Monte Carlo Simulations of Conformal Theory Predictions for
the 3-state Potts and Ising Models

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Abstract

The critical properties of the 2D Ising and 3-state Potts models are investigated using Monte Carlo simulations. Special interest is given to measurement of 3-point correlation functions and associated universal objects, i.e. structure constants. The results agree well with predictions coming from conformal field theory confirming, for these examples, the correctness of the Coulomb gas formalism and the bootstrap method.

I. INTRODUCTION

Conformal field theory has produced many precise predictions for 2-dimensional, equilibrium, critical systems. They fall into two large groups: critical exponents and operator-product structure constants. Theoretical calculations of these quantities are based on very special properties of the representations of the conformal group that are be-

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lieved to be relevant to 2D critical statistical systems [4] – degenerate Verma modules [3] and modular invariance [3]. The calculation of structure constants exploits indirect techniques of constructing correlation functions – the bootstrap equation [5] and the Coulomb gas formalism [3]. For many important systems, like the Potts model, the only method available to calculate these universal constants relies on conformal field theory. Though there is widespread sentiment that these techniques are correct, the abstractness of their analyses and the absence of independent theoretical confirmation of their predictions justify an effort to obtain experimental confirmation.

Experimental tests of the predictions for the structure constants are very difficult and do not presently exist. They would necessitate the measurement of both 2-point and 3-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 two well-known models – the Ising and 3-state Potts models. The results will give “measured” structure constants that will be compared to predictions of conformal field theory [7,8]. They will provide us with both an “experimental” test of conformal field theory and an insight into the methods necessary to measure these new “universal” quantities that it predicts in 2D critical systems.

We will briefly summarize some facts about the Potts and Ising models that will be important to our analysis. A review of the statistical properties of these models can be found in Refs. [9,10]. Their identifications with conformal field theories are discussed in Refs. [4,5,7,8]. Since the theoretical tools necessary to perform the simulations are minimal, we refer to Refs. [5,8] 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, $\vec{n}$. The Hamiltonian of these models has the following form:

$$H = \sum_{\vec{x}} E(\vec{x}) = -J/2 \sum_{\vec{x},\vec{n}} \left[ S(\vec{x} + \vec{n}) + S(\vec{x} - \vec{n}) \right] S^*(\vec{x})$$

(1)

where $\vec{x}$ is a vector on the lattice. The spin density, $S(\vec{x})$, and the energy density, $E(\vec{x})$, 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 $S(\vec{x})$ takes the discrete values $\pm 1$ for the Ising model and $1, \exp(2\pi i/3), \exp(-2\pi i/3)$ for the 3-state Potts model. The energy density operator is defined locally by the value of $S(\vec{x})$ on five neighboring lattice sites, i.e.

$$E(\vec{x}) = -J \sum_{\vec{n}} \frac{1}{2} [S(\vec{x} + \vec{n}) + S(\vec{x} - \vec{n})] S^*(\vec{x}).$$

(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.

$$H = -J \sum_{\vec{x}, \vec{n}} \delta(S(\vec{x}), S(\vec{x} + \vec{n})).$$

(3)

The Hamiltonians (1) and (3) are equivalent, except for 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 non-aligned neighboring spins contributes -1/2 in (1) and 0 in (3).

The scaling behavior of 2-point correlations at a critical point defines the conformal dimension, $\Delta_i$, of a scaling field $\phi_i(\vec{x})$. For spinless fields like $S(\vec{x})$ and $E(\vec{x})$, it is given by:

$$\langle \phi_i(\vec{x})\phi^*_j(\vec{0}) \rangle = \frac{\delta_{ij} N^2}{|\vec{x}|^{1+\Delta_i}}.$$ 

(4)

True scaling fields (ex. conformal primary fields) have vanishing statistical averages at a critical point, e.g. $\langle \phi_i(\vec{x}) \rangle = 0$. To obtain such fields, one must subtract the thermal averages from lattice fields with non-zero averages, like $E(\vec{x})$. 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 (1) and all other equations for critical correlation functions manifestly respect the discrete symmetries of (1). The spin field, $S(\vec{x})$, transforms under the discrete symmetry $Z_2$ for the Ising and under $Z_3$ for the 3-state Potts model. Its
correlation functions will obey superselection rules, at the critical point, associated with these symmetries.

The conformal dimensions of $S(\vec{x})$ and $E(\vec{x})$ have been known for the Ising and Potts models for sometime [4,5,8,9]. Their explicit values are given in Table I.

Our main interest concerns the predictions from conformal field theory for the 3-point correlation functions. It is well-known that the 3-point correlations of conformally invariant theories have the following special form [1]:

$$\langle \phi_i(\vec{x}_i)\phi_j(\vec{x}_j)\phi_k(\vec{x}_k) \rangle = \frac{C_{ijk}N_iN_jN_k}{|\vec{x}_{ij}|^{2\Delta_i+2\Delta_j-2\Delta_k} \times \text{cyclic perms.}}.$$  \hspace{1cm} (5)

The quantities $C_{ijk}$ are the structure constants. Much of the revival of interest in conformal theories during the 1980’s was associated with the realization that, in 2D, the $C_{ijk}$’s were new universal quantities different from critical exponents. More importantly, they were shown to be calculable from symmetry considerations alone [5]. The $N_i$’s define the normalizations of the 2-point functions. They are not universal and must be measured in our simulations of 2-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 [3]. The critical point of the 3-state Potts model has been identified with a $Z_3$ symmetric version of the $D_5$ conformal minimal model [4,8]. 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. [7,8].

The structure constants not shown in table II vanish due to the discrete symmetries of the two models. The vanishing of $C_{EEE}$ is, however, less trivial. It results from a well-known fusion rule ($\Phi_{21} \times \Phi_{21} = 1$) whose discovery stimulated the revival of interest in 2D conformal symmetry [5] in 1984. We will compare this prediction of conformal field theory directly to simulations. The fusion rules only state when structure constants are non-zero. The actual
values for non-zero $C_{ijk}$'s of Table I 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]. Thus, the values of the non-zero $C_{ijk}$'s 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 constants of the Ising model were known before the arrival of conformal field theories [11], those for the 3-state Potts model have not been found by other methods [8]. Thus, the later model allows a real test of the methods of conformal field theory.

II. 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 2-point correlations of $S(\vec{x})$ 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 2-point correlation of $S(\vec{x})$ at $T_c$, we can measure the scaling dimension of $S(\vec{x})$ and the normalization constant $N_S$ in (1). Next, the thermal average of $E(\vec{x})$, $\langle E \rangle$, is measured at the critical temperature. Then, the critical 2-point correlation of $E(\vec{x})$ is simulated. The nonscaling contribution $\langle E \rangle^2$ is subtracted, and we then determine the scaling dimension of $E(\vec{x})$ and $N_E$. Finally, the 3-point correlations are simulated. The scaling exponents can be extracted and the structure constants are found with the help of (3) 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 simulations of the Ising model were carried out on a $512 \times 512$ square lattice with periodic boundary conditions. The algorithm used to generate sample configurations is a cluster algorithm, as outlined by Wolff [12]. 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 Ising simulations, we thermalized over 300 such time units and took 18000 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 determining the temperature at which the 2-spin correlation \( \langle S(\vec{x})S(\vec{0}) \rangle \) shows power-law scaling, we found that for our system size \( T_c/T_D = 1.0015 \pm 0.0002 \). All data reported in this work for the Ising model is obtained with this lattice size and at the above value for \( T_c \). There are two independent theoretical calculations of \( C_{SES} \) for the Ising model, and one does not rely on conformal theory [11]. Here, we are sure of the value of \( C_{SES} \) and the Ising model is a test of our procedure. It gives us more assurance when simulating the Potts model where no independent checks exist. The simulations of the Potts model are the real experimental tests of conformal field theory.

Fig. 1 shows the 2-point correlations for the Ising model. It is of particular importance to mention that the vacuum expectation value, \( \langle E \rangle^2 \), has already been subtracted in graphs of correlation functions of \( E(\vec{x}) \). The measured exponents \( \eta_{SS} = 0.26 \pm 0.01 \) and \( \eta_{EE} = 2.01 \pm 0.05 \) are in agreement with the values presented in Table I, i.e. four times the conformal dimensions for each field. More importantly, Fig. 1 tells us that \( N_{SS}^2 = 0.704 \pm 0.004 \) and \( N_{EE}^2 = 0.42 \pm 0.02 \).

The 3-point correlations were measured by placing one operator at \( \vec{0} = (0, 0) \) (the center of the lattice), and the two others at \( \vec{r}_1 = (r, 0) \) and \( \vec{r}_2 = (0, r) \), i.e. two vectors along the two perpendicular lattice directions at a distance \( r \). Fig. 2 shows this correlation for the Ising model as a function of \( r \). Conformal field theory, eq. (3) and Table I, predicts that for the Ising model:

\[
\langle S_{r_1} E_0 S_{r_2} \rangle = 2^{3/8} N_{SS}^2 N_{EE} C_{SES} r^{-5/4}.
\]

The observed power law behavior \( \eta_{SES} = 1.30 \pm 0.05 \) is in agreement with the predicted exponent. The prefactor \( k_{SES} = 0.33 \pm 0.02 \) and the measured values of \( N_S \) and \( N_E \) allow us to calculate the structure constant. We find that \( C_{SES} = 0.54 \pm 0.05 \). This measured value
compares well with the theoretical value of Table II. Having shown that our simulations work for the Ising model, we can proceed to simulating the Potts model with some confidence.

For the 3-state Potts model, we repeat the analysis. The Monte Carlo simulations were performed on a $500 \times 500$ lattice with the Wolff algorithm. Again, we thermalized over 300 time units, and took samples separated by 20 time units. For the Potts model, the total number of samples was 21000. As for the Ising model, these samples were blocked in groups of 150 to obtain statistical errors.

By determining the temperature at which the 2-spin correlation $\langle S(\vec{x})S^*(\vec{0})\rangle$ shows power-law scaling, we found that for our system size $T_c/T_D = 1.0005 \pm 0.0003$. The simulations of the 2-point functions give $N^2_S = 0.54 \pm 0.03$ and $N^2_E = 0.125 \pm 0.005$ (Fig. 3). The power-law dependence of these correlations were measured as $\eta_{SS^*} = 0.26 \pm 0.02$, in agreement with Table II, and $(\eta_{SS^*} = 1/4)$, and $\eta_{EE} = 1.66 \pm 0.04$, in slight disagreement with Table II $(\eta_{EE} = 8/5)$. If we again place one operator at $\vec{0} = (0,0)$ (the center of the lattice), and the two others at $\vec{r}_1 = (r,0)$ and $\vec{r}_2 = (0,r)$, the values of Table II in combination with (5) predict that for the Potts model:

$$\langle S_{r_1} S_0 S_{r_2} \rangle = 2^{-1/15} N^3_S C_{SSS} r^{-2/5}. \quad (7)$$

and

$$\langle S_{r_1} E_0 S_{r_2}^* \rangle = 2^{4/15} N^2_S N_E C_{SES^*} r^{-16/15}. \quad (8)$$

The measurements shown in Fig. 4 fit this power-law behavior well: $\langle S_{r_1} S_0 S_{r_2} \rangle = k_{SSS} r^{-\eta_{SSS}}$, 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 $\eta_{SES^*} = 1.11 \pm 0.04$, respectively. The exponents agree with the theoretical values $2/5$ and $16/15$. Combining these results with (5), we obtain measured values for the two non-zero structure constants of the 3-state Potts model, $C_{SES^*} = 0.61 \pm 0.06$ and $C_{SSS} = 1.16 \pm 0.14$. Again, the agreement with the predictions of Table II is quite good.

Finally, we show in Figs. 5, 6 the simulations of the 3-point correlation $\langle E_{r_1} E_0 E_{r_2} \rangle$. For both the Ising and the Potts models, this correlation should vanish due to the conformal
fusion rule $\Phi_{21} \times \Phi_{21} = 1$ [4,5]. As these graphs show, the 3-point correlation functions are consistent with zero when the distances between the operators are as small as 5 lattice spacings (Note that the scale of the graphs is greatly magnified.). At very short distances the correlations do not vanish, because the system sees the discreteness of the lattice and is thus not described by conformal theory. The vanishing of these correlations at distances greater than a few lattice spacings is strong evidence for the correctness of the conformal fusion rule.

In summary, we have measured 2- and 3-point correlations for the two-dimensional Ising and 3-state Potts models and have compared both their exponents and prefactors, e.g. structure constants, with predictions from conformal field theory. All measured exponents, except one, are within one standard deviation of theoretical predictions, and the remaining one is within two standard deviations. Far more interesting is the fact that the structure constants are also in good agreement with conformal theory predictions. For $C_{EEE}$, this gives us a verification of one fusion rule of conformal models. For $C_{SES}$ and $C_{SSS}$, this gives a direct test of the screened Coulomb gas and bootstrap equation formalisms which were necessary to obtain their 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.

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TABLES

TABLE I. Scaling dimensions of the Spin and Energy Density Fields

| Model: Ising | 3-state Potts |
|-------------|--------------|
| $S(\vec{x})$ | 1/16         | 1/15         |
| $E(\vec{x})$ | 1/2          | 2/5          |

TABLE II. Predictions of structure constants from conformal theory

| Model        | Structure constant | value     |
|--------------|--------------------|-----------|
| Ising        | $C_{SES}$          | 1/2       |
|              | $C_{EEE}$          | 0         |
| 3-state Potts| $C_{SES^*}$        | 0.546     |
|              | $C_{EEE}$          | 0         |
|              | $C_{SSS}$ (=$C_{S\cdot S\cdot S}$) | 1.092     |
FIGURES

FIG. 1. 2-spin correlations (top) and energy density 2-point correlations (bottom) in the Ising model on a $512 \times 512$ lattice 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 $k_{SS} = 0.704 \pm 0.004$ and $\eta_{SS} = 0.26 \pm 0.01$, and $\langle E_0 E_r \rangle = k_{EE} r^{-\eta_{EE}}$, where $k_{EE} = 0.42 \pm 0.02$ and $\eta_{EE} = 2.01 \pm 0.05$.

FIG. 2. Mixed 3-point correlations of the Ising model on a $512 \times 512$ lattice at $T = T_c$. The dashed line is our fit to the power-law behavior, given by: $\langle S_r E_0 S_r \rangle = k_{SES} r^{-\eta_{SES}}$, where $k_{SES} = 0.33 \pm 0.02$ and $\eta_{SES} = 1.30 \pm 0.05$.

FIG. 3. 2-spin correlations (top) and energy density 2-point correlations (bottom) in the 3-states Potts model on a $500 \times 500$ lattice 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 $\eta_{EE} = 1.66 \pm 0.04$.

FIG. 4. 3-spin correlations (top) and mixed 3-point correlations (bottom) in the Potts model on a $500 \times 500$ lattice at $T = T_c$. The dashed lines are our fit to the power-law behavior, given by: $\langle S_r S_0 S_r \rangle = k_{SSS} r^{-\eta_{SSS}}$, where $k_{SSS} = 0.44 \pm 0.04$ and $\eta_{SSS} = 0.39 \pm 0.02$, and $\langle S_r E_0 S_r^* \rangle = k_{SES} r^{-\eta_{SES^*}}$, where $k_{SES^*} = 0.14 \pm 0.01$ and $\eta_{SES^*} = 1.11 \pm 0.04$.

FIG. 5. Energy-density 3-point correlations of the Ising model on a $512 \times 512$ lattice at $T = T_c$. For $r > 10$, $\langle E_r E_0 E_r \rangle < 2 \cdot 10^{-4}$.

FIG. 6. Energy-density 3-point correlations of the Potts model on a $500 \times 500$ lattice at $T = T_c$. For $r > 10$, $\langle E_r E_0 E_r \rangle < 10^{-5}$.
Barkema/McCabe Fig. 3
Barkema/McCabe Fig. 4
$\langle E_{r_1} E_0 E_{r_2} \rangle$