Extended Scaling Scheme for Critically Divergent Quantities in Ferromagnets and Spin Glasses

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From a consideration of high temperature series expansions in ferromagnets and in spin glasses, we propose an extended scaling scheme involving a set of scaling formulas which expresses to leading order the temperature (T) and the system size (L) dependences of thermodynamic observables over a much wider range of T than the corresponding one in the conventional scaling scheme. The extended scaling, illustrated by data on the canonical $2d$ ferromagnet and on the $3d$ bimodal Ising spin glass, leads to consistency in the estimates of critical parameters obtained from scaling analyses for different observables.

Critical divergences of thermodynamical quantities $F(T)$ at continuous phase transitions are conventionally quoted in terms of the normalized scaling variable $t = (T - T_c)/T_c$, i.e., in the form

$$F(T) \simeq A_F[(T - T_c)/T_c]^{-\rho}, \qquad (1)$$

where T_c, ρ, and A_F are the transition temperature, the critical exponent, and the critical amplitude, respectively. There exist associated finite size scaling (FSS) rules. It has been clearly underlined (see, e.g., [1]) that this representation is valid only in the immediate vicinity of T_c, which is a very restrictive condition for both numerical simulations and experiments. In particular, for the analysis of finite size numerical data on complex systems such as Ising spin glasses (ISGs), where simulations have many intrinsic limitations, it is difficult to analyze data while strictly complying with this condition.

Other scaling variables can be used. In all modern theoretical and numerical analyses on ferromagnets, e.g., Refs. [2,3], as well as in some experimental analyses, e.g., Refs. [4,5], the scaling variable $\tau = 1 - \beta/\beta_c \equiv (T - T_c)/T$ is used instead of t. Although no general rationalization seems to have been published yet explaining why one scaling variable should be chosen rather than another, in this Letter we propose a coherent scaling scheme for critically divergent quantities derived from a systematic consideration of high temperature series expansions (HTSE) which naturally leads us to use the variable τ. In addition to this, the HTSE analysis leads us to properly define singular terms of interest in such a way that they themselves reproduce appropriate temperature dependence at the highest temperatures, i.e., in the limit $\beta \rightarrow 0$. We call this the *extended* scaling scheme, which we demonstrate below to be quite powerful at temperatures close to T_c where in practice one makes critical analyses for divergent quantities.

For a ferromagnet and, in particular, an Ising ferromagnet (IF), our extended scaling scheme is explicitly described as follows. (i) We use τ as the normalized scaling

variable and write

$$\chi(\beta) \simeq A_\chi \tau^{-\gamma}, \qquad (2)$$

for the reduced susceptibility χ following the standard definition without a prefactor β, which is in fact consistent with the idea of our extended scaling. (ii) Defining the second moment correlation length ξ through $\mu_2 = \sum_r r^2 \langle S_0 S_r \rangle = 2d\chi\xi^2$, with d the spatial dimension [3], we write ξ as

$$\xi(\beta) \simeq \beta^{1/2} A_\xi \tau^{-\nu}. \qquad (3)$$

(iii) Using this form of $\xi(\beta)$, we rewrite the FSS ansatz, $F(L, \beta) \sim L^{\rho/\nu} \tilde{F}[L/\xi(\beta)]$, as

$$F(L, \beta) \sim [L/\beta^{1/2}]^{\rho/\nu} \mathcal{F}[(L/\beta^{1/2})^{1/\nu}(1 - \beta/\beta_c)]. \qquad (4)$$

For the $2d$-IF, where the confluent corrections to scaling are known to be zero [2,6,7], we demonstrate that the above critical expressions with the known exact values of the critical parameters reproduce $\chi(\beta)$ and $\xi(\beta)$ to a good approximation right up to high temperatures, and that our FSS form Eq. (4) holds to a high approximation over a very much wider range of L and T than the conventional one. For the ISG, β^2 replaces β throughout in (i), (ii), and (iii), giving an entirely novel set of expressions. The use of our FSS form appropriately modified for the ISG resolves a long-standing puzzle in the ISG critical analysis, i.e., published estimates for the critical exponent ν through χ scaling and through ξ (or the Binder parameter) scaling differ by a large factor [8,9]. We emphasize here that Eqs. (2)–(4) above are leading order expressions of the divergent quantities. This does not mean that we neglect even the confluent corrections to scaling, but that fits of the numerical data examined below to our extended scaling scheme only with the leading expressions are quite satisfactory. We will discuss separately [10] that analyses of published high-precision data on canonical ferromagnets using the present extended scaling scheme actually give

estimates of the confluent correction terms which improve considerably over those from standard analyses.

In standard spin 1/2 ferromagnets the HTSE for the susceptibility $\chi(\beta)$ is written as

$$\chi(\beta) = 1 + a_1\beta + a_2\beta^2 + a_3\beta^3 + \cdots, \qquad (5)$$

where $\beta = J/k_BT$ with the coupling constant J and k_B set to unity [3,11,12]. The asymptotic form of its factors a_n is eventually dominated by the closest singularity to the origin (Darboux's first theorem [13]) which in the simplest case is the physical singularity, i.e.,

$$[1 - \beta/\beta_c]^{-\gamma} = 1 + \gamma\left(\frac{\beta}{\beta_c}\right) + \frac{\gamma(\gamma+1)}{2}\left(\frac{\beta}{\beta_c}\right)^2 + \cdots, \qquad (6)$$

with β_c being the inverse critical temperature. One of the techniques to relate these two expressions is the ratio method, in which the recurrence relation $a_n/a_{n-1} = (1/\beta_c)(1 + (\gamma - 1)/n)$ for large n is used [14]. It is therefore natural to adopt $\tau = 1 - \beta/\beta_c$ as the scaling variable in critical analyses based on the HTSE theory.

The HTSE for the second moment $\mu_2(\beta)$ introduced above is of the form [3]

$$\mu_2(\beta) = (b_1\beta)[1 + (b_2/b_1)\beta + (b_3/b_1)\beta^2 + \cdots]. \qquad (7)$$

It diverges at T_c as $[T - T_c]^{-(\gamma+2\nu)}$. Then, invoking again Darboux's theorem to link the series within the brackets $[\cdots]$ to the critical divergence, the appropriate extended scaling form can be written as

$$\mu_2(\beta) \simeq \beta A_\mu(1 - \beta/\beta_c)^{-(\gamma+2\nu)}. \qquad (8)$$

By combining this with Eq. (2) for $\chi(\beta)$, Eq. (3) for $\xi(\beta)$ is derived. With this expression for ξ the FSS form becomes Eq. (4). At the limit $\beta \to 0$, Eqs. (2), (3), and (8) have the same β dependence as the leading terms of the corresponding HTSE. This implies that they merge smoothly to the analytic corrections to scaling to yield the proper expressions at highest temperatures. Similar expressions are expected also for confluent corrections to scaling if they exist.

We exhibit in Figs. 1(a) and 1(b) log-log plots of the susceptibility χ of the canonical 2d-IF in the thermodynamic limit, plotted against $\log(t)$ and $\log(\tau)$, respectively. The data points in the figure are the high-precision results of the critical [2] and HTSE [12] analyses. The line in Figs. 1(a) and 1(b) is the power-law expression of χ as a function of t and τ, respectively, with $\gamma = 7/4$ and the critical amplitude $A_\chi = 0.962581\ldots$ [2]. By the τ scaling, all the data points up to nearly $\tau = 1$, i.e., to almost $T = \infty$, lie on the scaling expression of Eq. (2) within the accuracy of the figure. This result reflects the weakness of corrections to scaling in this system as mentioned above. On the other hand, the deviation of the true χ data from the t scaling line, $\chi = A_\chi t^{-\gamma}$, is significant already at, say, $t \simeq 0.2$ (or $T \simeq 1.2T_c$). Thus if the scaling variable t rather than
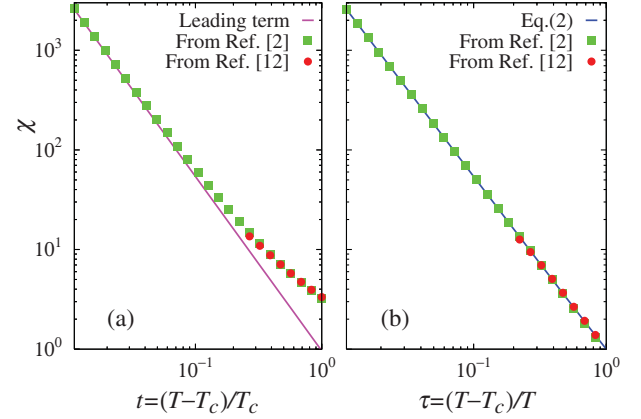

FIG. 1 (color). Susceptibility χ of the 2d-IF as a function of $\log(t)$ (a) and $\log(\tau)$ (b).

τ were used for a critical analysis on this system, there would appear to be very strong "correction" terms, which would pollute the evaluation of the γ value.

Figure 2 shows the FSS plots for the 2d-IF susceptibility, the standard one in the inset and the extended one in the main panel. It is clear that the standard form, as expected, gives acceptable scaling only extremely close to T_c, while the extended form gives high quality scaling for all temperatures above T_c examined. In Fig. 3 we show the conventional and extended FSS plots of $\chi(T, L)$ as a function of $\xi(T, L)/L$. Note that, since the value T_c is not involved in this analysis at all (also in Fig. 6 below), one can judge straightforwardly our proposal (iii) by this comparison. The consequence is that the extended FSS plot is definitely better than the conventional one. We thus conclude that, at least for the 2d-IF, our extended scaling scheme does indeed work much better than the conventional one.
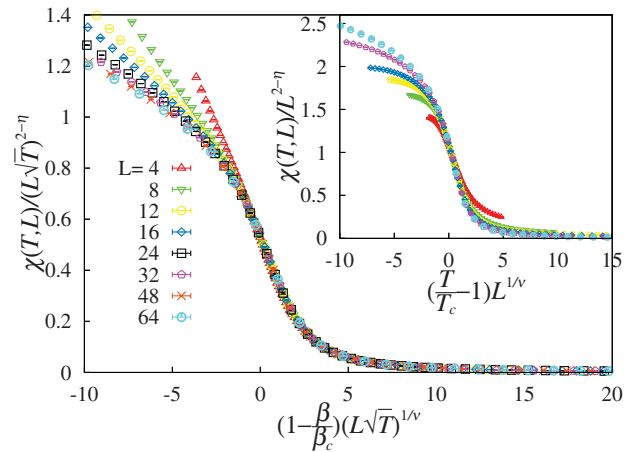

FIG. 2 (color). An extended FSS plot for the 2d-IF susceptibility χ. The points are data obtained by our Monte Carlo simulation at temperatures $0.46 \leq T/T_c \leq 1.86$. The inset presents a standard FSS plot for the same χ. For both plots the exact scaling parameters are used.
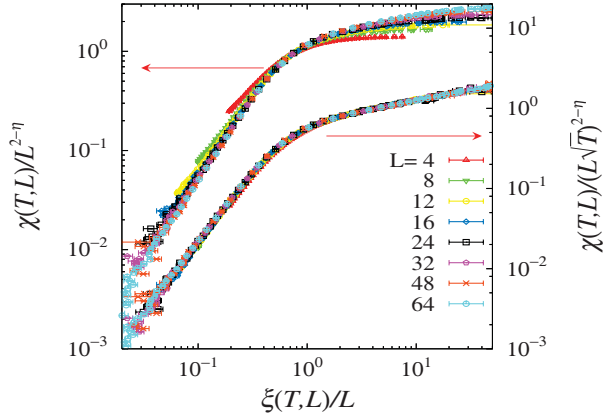
FIG. 3 (color). An extended (conventional) FSS plot for the 2d-IF susceptibility χ normalized by $(L\sqrt{T})^{2-\eta}$ $(L^{2-\eta})$ as a function of $\xi(T,L)/L$.

Let us next discuss an extension of our extended scaling scheme to the Edwards-Anderson 3d-ISG model having a symmetric interaction distribution with zero mean. Because of the symmetry, as stated by Daboul *et al.* [15], only even powers of β enter into the HTSE for thermodynamic quantities, and the HTSE for the reduced spin glass (SG) susceptibility χ_{SG} (the ordinary one multiplied T^2) is of the form

$$\chi_{SG}(\beta) = 1 + c_1(\beta^2) + c_2(\beta^2)^2 + c_3(\beta^2)^3 + \cdots. \quad (9)$$

Hence once again invoking the Darboux theorem, but this time with $(\beta/\beta_c)^2$ replacing β/β_c, or $\tau' = 1 - (\beta/\beta_c)^2$, we adopt the following scaling form for $\chi_{SG}(\beta)$ [15]:

$$\chi_{SG}(\beta) \simeq A_{\chi_{SG}}[1 - (\beta/\beta_c)^2]^{-\gamma}. \quad (10)$$

The μ_2 in spin glasses, again due to the symmetry, can be expressed as even powers of β starting from the β^2 term, though the coefficients have not been explicitly evaluated yet. Hence the scaling form for $\xi(\beta)$ in spin glasses can be taken to be

$$\xi(\beta) \simeq \beta A_{\xi_{SG}}[1 - (\beta/\beta_c)^2]^{-\nu}. \quad (11)$$

Then the extended FSS for ISGs can be written as

$$F(L, \beta) \sim [L/\beta]^{\rho/\nu} \mathcal{F}\{(L/\beta)^{1/\nu}[1 - (\beta/\beta_c)^2]\}. \quad (12)$$

In contrast to the 2d-IF, analytical theories are very limited for ISGs. Daboul *et al.* [15] were able to make accurate estimates of β_c and γ of the models by the HTSE method but only in dimension 4 and above. We therefore compare our extended τ scaling scheme with the conventional one with a variable t, without introducing corrections to scaling in either analysis. The numerical data used are obtained on the 3d-ISG system with bimodal interactions by the exchange Monte Carlo method.

In Fig. 4 we show an extended FSS plot for the correlation length $\xi(L, T)/L$ as a function of the scaling variable $x = |\tau'|(TL)^{1/\nu}$ based on Eq. (12). In this plot we fix $T_c =$
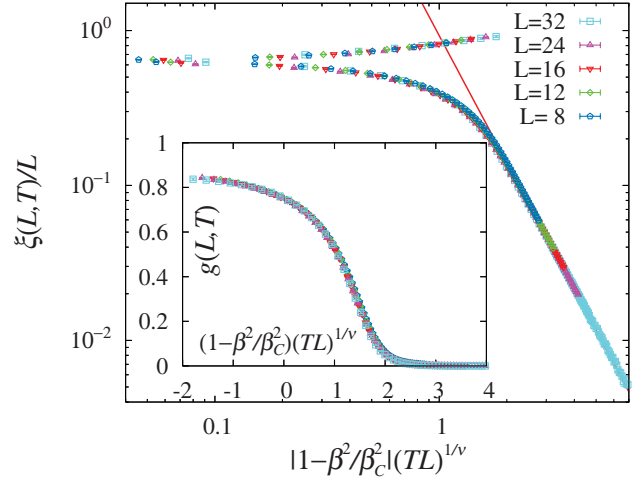

FIG. 4 (color). An extended FSS plot of $\xi(L, T)/L$ of 3d-ISG. The straight line with slope 2.72 ($= \nu$) represents an expected asymptotic form of the scaling function. The inset shows the FSS plot of the Binder parameter.

1.11, which is the optimal value from our analyses and is consistent with that of Ref. [8], and adjust ν to obtain the best scaling fit. We end up with $\nu = 2.72(8)$. The fit is surprisingly good for all the data with L's indicated in the figure and at T from $0.81T_c$ to $7.2T_c$. The slope of the straight line in the range $|x| \gg 1$ is 2.72 $(= \nu)$. Note that data points on the line are not only those at sufficiently high temperatures with $\xi \simeq \beta$ from Eq. (11) but also those in the critical range with $\beta \ll \xi \ll L$.

Figure 5 shows an extended FSS plot for χ_{SG}. This plot is obtained by fixing $T_c = 1.11$ and $\nu = 2.72$ and by adjusting η to give $\eta = -0.40(4)$. We obtain quite satisfactory scaling for all our data. In contrast, a conventional FSS plot using the variable t as shown in the inset is rather poor except for the immediate vicinity of $x = 0$. The fit yields a small apparent value of $\nu = 1.47(3)$ similarly to
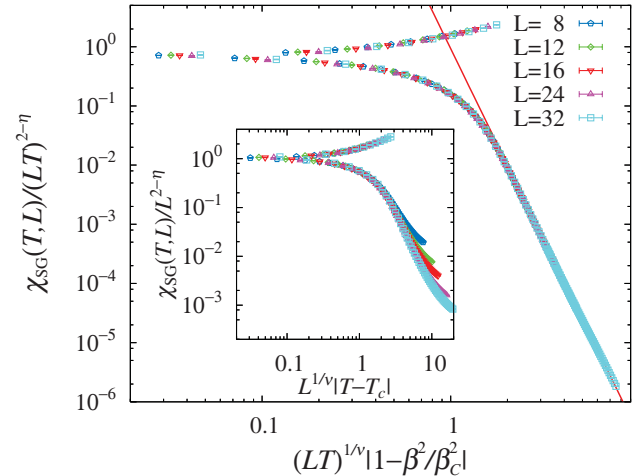

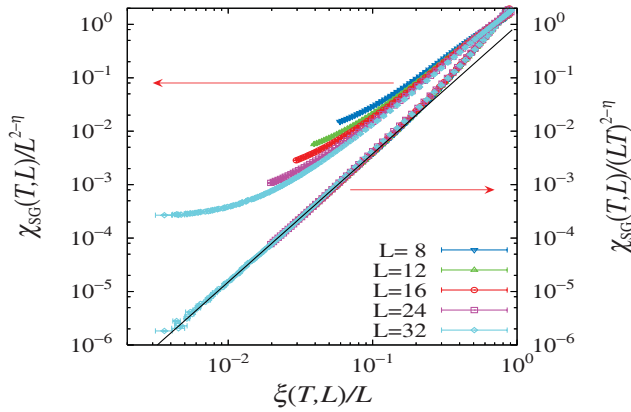FIG. 5 (color). An extended FSS plot of χ_{SG}. The inset is the corresponding conventional FSS plot.

FIG. 6 (color).   An extended (conventional) FSS plot for the 3d-ISG susceptibility χ_{SG} normalized by $(LT)^{2-\eta}$ ($L^{2-\eta}$) as a function of $\xi(T, L)/L$.

the previous conventional FSS analyses [8,9]. In Fig. 6 we demonstrate conventional and extended scaling plots for χ_{SG} versus ξ. The comparison of the two implies that our scaling scheme with (ii) and (iii) is definitely more appropriate also for the 3d-ISG.

One can remark that our extended scaling scheme with only the leading term for each divergent observable gives a high quality fit over the entire range of L and T examined. Another important result here for the SG study is that the extended FSS analyses on ξ, g, and χ_{SG} with the implicit assumption that corrections to scaling are weak yield a unique critical parameter set. This is in sharp contrast to standard FSS methods for which the estimate for ν obtained from χ scaling with the same assumption is considerably smaller than that from ξ or g scaling [8,9]. In this context, we note that numerical data on the same 3d-ISG model have also been analyzed using t scaling together with strong correction to scaling terms [16,17]. We have checked that our data can be analyzed equally well using a very similar method to that of Ref. [16], and the excellent fit to the data from the extended scaling without corrections to scaling is obtained with two fewer fitting parameters. This does not imply that corrections to scaling are absent, but just that their influence on the fits examined here is rather weak.

In conclusion, by considering the intrinsic structural form of high temperature series developments, we have proposed an extended scaling scheme with appropriate scaling expressions for thermodynamic observables in ferromagnets and spin glasses, and have demonstrated the

results which support it strongly. One of them is the direct comparison of our extended scaling on χ vs ξ with that of the conventional one. Another is the result that, within our scheme, the leading order critical power-law expressions with a coherent set of critical parameters remain good approximations to the true behavior over a much wider temperature range than with the standard t scaling. From these results we consider that our extended scaling scheme with the variable τ is more fundamental than the conventional t scaling.

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