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Au Effkient Monte Carlo Technique for Continuous Functions and Universal Scaling Functions†

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The functional Monte Carlo method devised by one of the authors for the efficiency and accuracy can be used to calculate universal scaling functions. In order to demonstrate the technique we take 3-state Potts model for which many of the exact critical properties are known. Various thermodynamic functions of Potts model on square lattice of sizes ranging from 6 X 6 to 33 X 33 are calculated and the two scale factor universality (or hyperuniversality) theory put forward by Privman and Fisher is tested and verified. We also estimate the higher order derivatives of universal function using hyperuniversality hypothesis.

I. INTRODUCTION

A very efficient Monte Carlo technique developed recently by one of the authors[1-2] which calculates continuous thermodynamic functions of continuous thermodynamic variables can be used to estimate the universal functions of the two scale factor universality theory introduced by Privman and Fisher.[3-4] In the functional Monte Carlo technique we take independent samples in very short time interval typically of a few hundredths of a Monte Carlo step per spin and it is so fast and efficient that we can calculate whole thermodynamic functions in a time that takes to obtain a single thermodynamic point by conventional Metropolis algorithm. This technique not only is efficient and accurate but also furnishes primary thermodynamic functions such as free energy directly from the Monte Carlo data, a feature not available in the conventional Monte Carlo method?"

In this talk we present a brief account of my Monte Carlo technique (which will be abbreviated as M.C.t. hereafter) together with results of the 3-state Potts model on a square lattice. Since we can calculate free energy in continuous form in the functional Monte Carlo technique, we can extract singular part of various thermodynamic functions from the simulation results and we can estimate universal functions eventually. In section II we will explain the essence of the functional Monte Carlo technique and in section III, we will discuss the new technique analyzing

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critical behavior using the functional Monte Carlo results. In section IV we will present the calculations done on the 3-state Potts model on a square lattice and finally we devote section 5 to a summary and further remark concerning this new technique.

II. FUNCTIONAL MONTE CARLO METHOD

In order to illustrate the new method let us take as an example a spin-l/2 Ising model of N spins in the absence of an external field. The energy of the system can be written as

$$E(\{S_i\}) = -J \sum_{<i,j>} S_i S_j, \tag{1}$$

where S_i is the spin variable assuming $\pm$ 1 values, J is the exchange energy and $<i,j>$ runs over interacting nearest neighbor pairs i,j. The canonical average $<A>$ of any thermodynamic quantity $A(\{S_i\})$ is defined by

$$<A>= \sum_{\{S_i\}}^{2^N} A(\{S_i\}) \exp(-\beta E(\{S_i\}))/Q, \tag{2}$$

where β is the inverse temperature $1/kT$ with Boltzmann's constant k and Q is the partition function defined by

$$Q = \sum_{\{S_i\}}^{2^N} \exp(-\beta E(\{S_i\})). \tag{3}$$

We can rewrite Eq. (2) and (3) in slightly different forms as

$$<A>= \sum_{E=E_0}^{E_m} \Omega(E) \exp(-\beta E) \overline{A}(E)/Q, \tag{4}$$

and

$$Q = \sum_{E=E_0}^{E_m} \Omega(E) \exp(-\beta E), \tag{5}$$

where $\overline{A}(E)$ is the microcanonical average of the variable A defined by

$$\overline{A}(E) = \sum_{\{S_i\}}^{\Omega(E)\prime} A(\{S_i\})/\Omega(E), \tag{6}$$

and Q(E) is the total number of configurations with a fixed E. The prime in Eq. (6) indicates that the summation is over microscopic configurations with the fixed E. In this point of view, the calculation of $<A>$ is reduced to the calculations of $Q(E)$ and microcanonical average $\overline{A}(E)$.

Let γ, N+, and N^{++} be the coordination number, the total number of up-spins, and the total number of interacting up-spin pairs respectively. Then the energy of the system can be written as

$$E = -4J(N^{++} - \frac{1}{2}\gamma N^{+}), \tag{7}$$

where the constant term $-1/2\,J\gamma N$ has been dropped. Therefore configurations with constant E can be generated by keeping $N^{++} - 1/2\,\gamma N^{+}$ constant. In this description, the lowest energy, $E_0 = E(N^{++} = 0, N^{+} = 0) = 0$ and highest energy, $E_{\max} = E(T = \infty) = 1/2\,J\gamma N$ so that there are only $\gamma N/8$ discrete energies separated by $\Delta E \equiv 4J$. Therefore we only need to generate $\gamma N/8$ independent sets of configurations to evaluate $Q(E)$ and $\overline{A}(E)$.

The crux of new technique is how to evaluate $\overline{A}(E_j)$ and $\Omega(E_j)$ efficiently. We set up a random walk through configuration space restricted to narrow energy band given by

$$E_j - \frac{1}{2}\gamma\Delta E \le E(\{S_i\}) \le E_j + (\frac{1}{2}\gamma + 1)\Delta E, \tag{8}$$

and use, for data taking, configurations which satisfy

$$E(\{S_i\}) = E_j \quad \text{and} \quad E(\{S_i\}) = E_j + \Delta E. \tag{9}$$

As will be explained later, only by this elaboration it is guaranteed that samples from which data are taken are independent configurations.

We will sketch briefly the new algorithm. We first generate an initial spin configuration $\{S_i\}$ with given energy $E(\{S_i\})$. We start a random walk by single spin flip algorithm as follows. We select a single spin out of N spins either randomly or sequentially and attempt to flip it. Whenever the attempted move takes the walker to a spin configuration $\{S_i\}$ which lies within the energy band (8) the move is allowed; otherwise the move is rejected. Whenever the walker visits points in the configuration space satisfying the energy value given by (9), relevant information such as N^{+} is sampled together with the total number of visits. The last information is vital and a key to the new method which allows us to evaluate canonical averages.

The allowance of $1/2\,\gamma E$ energy width in (8) is crucial for the accurate determination of distribution of N^{+} although it is less so for the estimate of $\Omega(E + \Delta E)/\Omega(E)$. The reason is as follows. Since the energy change δE produced by the single spin flip move from the original configuration is restricted to a range $[-1/2\,\gamma\Delta E, 1/2\,\gamma\Delta E]$, the allowance of the energy width makes the next spin flip move after sampling always lie within the energy band given by (8). Therefore

the walker moves away immediately from the previously sampled configuration thereby eliminating the possibility of repeated sampling of the same configuration. The possibility of such repeated sampling is especially severe at low E values where the rejection rate is very high. This allowance of the energy width also lets the walker escape trapping in metastable states if any. However allowance of energy width larger than l/2 $q\Delta E$ *makes* the M.C. process rapidly inefficient as was discussed in Ref. 1.

As far as we are interested in macroscopic thermodynamic functions or derivatives such as internal energy or susceptibility we only need calculate the number of configurations, $\omega(E, N^+)$ of fixed E and N^+ since $A(\{S_i\})$'s corresponding to these quantities depend only on N^+, so that $\Omega(E)$ and $\bar{A}(E)$ are calculable from $\omega(E, N^+)$ by

$$\Omega(E) = \sum_{N^+} \omega(E, N^+),$$

and

$$\bar{A}(E) = \sum_{N^+} A(E, N^+)\omega(E, N^+)/\Omega(E).$$

In order to calculate $\omega(E, N^+)$, *we* run this random walk starting from the lowest energy E_0 to the highest energy $E_{\max}$. Since we know $\omega(E_0, N^+)$, namely $\omega(E, N^+) = \delta_{N^+,0} + \delta_{N^+,N}$ *so* that $\Omega(E_0) = 2$, (in practice we can calculate some more $\omega(E, N^+)$ for low lying E's by hand so that we can start the random walk and data taking from some higher *E.) we* can estimate $\omega(E, N^+)$ successively by the following way.

We count $n(E, N^+)$ and $n(E + \mathrm{AE}, N^+)$, the numbers of configurations of two neighboring energies with given N^+ visited by the random walker in the configuration space given by (9). Let N_d and $N_d{}^+$ be the total number of points visited with energy E and $E + AE$, i.e., $N_d = \Sigma n(E, N^+)$ and $N_d{}^+ = \Sigma n(E + AE, Nf)$. Then we have $\Omega(E + \mathrm{AE}) = \Omega(E)N_d{}^+/N_d$, and $\omega(E, N^+) = \Omega(E)n(E, N^+)/N_d$. This completes the functional Monte Carlo technique.

The first test of the new method I took an Ising model on an N = 30 x 30 square lattice with toroidal boundary condition and obtained data and compared the results from the data with the well known exact results for finite sized lattices.

We also calculated the magnetization and susceptibility and compared with 'Onsagar's exact magnetization for infinite system and known asymptotic susceptibility expression for infinite system. The typical relative deviations from the exact values, $(A_{,,} - A_{\mathrm{exact}})/A_{\mathrm{exact}}$ for the free energy, internal energy, entropy and specific heat are around $10^{-4}, 10^{-3}, 10^{-3}$ and 10^{-2} respectively.

The advantage of this new method beside the points we mentioned already is 1) the algorithm consists of only integer operations which best suit digital computers, 2) it is extremely

lenient in its demands on the random number generator since the complexity of the system itself serves as a random number generator and 3) there is no critical slowing down because the configuration space is restricted to a narrow energy band at each separate energy.

III. UNIVERSAL SCALING FUNCTION ENTAILING HYPERUNIVERSALITY

Thermodynamic functions calculated from the Monte Carlo data can be used 1) to test the finite size scaling theory, 2) calculating various critical parameters and 3) ultimately to estimate the universal scaling functions. In this paper we will be mainly concerned to the test of two scale factor universality or hyperuniversality hypothesis put forward by Privman and Fisher. Privman and Fisher-3 assert that the singular part of free energy density has the form

$$f_s(t, H; L) \approx L^{-d} Y(atL^{1/\nu}, bHL^{\Delta/\nu}), \tag{10}$$

where the scaling function Y is universal for all universality class. In the above equation L is the side of d dimensional cube and t and H are two scaling fields and $1/\nu$ and Δ/ν are corresponding critical exponents. The theory asserts that two metric scale factors a and b are the only nonuniversal numbers which depends on the particular system and no further nonuniversal scale factors needed in describing scaling behavior near the critical point. Since finite system is analytic, the scaling function Y is analytic around and at the bulk critical point, $t = 0$ and $H = 0$. In this form the hyperscaling relation

$$2 - \alpha = d\nu \tag{11}$$

is already built in and the no $\pm$ functions differentiating above and below the critical temperature is needed. Asymptotic behavior such as

$$Y(\tau, \omega) \approx (\pm\tau)^{d\nu} Q_{\pm}(\omega(\pm\tau)^{-\Delta}), \text{ for } \tau \to \pm\infty, \tag{12}$$

of the scaling function Y eventually leads to two $\pm$ amplitudes in the t- scaled form

$$f_s(t, H; \infty) \approx a^{2-\alpha}|t|^{2-\alpha} Q_{\pm}(ba^{-\Delta} H|t|^{-\Delta}). \tag{13}$$

The two scale factor universality form given by Eq. (10) is best suited for the analysis of critical behavior for the data obtained using functional Monte Carlo technique. This is because in Monte Carlo method we can only calculate thermodynamic functions of finite size and these functions contain the singular part which is the universal scaling function Y given by Eq. (10) and its derivatives.

In order to explain the technique of extracting the universal scaling function, let us start

from the definition of free energy density. It is

$$f = -\frac{1}{V} \ln \left[\sum_{N_e=0}^{N_e^{\max}} \Omega(E) \exp(-K N_e) \right], \tag{14}$$

where K is $K = \beta \Delta E$ with the minimum energy spacing AE and V is the volume of the system, L^d. In this paper we will consider only the case with no external field so that the magnetic scaling field is suppressed.

We will define temperature scaling field by $\varepsilon = K_c - K$ instead of usual $t = |T/T_c - 1|$ for the reason which will be clear as we proceed. The temperature scaling variable now becomes $\tau = a\varepsilon L^{1/\nu}$ with the nonuniversal metric factor a. This free energy is a sum of two parts, namely analytic part, f_a and singular part f_s, i.e., $f = f_a + f_s$. Following Privman and Fisher we can write the singular part of the free energy as $f_s = L^{-d} Y(\tau)$.

Let us denote the n-th order derivative of the free energy density with respect ε by $f^{(n)}$. Then we have

$$f^{(n)} = f_a^{(n)} + a^n L^{-d+n/\nu} Y^{(n)}(\tau), \tag{15}$$

where $f_a^{(n)}$ is n-th derivative of the analytic part of the free energy density with respect 'temperature', ε and $Y^{(n)}(\tau)$ is n-th derivative of the universal scaling function Y(r) with respect variable τ. Since Y(r) is universal its derivatives $Y^{(n)}(\tau)$ are also universal. In the functional Monte Carlo technique one calculates total thermodynamic functions of the finite system and variables for analytic part, ε and for the singular part, τ are different. Therefore it is not a straight forward matter to isolate the singular part from the sum. However two factors can be taken into account. 1) For the higher order derivatives where thermodynamic quantities diverge at the critical point, the normal part will be negligibly small compared with the singular part near and at the critical point. 2) It is expected that the analytic part would well be slowly varying so that it can be assumed to be a constant in the narrow temperature range around the bulk critical point. These observations are confirmed by our simulation data as we see in the next section.

Since thermodynamic functions of interest in analyzing critical behavior are free energy and derivatives of $-f$, we define Γ_0 by $-f$. Then the higher order derivatives of rO is nothing but cumulants of the canonical weight factor

$$\Phi(N_e) = \Omega(N_e) \exp(-K N_e)/Q, \tag{16}$$

because of the fact that $\partial\varepsilon = \partial(-K)$. In the above Eq. Q is the partition function. For example the second derivative of the Γ_0 with respect to ε is Γ_2 whose singular part is $-a^n L^{-d+2/\nu} Y^{(2)}(\tau)$, which in turn is proportional to the singular part of the specific heat.

In extracting the singular part of the thermodynamic functions we take as the first ap-

proximation analytic part of thermodynamic functions to be a constant identical to the value at the bulk critical temperature. These values are estimated fitting thermodynamic functional values at the bulk critical temperature using usual finite size scaling prediction. After subtracting analytic part of the cumulant from the total cumulants, remnants are first approximants of the singular part of the cumulants. We next perform size dependent transformation of the singular part of cumulants from variable ε to variable τ. This transformation makes, for a fixed range oft, the ε range smaller and smaller as L grows larger and larger. Therefore as the system size becomes reasonably large, constant value approximation of the analytic part of the thermodynamic functions in ε variable becomes better better provided that analytic part is smoothly varying. Thirdly we multiply size dependent factor $L^{-d+n/\nu}$ to the n-th cumulant. Asymptotic limit of this function in the limit for large L will furnish first approximant of the n-th derivative of the universal scaling function Y(z).

IV. SCALING FUNCTION FOR THE 3-STATE POTTS MODEL ON A SQUARE LATTICE

We performed Monte Carlo simulation for 3-state Potts model on a square lattice with periodic boundary conditions, of sizes ranging from 6 x 6 to 33 x 33 The canonical distribution function is calculated and first order approximants of the universal function and its derivatives are estimated.

The energy of the Potts model can be written as

$$E(\{\sigma_i\}) = -J \sum_{<i,j>} \delta(\sigma_i, \sigma_j), \tag{17}$$

where spin variables σ_i at i-th lattice site can take $0 \cdots q-1$ values for the q-state model. $\delta(\sigma_i, \sigma_j)$ is usual Kronecker delta function which take a value 1 if the two arguments are equal, 0 otherwise. The ground state is q-fold degenerate takes energy $-\gamma N/2$ for N spin system, where γ is the coordination number. We substract this number from the energy expression to make the ground state $E_0 = 0$. The energy spacing is AE = J and the maximum energy $E_{\max} = (q-1)/2q\, J\gamma N$. The energy labeling integer number, $N_e \equiv E/J$, now runs from 0 to $N_{e\max} = (q-1)/2q\, \gamma N$ and moments of the canonical distribution function (16) can now be calculated from the Monte Carlo data $\{\Omega(N_e)\}$ as

$$\alpha_n \equiv \sum_{N_e} N_e^n \Phi(N_e) \tag{18}$$

From these moments, we can calculate various cumulants Γ_n. We calculate them upto 4-th order using formula

$$\Gamma_1 = \frac{\alpha_1}{V},$$

$$\Gamma_2 = \frac{(\alpha_2 - \alpha_1^2)}{V},$$

$$\Gamma_3 = \frac{(\alpha_3 - 3\alpha_2\alpha_1 + 2\alpha_1^3)}{V}, \tag{19}$$

$$\Gamma_4 = \frac{(\alpha_4 - 3\alpha_2^2 - 4\alpha_3\alpha_1 + 12\alpha_2\alpha_1^2 - 6\alpha_1^4)}{V}$$

Since the singular part of the Γ_0 is defined by $-f_s$, it is related to the universal scaling function Y(r) by

$$\Gamma_{0s} = -L^{-d}Y(\tau) \tag{20}$$

where we define τ by $\varepsilon L^{1/\nu}$. Nonuniversal metric factor a has been absorbed into τ. In our calculation we used for the length parameter ***L,*** 1/3 of side of lattices so that ***L*** ranges from 2 to 11.

Since

$$\Gamma_{ns} \quad \frac{\partial^n \Gamma_{0s}}{\partial \varepsilon^n} = -L^{-(d-n/\nu)}Y^{(n)}(\tau), \tag{21}$$

we have

$$\Gamma_{ns}L^{d-n/\nu} = -Y^{(n)}(\tau), \tag{22}$$

where $Y^n(\tau)$ is the n-th derivative of $Y(\tau)$. In plot of various cumulants we used another variable s related to τ by the relation

$$s \equiv \frac{\tau}{KK_c}.$$

In Fig. 1, Fig. 2, $\cdots$, Fig. 5, we plot total Γ_0 and its derivatives, Γ_1 through Γ_4, for sizes ranging from 6 **x** 6 to 33 **x** 33 against temperature K^{-1}. Typical precision is 10^{-4} for free energy, 10^{-3} for Γ_1, 10^{-2} or better for Γ_2 and around 5% for Γ_3, 10% of better for Γ_4.

In Fig. 6, we replot Fig. 3 to mark the temperature range in ε variable which will be transformed into s variable of fixed range [-0.8,1.2]. In subsequent figures, Fig. 6 through Fig. 11, we plot the scaled singular part of cumulants given by Eq. (22) against s.

In this figures we took analytic part of the cumulants, as 0.0601 for Γ_{0a}, 0.4266 for Γ_{1a}, -1.4

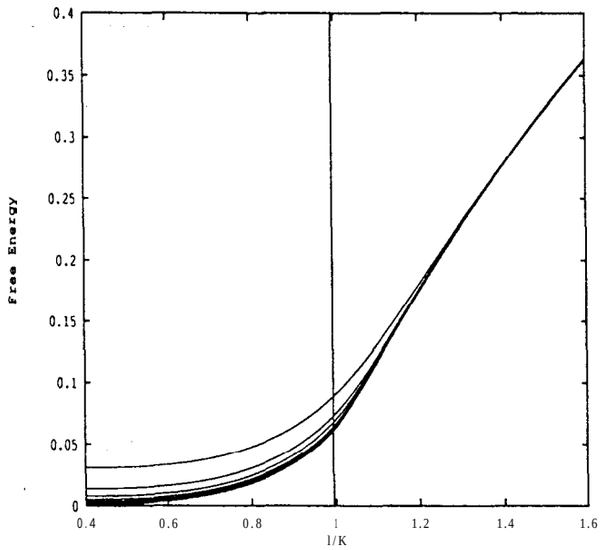

FIG. 1. $-f$ (free energy density) against K^{-1}. Vertical line in the middle marks the critical temperature K_c^{-1} = 0.99497. Large L curves sink to the bottom in the righthand side (low temperature side).

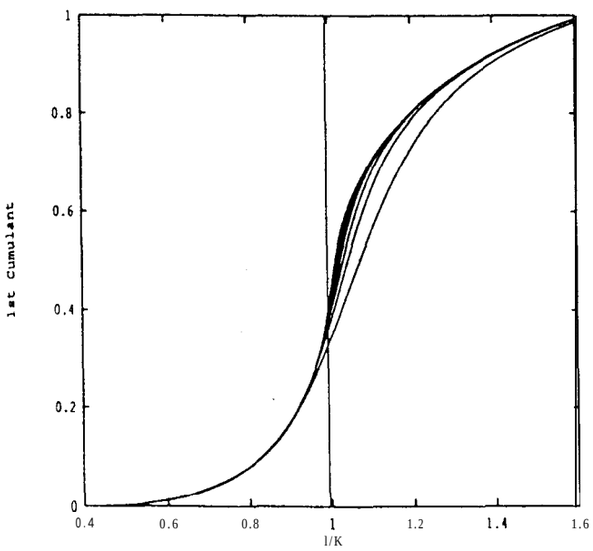

FIG. 2. Γ_1 (internal energy density) against temperature K^{-1}. Vertical line marks the critical temperature K_c^{-1} = 0.99497. Large L curves stack on top of lower L curves in the righthand side (high temperature side).

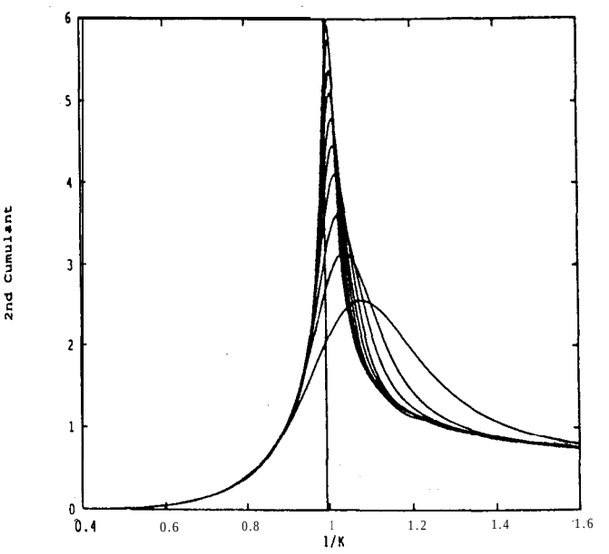

FIG. 3. Γ_2 (proportional to specific heat) against temperature K^{-1}. Vertical line marks the critical temperature $K_c^{-1} = 0.99497$. As L grows, the position of peaks moves toward the bulk critical temperature.

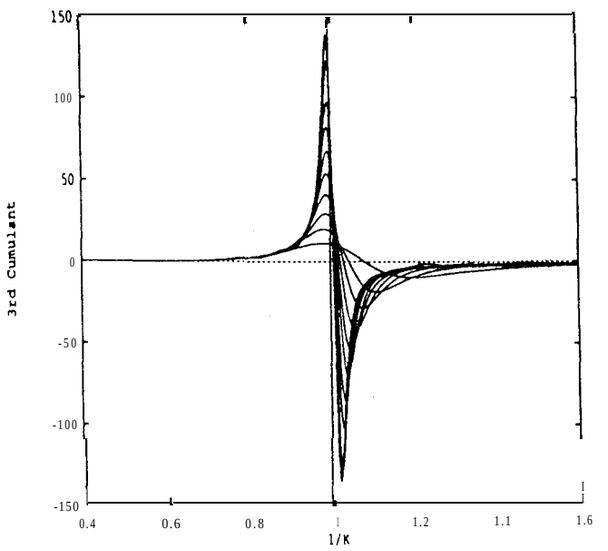

FIG. 4. Γ_3 (proportional to the first derivative of specific heat) against temperature K^{-1}. Vertical line marks the critical temperature $K_c^{-1} = 0.99497$. The vertical scale is order of 100.0 while analytic part of this quantity is estimated to be about 2.6.

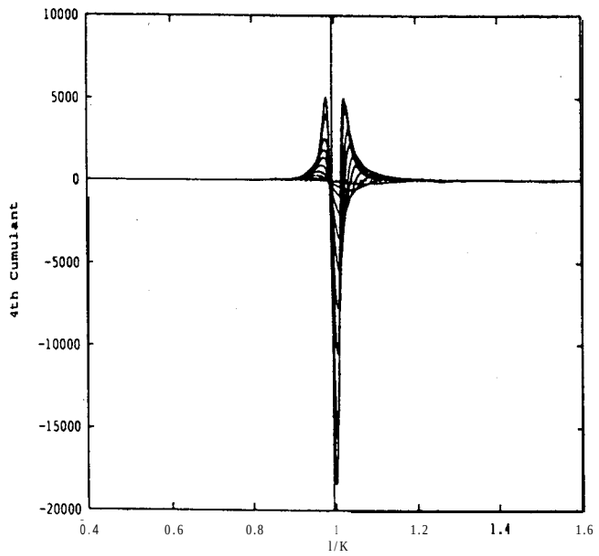

FIG. 5. Γ_4 (proportional to the second derivative of specific heat) against temperature K^{-1}. Vertical line marks the critical temperature K_c^{-1} = 0.99497. The vertical scale is order of 10000.0 while analytic part of this quantity can be neglected in the estimating scaling function.

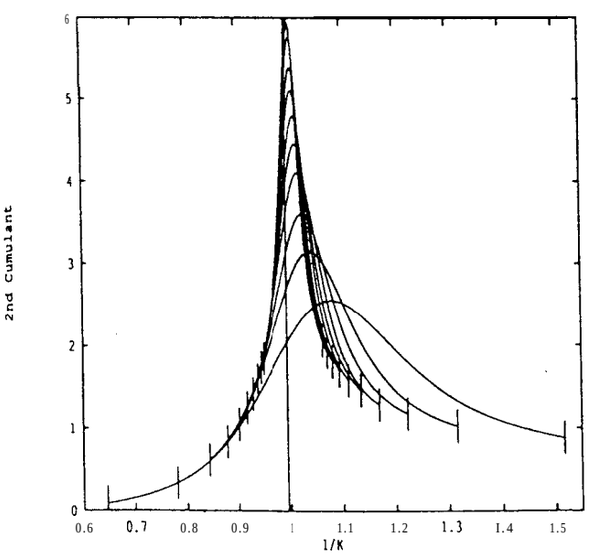

FIG. 6. Γ_2 (proportional to specific heat) against temperature K^{-1}, are redrawn to mark the range of temperature which transform to a fixed range of s, [-0.8, 1.2].

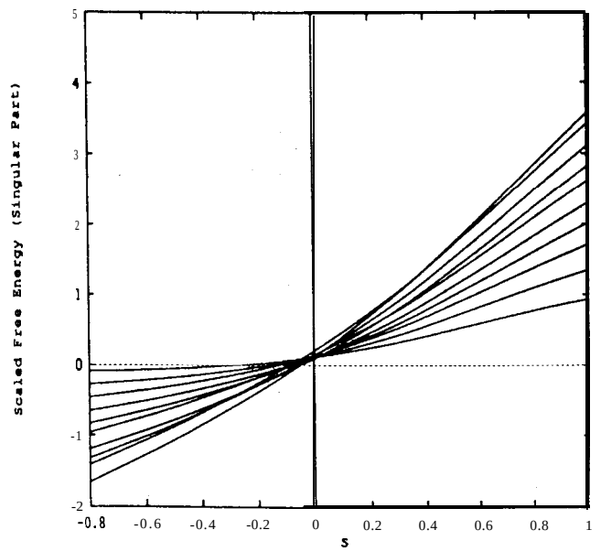

FIG. 7. $\Gamma_{0s}L^2$ againsts. Asymptotic limit of the family curves as L grows to infinity should give the universal function -Y(s). 0.601 is used for Γ_{0a}.

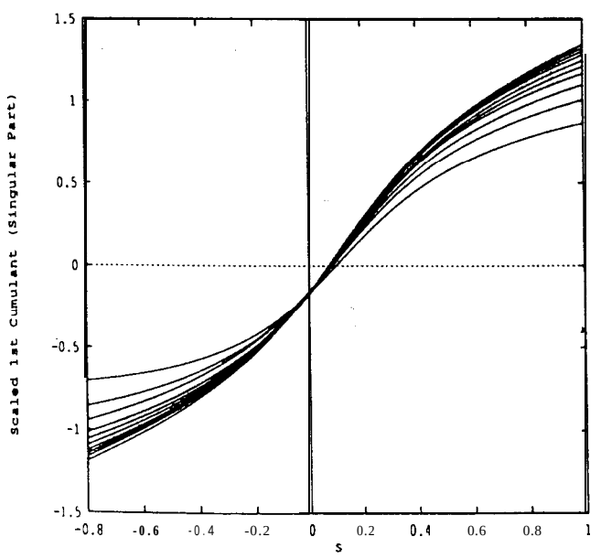

FIG. 8. $\Gamma_{1s}L^{2-1/\nu}$ against s. Asymptotic limit of the family curves as L grows to infinity should give the first derivative of universal function $-Y^{(1)}(s)$. 0.4266 is used for Γ_{1a}.

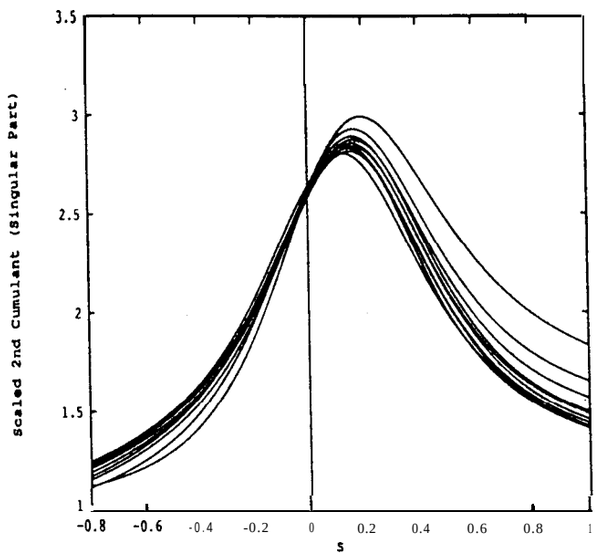

FIG. 9. $\Gamma_{2s}L^{2-2/\nu}$ against s. Asymptotic limit of the family curves as L grows to infinity should give the second derivative of universal function, $-Y^{(2)}(s)$. -1.4 is used for Γ_{2a}. It is noteworthy that the analytic part of the specific heat is negative.

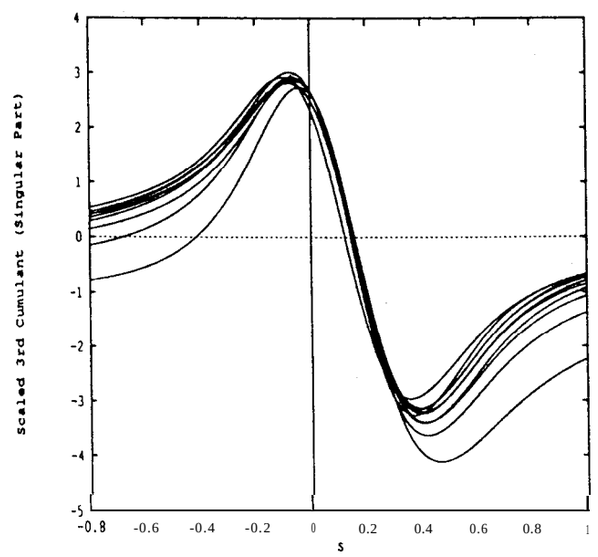

FIG. 10. $\Gamma_{3s}L^{2-3/\nu}$ against s. Asymptotic limit of the family curves as L grows to infinity should give the third derivative of universal function, $-Y^{(3)}(s)$. Accuracy in measurement of 3rd cumulant is not so good although the unscaled Γ_{3s}'s diverge rather rapidly as L grows large Here 2.8 is used for Γ_{2a}.

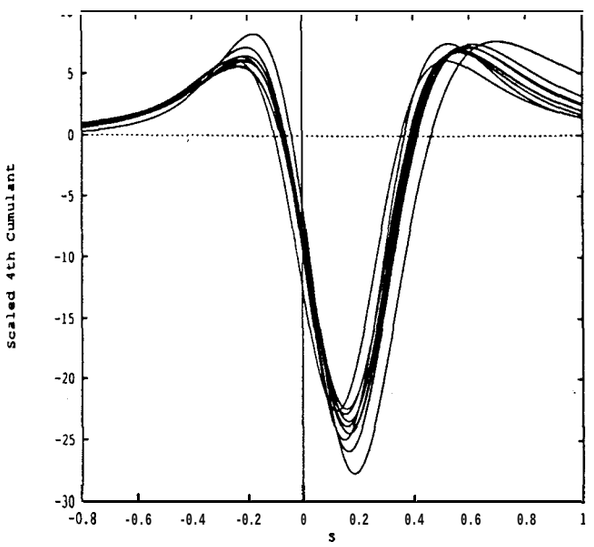

FIG. 11. $\Gamma_{4s}L^{2-4/\nu}$ against s. Asymptotic limit of the family curves as L grows to infinity should give the third derivative of universal function, $-Y^{(4)}(s)$. Accuracy in measurement of 4th cumulant is not good although the unscaled Γ_{4s}'s diverge enormously as L grows large. Analytic part if any would be drowned in the statistical errors. However scaling behavior of this quantity may be used for an estimation of the exponent, ν since $L^{2-4/\nu}$ is rather sensitive to the value of ν.

for Γ_{2a}, 2.8 for Γ_{3a}, 0.0 for Γ_{4a}.

These values are obtained using finite size scaling prediction at the bulk critical temperature $\varepsilon = s = 0$ so that scaled Γ_{ns} all fall into a single point at the bulk critical temperature. In this paper we are mainly concerned to the test. whether the result of the continuous functional Monte Carlo technique confirms the two scale factor universality prediction, we used exact critical temperature I&-1 = 0.99497 and the exponent v = 5/6.[7] Since $1/\nu$ is less than 2, singular part of both Γ_{0s} and Γ_{1s} vanish in the large L limit making analytic parts just bulk values. They are simply critical values of - free energy and internal energy as we can see from the Eqs. (18) and (19). These values are exactly known to be,[7] -2.0702(1) and -1.5447.

Since our energy density is measured 2.0 above the ground state, our estimated critical bulk free energy density and internal energy are -2.0702(1) and -1.5447 and they agree with the exact values almost to the machine precision.

Figs. 6-10 shows general tendency that we have claimed in section 3. As the size L grows large the scaled cumulants Eq. (22) approach to the $-Y^{(n)}$ since the approximation of constant analytic part over the fixed range of τ holds better and better. It should be also noted that the analytic part of 3rd cumulant is about 2.8 that it can almost negligible. In fact in the 4th cumulant

we have neglected analytic part altogether since the effect of the analytic part could well be drowned inside of statistical error of the simulation.

It should be remarked that while the accuracy of simulation is better for lower order cumulants, the singular part of these functions either diminish or grows moderate rate even if it diverges as the system size grows. On the other hand we have less precision for higher order cumulants although they diverge enormous rate. In the case of free energy the singular part is only a minute fraction of the total free energy and it would easily be drowned into the error bound of simulation as the system size grows. These two trends are competing each other so that optimum order of the cumulant which furnish best result in estimating scaling function would be either lst, or 2nd cumulant, namely internal energy or specific heat.

V. CONCLUSION AND DISCUSSION

We have demonstrated from the continuous functional Monte Carlo data not only that the two scale factor universality hypothesis holds good but also the scaling functions can be estimated from the data. In fact as a first approximants for these quantities we could take the scaled cumulants of the largest L. In fact the deviation of the last two scaled cumulants are almost within statistical deviation.

Next improvement in estimating scaling functions $Y^{(n)}$ is to use of linearly varying analytic part near the bulk critical point. Using the first approximant for $Y_1^{(n)}$, we can reverse the transformation given by Eq. (22) and subtracting $-L^{-(d-n/\nu)}Y_1^{(n)}(\tau)$ from the unscaled cumulants we can estimate the analytic parts of the cumulant in τ scale. Transforming τ variable back to ε variable, we can obtain the slowly (linearly) varying analytic parts of cumulants. We may use these analytic parts in estimating next order approximants of scaling functions.

In the above consideration we have altogether neglected any correction to scaling occurring either from nonlinear field or from irrelevant scaling field. In the above analysis the numerical evidence indicate that these corrections are indeed negligible. However in general case, these corrections may be necessary in estimating scaling functions.

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