Monte Carlo Technique for Universal Finite-Size-Scaling Functions: Application to the 3-State Potts Model on a Square Lattice

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We present a method which allows calculation of whole universal finite-size-scaling functions from Monte Carlo data. The crux of the new method is a technique of isolating the singular part from the total free energy. We apply this method to the 3-state Potts model on a square lattice and find the normalized scaling function $Y(x)$ in the form $1+x+5.31x^2-1.2x^3-0.67x^4\ldots$ near the bulk critical point $x=0$, together with the normalizing universal amplitude $E=1.053$ and a nonuniversal metric factor $D=-0.387$. It also behaves as $Y(x)\approx(\pm x)^{d\nu}Q_\pm$ for large x in agreement with the hyperuniversality hypothesis with $Q_+/Q_-\approx 1$.

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Computer simulations on statistical mechanical problems are inherently restricted to systems of finite size, in spite of recent development of enormously high-speed and large-capacity computers. On the other hand, to study problems like phase transitions and critical phenomena, one clearly needs to consider systems of finite size. Fortunately, the recent progress of finite-size-scaling theory [1,2] allows one to infer infinite size or bulk properties from the properties of relatively small-size systems even at the critical point. So far, however, no computer simulations have been efficient or accurate enough to determine the behavior of the universal scaling functions.

In this paper we present a Monte Carlo (MC) technique by which one can calculate universal finite-size-scaling functions and thereby predict thermodynamic functions appropriate to the bulk system. The method is successfully applied to the calculation of the universal scaling function of the 3-state Potts model on a square lattice. Aside from verifying the hyperuniversality hypothesis we obtain the whole universal function and its derivatives up to the fourth order. We also find that our results are in good agreement with available exact theoretical results.

According to the two-scaling-factor universality hypothesis put forward by Privman and Fisher [1], the free-energy density f consists of the analytic part f_a and the singular part f_s, i.e.,

$$f=f_a+f_s\,. \tag{1}$$

The singular part behaves as

$$f_s(t;L)\approx L^{-d}EY(DtL^{1/\nu})\,, \tag{2}$$

where L is the side of d-dimensional cube (in some arbitrary unit of length scale), t is the thermal scaling field, $1/\nu$ is the corresponding critical exponent, and the normalized scaling function Y is believed to be universal within a universality class of given geometry. In this paper we will consider only the zero-field case. The above scaling form contains the hyperscaling relation, $2-\alpha=d\nu$. Following the suggestion of Fisher [3], we will determine the amplitude E and the nonuniversal metric factor D by imposing the normalization condition $Y(0)=1$ and $Y'(0)=1$. It should be noted that for two-dimensional systems under toroidal boundary conditions, the normalization constant E is related to the logarithm of the modular covariant partition functions [4,5].

Since the free energy of a finite system is analytic, the scaling function Y is also analytic. Only asymptotic behaviors such as $Y(x)\approx(\pm x)^{d\nu}Q_\pm$, for $x\to\pm\infty$, eventually lead to two $\pm$ amplitudes in the t-scaled form as $f_s(t;\infty)\approx ED^{d\nu}Q_\pm|t|^{2-\alpha}$.

In order to illustrate the new method, let us take as an example the q-state Potts model in the absence of an external field. The energy of the Potts model with the interaction strength J can be written as

$$\mathcal{E}(\{\sigma_i\})=-J\sum_{\langle i,j\rangle}\delta(\sigma_i,\sigma_j)\,, \tag{3}$$

where the spin variable σ_i at the ith lattice site can take q values $(0,\ldots,q-1)$, and $\delta(\sigma_i,\sigma_j)$ is the usual Kronecker delta function.

We define the *free energy* by

$$f=\frac{1}{V}\ln\left[\sum_{\mathcal{E}=\mathcal{E}_{\min}}^{\mathcal{E}_{\max}}\Omega(\mathcal{E})\exp\{-K(\mathcal{E}/J)\}\right]\,, \tag{4}$$

where $K\equiv J/k_BT$ with the temperature T and Boltzmann constant k_B, $V\equiv L^d$ is the volume of the isotropic d-dimensional system, and $\Omega(\mathcal{E})$ denotes the number of configurations at fixed energy $\mathcal{E}$.

Thermodynamic functions of interest are all calculable from the free-energy density (4) by taking appropriate derivatives, and they are cumulants of the canonically weighted distribution function,

$$\Phi(\mathcal{E})=\Omega(\mathcal{E})\exp\{-K(\mathcal{E}/J)\}/Z\,, \tag{5}$$

where $Z\equiv\exp(Vf)$ is the partition function.

We denote the nth order cumulant by Γ_n, i.e.,

$$\frac{\partial^n f}{\partial t^n}=\frac{\partial^n f}{\partial(-K)^n}\equiv\Gamma_n \tag{6}$$

with $\Gamma_0\equiv f$. As we know from elementary statistical mechanics, Γ_1 is the internal energy density while Γ_2 is proportional to the specific heat. We define the temperature scaling field by $t = K_c - K$ instead of usual $|T/T_c - 1|$ so as to make entailing expressions simpler. The scaled temperature variable x then can be written as

$$x = DtL^{1/\nu}. \quad (7)$$

Now all cumulants can be expressed as sums of two parts, namely, the analytic and the singular parts,

$$\Gamma_n = \Gamma_{na} + \Gamma_{ns}, \quad (8)$$

where the singular parts are related to the universal scaling function Y and its higher-order derivatives. If we can neglect corrections to scaling, we have

$$\Gamma_{ns} = L^{-d+n/\nu} ED^n Y^{(n)}(x). \quad (9)$$

In this point of view, the calculation of Y ($\equiv Y^{(0)}$) and its derivatives $Y^{(n)}$ ($\equiv \partial^n Y/\partial x^n$) reduces to the calculation of $\Phi(\mathcal{E})$, in Eq. (5), which in turn reduces to the calculation of $\Omega(\mathcal{E})$. The efficient and accurate algorithm developed recently [6,7] allows us to calculate $\Omega(\mathcal{E})$ and consequently $\Phi(\mathcal{E})$ and the Γ_n's accurately. However, we have total Γ_n's in the K or t variable while we need the singular part of the Γ_n's in the scaled variable x, and it is not a straightforward matter to separate the singular part from the analytic part of the Γ_n's.

The separation of the singular part of the free energy can be done by the following scheme.

We first calculate the analytic part of the free energy f_a. To do this we expand both f_a and f_s in t and x variables, respectively: $f_a = \sum_{n=0} a_n t^n/n!$ and $f_s = \sum_{n=0} c_n x^n/n!$. From Eqs. (6), (8), and (9), we have the relation

$$\Gamma_n(K_c;L) = a_n + L^{-d+n/\nu} ED^n c_n, \quad (10)$$

among the expansion coefficients a and c. Therefore we can estimate a pair of numbers $(a_n, ED^n c_n)$ for each n, from a set of bulk critical values $\Gamma_n(K_c;L)$ for different sizes L, for example, using the χ^2 fit method in Eq. (10).

Although both expansions have a common origin about which the Taylor series are made, the radii of convergence are expected to be different for large L. Furthermore, since we expect that the analytic part of the free energy is smooth and slowly varying near the bulk critical point and L independent, we can assume that the first few terms of the Taylor series are good enough for representing the analytic part of the free energy of a moderate-sized system in the scaling regime. On the other hand, the scaling regime, the range of x on which the scaling function Y contains information about the bulk system, consists of a narrow range of t variable as L becomes large, which can be seen in Eq. (7). For these reasons we may take the analytic part f_a and its derivatives $f_a^{(n)}$ or Γ_{na} as the Taylor series approximation and its derivatives. Then by subtracting them from the total cumulant Γ_n, we can isolate Γ_{ns}, the singular part of the cumulant. Finally, multiplying $\Gamma_{ns}(x)$ by $L^{d-n/\nu}E^{-1}D^{-n}$, we obtain a series of functions for each n, $L^{d-n/\nu}E^{-1}D^{-n}\Gamma_{ns}(x)$, which should collapse into $Y^{(n)}(x)$, the nth derivative of the scaling function, for all L.

In the above scheme, corrections to scaling may become important in estimating a_n's for $n \geq 3$ and for large L. Although it is possible to include the corrections to scaling in Eq. (10) we neglected the effect in the following analysis since the statistical uncertainties in Γ_n ($n \geq 3$) are so large and there are not enough data points (of different sizes L) available. In any case they are significant only for large values of L while the a_n's for $n \geq 3$ become less significant in estimating Γ_{na} as L grows large for the reason stated in the previous paragraph.

We have performed MC calculations on the 3-state Potts model on a square lattice with periodic boundary conditions, of sizes $L \times L = 3l \times 3l$, with $l = 2,3,\ldots,11$. In measuring $\Omega(\mathcal{E})$, we have used the algorithm developed in Ref. [6]. Although we can determine from our MC data the critical temperature and the exponent ν, we have used the known exact values [8], $K_c^{-1} = 0.99497$ and $\nu = \frac{5}{6}$. These two numbers and the finite-size-scaling form in Eq. (2) are the only inputs in obtaining the following output from our MC data for $\Omega(\mathcal{E})$.

The Γ_n's are calculated from the moments of energy $\langle \mathcal{E}^n \rangle$ which can be evaluated from $\Omega(\mathcal{E})$ directly. In Fig. 1 we plot the total cumulant Γ_n versus the temperature K^{-1}. The vertical line in the middle represents the critical temperature K_c^{-1}. We have defined the scaling functions on a range of $x \in [1.94, -1.94]$, and the vertical ticks of growing height mark the corresponding range in t for growing L. Only curves for $L \geq 15$ are shown in this

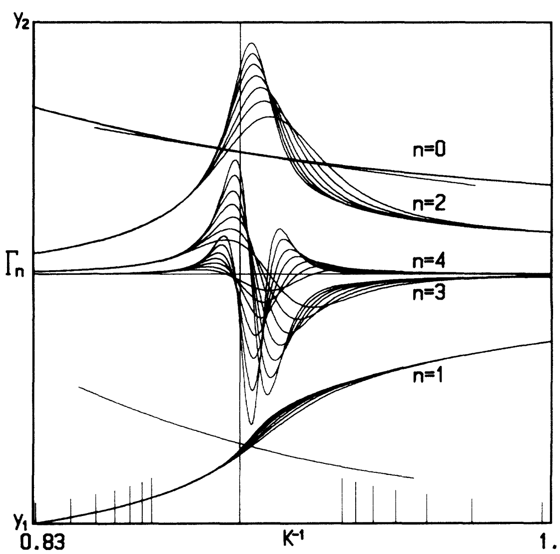

FIG. 1. Cumulants Γ_n vs temperature K^{-1}. The ordinates (y_1, y_2) are $(-0.9, 3.1)$, $(-1.9, 0.1)$, $(-6.5, 6.5)$, $(-300, 300)$, and $(-32000, 32000)$ for $n = 0$, 1, 2, 3, and 4, respectively. The horizontal line in the middle marks the midpoint between y_1 and y_2.

figure and in Fig. 2.

Using total cumulant values at the critical point, we obtain 2.0700(1), $-1.577(1)$, $-1.40(5)$, 3.1(5), and 21(6) for a_n $(n=0,\dots,4)$ and 1.053(7), $-0.408(7)$, 1.68(2), 0.45(1), and $-0.38(2)$ for $ED^n c_n$ $(n=0,\dots,4)$. Together with the normalization condition $c_0=1.0$ and $c_1=1.0$, these results in turn yield $E=1.053(7)$ and $D=-0.387(4)$. In fact, a_0 and a_1 are critical values of the free energy and of the internal energy, known exactly: 2.0701... and $-1.5774\dots$, respectively [8]. Comparison of our data with these values would give a general idea about the accuracy of this analysis. The conformal field theory also predicts the exact value of E in this case. It is given by $E=\ln\bar{Z}(1)=1.0479\dots$, where $\ln\bar{Z}(\delta)$ is the modular invariant partition function (including the central charge factor) of the 3-state Potts model with aspect ratio δ [4,5]. This value also falls within the error bound of our estimate.

A short curve tangent to Γ_0 and another crossing Γ_1 in Fig. 1 are their analytic parts found by the above analysis. It should be noted that the analytic part Γ_{1a} is not tangent to Γ_1 although $\Gamma_{1a}(K_c)$ should converge to $\Gamma_1(K_c)$. This behavior is a natural consequence of the fact that $2-d\nu>0$ and has important implications in estimating amplitudes $Q_\pm$ as we shall see shortly.

In Fig. 2 we plot $L^{d-n/\nu}\Gamma_{ns}(x)$ for $n=0,\dots,4$, each of which should collapse into a single curve $ED^nY^{(n)}(x)$ for all L. We can see by inspection that on the low-temperature side this size is good enough for representing asymptotes of scaling functions, although we may need a little larger size to calculate the true asymptote of $ED^nY^{(n)}$ for all n, except possibly $EDY^{(1)}$, on the high-temperature side. Two short curves tangent to EY and $EDY^{(1)}$ are their Taylor series approximations calculated above. The vertical lines near both sides mark the asymptotic region used for the log-log plot in Fig. 3.

In Fig. 3 we plot $\ln(|Y^{(n)}|)$ vs $\ln(|x|)$ in the region marked in Fig. 2 so as to see whether the $Y^{(n)}$'s behave as predicted by the hyperuniversality hypothesis, namely, $Y^{(n)}(x)\approx Q_\pm^{(n)}(\pm x)^{(d\nu-n)}$ for large x. Here the $Q_\pm^{(n)}$'s are related to each other recursively via $Q_\pm^{(n+1)}=(d\nu-n)Q_\pm^{(n)}$. For this plot we have taken, for the scaling function and its derivatives $Y^{(n)}$, $L^{d-n/\nu}E^{-1}D^{-n}\times\Gamma_{ns}(x)$ with the largest L, i.e., 33. In particular the low-temperature asymptotes of $Y^{(n)}$ for all n as well as the high-temperature asymptotes for $n=1$ and 2 are shown. The ordinates for $\ln(|Y^{(n)}|)$ are shifted for each n to absorb the multiplicative factors so that all asymptotes are made to converge to the two points, i.e., $\ln(Q_\pm)+\frac{5}{3}\ln(|\mp 1.94|)$ for $n=0$. The short solid lines display the predicted slope $(\frac{5}{3}-n)$. Although the $Q_\pm$'s from different n's except $n=1$ and 2 are somewhat scattered, the slopes follow the predicted exponents rarely nicely even for $n=4$. Ticks on the right axis mark the positions 5% above and below the expected convergence point of the high-temperature asymptotes. Our values of $Q_+=5.19(3)$ and $Q_-=5.13(3)$ are calculated from the asymptotic behavior of $Y^{(1)}$ since it displays the best asymptotic behavior in this plot. The ratio $Q_+/Q_-=1.01(3)$ is 1% off from the exact value of unity which is a consequence of the self-duality [9].

The reason that only $Y^{(1)}$ gives accurate asymptotic behavior can be understood as follows: First, since we

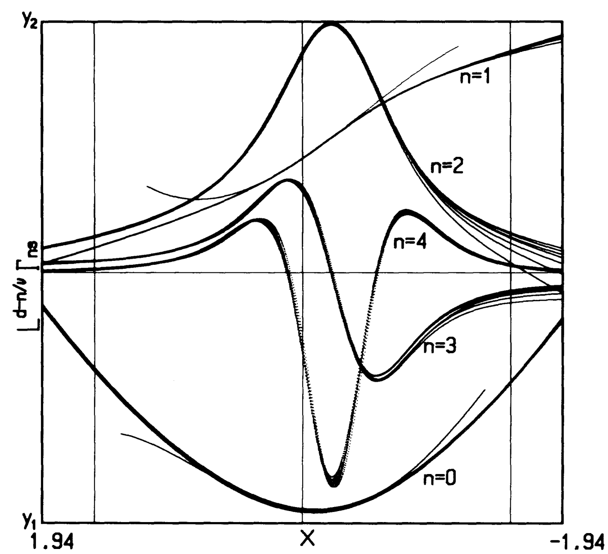

FIG. 2. $L^{d-n/\nu}\Gamma_{ns}(x)$ vs x for system sizes $L=15,18,\dots,33$. They are supposed to collapse into $ED^nY^{(n)}$. The ordinates (y_1,y_2) are (0,40), $(-17.88,6.12)$, $(-0.61,1.83)$, $(-1.35,1.35)$, and $(-1.3,1.3)$ for $n=0$, 1, 2, 3, and 4, respectively. The horizontal line in the middle marks the midpoint between y_1 and y_2.

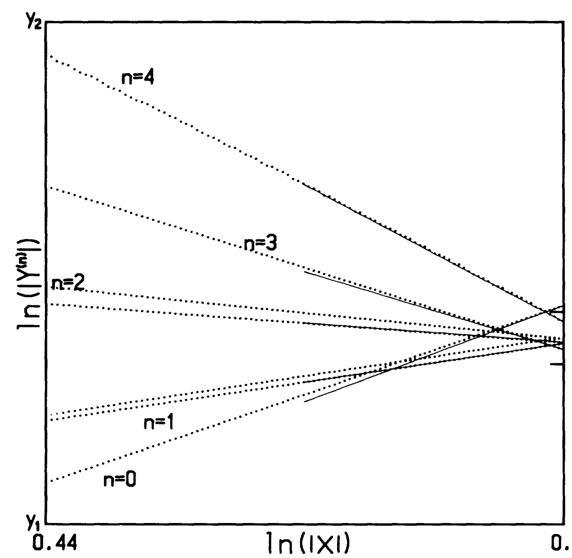

FIG. 3. $\ln(|Y^{(n)}|)$ vs $\ln(|x|)$. The ordinates (y_1,y_2) are (3.97,4.94), (2.88,3.83), (0.86,1.82), $(-1.85,-0.89)$, and $(-3.17,-2.21)$ for $n=0$, 1, 2, 3, and 4, respectively.

have taken only finite terms in the Taylor expansion of the analytic part of the free energy, the higher-order derivatives of the analytic part have even fewer terms so that they cannot represent the analytic part for the large x region correctly. Second, for higher-order cumulants, statistical uncertainty grows, and precision drops accordingly. In fact, in our data, the average relative standard deviation for sets of Γ_n are 10^{-4}, 10^{-3}, 10^{-2}, 10^{-1}, and 2.5×10^{-1} for $n=0$–4, respectively (see Ref. [6]). Then why is $Y^{(1)}$ better than Y? Since the analytic part of Y eventually falls to the total free-energy density in the limit of large L (see Fig. 1), the difference between the total free energy and the analytic part for large L becomes very small and is eventually drowned in the statistical error. On the other hand, $\Gamma_1-\Gamma_{1a}$ remains finite for all nonzero t (not x) even in the limit of large L as we noted previously, without much loss of accuracy in the Taylor series representation of Γ_{1a}.

It should be mentioned that the histogram technique recently developed by Ferrenberg and Swendsen [10,11] can also be used in the present method for the direct calculation of $Y^{(n)}$ for $n\geq1$ since the histogram yields the unnormalized distribution function $\Phi(\mathcal{E})$, in Eq. (5).

In conclusion, we have not only verified consequences of the hyperuniversality hypothesis in every detail with reasonable precision but also obtained the whole scaling function and its derivatives. One can even go further to try some closed-form expression for $Y(x)$ such as $a(x^2+b)^{5/6}[c+\tanh(dx)]+e$ for a starter, which exhibits all the characteristics found in this analysis. In any case our analysis suggests that combining the finite-size-scaling theory and a high-precision MC technique such as this in effect can *solve* statistical mechanical problems of bulk systems which exhibit critical phenomena.

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[1] V. Privman and M. E. Fisher, Phys. Rev. B **30**, 322 (1984).
[2] V. Privman, in *Finite Size Scaling and Numerical Simulation of Statistical Systems,* edited by V. Privman (World Scientific, Singapore, 1990).
[3] M. E. Fisher (private communication).
[4] J. L. Cardy, Nucl. Phys. **B270 [FS16]**, 186 (1986).
[5] H. W. J. Blöte, J. L. Cardy, and M. P. Nightingale, Phys. Rev. Lett. **56**, 742 (1986).
[6] K-C. Lee, J. Phys. A **23**, 2087 (1990).
[7] K-C. Lee, J. Korean Phys. Soc. **24**, 32 (1991).
[8] F. Y. Wu, Rev. Mod. Phys. **54**, 235 (1982).
[9] M. Kaufman and D. Andelman, Phys. Rev. B **29**, 4010 (1984).
[10] A. M. Ferrenberg and R. H. Swendsen, Phys. Rev. Lett. **61**, 2635 (1988).
[11] A. M. Ferrenberg and R. H. Swendsen, Phys. Rev. Lett. **63**, 1195 (1989).