES^*} r^{-\eta_{SES^*}}$$

with $k_{SES^*} = 0.14 \pm 0.01$ and $\eta_{SES^*} = 1.11 \pm 0.04$, respectively. The exponents agree with the theoretical values 2/5 and 16/15. Combining these results with (5) and the results for N_E and N_S, we obtain measured values for the two nonzero structure constants of the three-state Potts model, $C_{SES^*} = 0.61 \pm 0.06$ and $C_{SSS} = 1.16 \pm 0.14$. The measured values compare quite well with the predictions of Table II.

Finally, there are theoretical calculations of C_{SES} in the Ising model that do not rely on conformal theory.[13] The measurement of this structure constant allows an independent test of the validity of our procedure. Employing the method used above, we found that $C_{SES} = 0.54 \pm 0.05$ for the Ising model. This result is in good agreement with the correct theoretical value of 1/2.[7, 13]

In summary, we have measured two- and three-point correlations for the two-dimensional three-state Potts model and have compared both their exponents and prefactors, i.e., structure constants, with predictions from conformal field theory. All measurements, except one, are within one standard deviation of theoretical predictions. The remaining one is within two standard deviations. This gives a test of the screened Coulomb gas and bootstrap equation formalisms that were used to obtain the theoretical values.

Our Monte Carlo simulations strongly support the validity of the detailed conformal theory methods that have allowed the calculation of higher correlation functions at critical points. This work has extended the results of ref. 7, which measured a ratio of two structure constants for the three-state Potts model.

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