Correlations in Ising chains with nonintegrable interactions

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Two-spin correlations generated by interactions that decay with distance r as $r^{-1-\sigma}$ with $-1 < \sigma < 0$ are calculated for periodic Ising chains of length L. Mean-field theory indicates that the correlations $C(r, L)$ diminish in the thermodynamic limit $L \to \infty$, but that they contain a singular structure for $r/L \to 0$ that can be observed by introducing magnified correlations $LC(r, L) - \sum_r C(r, L)$. The magnified correlations are shown to have a scaling form $\Phi(r/L)$ and the singular structure of $\Phi(x)$ for $x \to 0$ is found to be the same at all temperatures, including the critical point. These conclusions are supported by the results of Monte Carlo simulations for systems with $\sigma = -0.50$ and -0.25 both at the critical temperature $T = T_c$ and at $T = 2T_c$.

I. INTRODUCTION

The Ising model in $d = 1$ dimension with long-range interactions decaying with distance r as $J(r) \sim r^{-1-\sigma}$ has been much studied. Dyson [1] showed that there is no phase transition for $\sigma > 1$, while there is long-range order at low temperatures when the interactions are ferromagnetic and $\sigma \leq 1$. The borderline case of $\sigma = 1$ was studied by several authors [2], who found a one-dimensional version of the Kosterlitz-Thouless transition [3] in the system. A variety of methods [4-7] have been used to show that the transition is of second order with continuously varying critical exponents in the region $\frac{1}{2} < \sigma < 1$. For $0 < \sigma < \frac{1}{2}$, it has been found that the critical exponents are mean-field-like for thermodynamic quantities, but the spin-spin correlations at the critical temperature

$$C(r) \propto \frac{1}{r^{d-2+\eta}} = \frac{1}{r^{\eta-1}} \tag{1}$$

have a nonclassical critical exponent $\eta = 2 - \sigma$ [8,9]. The case $\sigma = \frac{1}{2}$ is somewhat special in that the mean-field exponents are modified by logarithmic corrections [4] in analogy to the situation with the short-range Ising model for $d = 4$ or the $d = 3$ Ising model with dipolar interactions [10].

The case $\sigma < 0$ does not appear to have been investigated except for $\sigma = -1$. The reason perhaps is the fact that the interaction potential $J(r)$ becomes nonintegrable for $\sigma < 0$ and then the energy of the system is nonextensive. The textbook example of $\sigma = -1$ has attracted much attention since it corresponds to an Ising model in which every spin interacts equally with every other spin. The problem of nonextensive energy is solved by rescaling the coupling strength by the number of spins and the result is a mean-field exact solution. Spatial correlations have no meaning in this system.

For $\sigma < 0$ and $\sigma \neq -1$ one can still consider spatial correlations and this is what we shall do in this paper. The reason for doing it is partly that there are interactions in nature that are nonintegrable. The gravitational interaction is a prominent example, but there are many systems that contain topological defects with nonintegrable effective interactions between the defects. Our original motivation, however, comes from the studies of nonequilibrium steady states. The main difficulty with nonequilibrium steady states is that their properties depend not only on the interactions but also on the details of the underlying dynamics. In order to get a handle on the effect of dynamics, there have been several works [11-14] in which the goal was to determine the effective interactions that are generated by the interplay of various dynamical processes. A way to achieve this goal is to investigate the phase transitions occurring in nonequilibrium steady states and deduce the effective interactions from the universality class the transitions fall into. For example, a combination of spin flips and Levy-flight spin exchanges in a $d = 1$ kinetic Ising model produces a steady state with effective long-range interactions and this steady state displays a critical phase transition. In this case, the large-distance behavior of the interactions $J(r) \sim r^{-1-\sigma}$ can be deduced [12] from measuring critical exponents. Of course, this can be done only if σ is in a range $0 < \sigma < 1$ where either the correlation exponent η or the thermodynamic exponents depend on σ. In order to extend this method to nonintegrable interactions ($\sigma < 0$), we must investigate the correlations since measuring thermodynamic exponents yield mean-field values independently of σ. Thus we can see that in order to extract information about nonintegrable effective interactions in nonequilibrium steady states, we must first understand the *equilibrium* correlations in systems with nonintegrable interactions.

Since mean-field theory is expected to describe the critical behavior correctly for $\sigma < 0$, we used it to calculate the correlations for finite size systems (Sec. II). Our main result is that the singular part of the correlations

appears to have universal features that make it useful in deducing effective interactions in nonequilibrium steady states. We check our mean-field results against simulations in Sec. III and a final discussion is given in Sec. IV.

II. CALCULATION OF THE CORRELATION FUNCTION IN MEAN-FIELD THEORY

We consider a one-dimensional Ising model of $L = 2N + 1$ spins $s_i = \pm 1$ at sites $i = -N, -N+1, ..., N$ and impose periodic boundary conditions. The energy of the system is given by

$$\mathcal{H} = -\sum_{i<j} J_{i,j} s_i s_j - \sum_i H_i s_i \qquad (2)$$

and the interaction is assumed to decay with distance as a power-law but it is cut off at $|i - j| = N$:

$$J_{i,j} = \begin{cases} J/|i-j|^{1+\sigma} & \text{for } 1 \le |i-j| \le N \\ 0 & \text{otherwise.} \end{cases} \qquad (3)$$

Here $J > 0$ and the parameter σ is assumed to be in the range $-1 < \sigma < 0$. The inhomogeneous external field H_i is included in order to calculate the susceptibility $\chi_{i,j} = \partial \langle s_i \rangle / \partial H_j$, which, at temperature $\beta^{-1} = k_B T$, is related to the two-spin correlation function $C_{i,j} = \langle s_i s_j \rangle$ through

$$C_{i,j} = k_B T \left. \frac{\partial \langle s_i \rangle}{\partial H_j} \right|_{\{H_l\} \to 0} , \qquad (4)$$

where $\{H_l\} \to 0$ means that the susceptibility and, consequently, the correlation functions are evaluated in the limit of vanishing fields.

In the mean-field approximation, $\chi_{i,j}$ is obtained from the self-consistency equation for the average magnetization:

$$\langle s_i \rangle = \tanh\left(\sum_l \beta J_{i,l} \langle s_l \rangle + \beta H_i \right) . \qquad (5)$$

Taking a derivative of both sides of this equation with respect to H_j and letting $\{H_l\} \to 0$, we obtain

$$C_{i,j} = \left[\sum_l \beta J_{i,l} C_{l,j} + \delta_{i,j} \right] (1 - \langle s_i \rangle^2) . \qquad (6)$$

Equations (5) and (6) form a closed set of equations for $C_{i,j}$ and $\langle s_i \rangle$. In zero field, the system is expected to be homogeneous and thus $C_{i,j} = C_{i-j}$ and $\langle s_i \rangle = m$, where m is given by the stable solution of (5). Assuming this homogeneity, Eq. (6) is solved by Fourier transformation. Introducing

$$C(k) = \sum_{l=-N}^{N} C_l \exp(-ikl), \quad k = \frac{2\pi n}{2N+1},$$

$$n = 0, \pm 1, ..., \pm N \quad , \quad (7)$$

one finds

$$C(k) = \frac{1 - m^2}{1 - (1-m^2)\beta J(k)} , \qquad (8)$$

where $J(k)$ is the Fourier transform of $J_{i,j} = J_{i-j}$.

Up to this point, the derivation followed along standard lines. The nonintegrability of the interaction starts to play a role when we try to find the critical temperature T_c. Since $C(k = 0)$ is proportional to the fluctuation of magnetization, its divergence determines T_c in the thermodynamic limit $N \to \infty$. Thus setting $m = 0$ in Eq. (8), one finds

$$k_B T_c = J(0) = \lim_{N \to \infty} \sum_{n=1}^{N} \frac{2J}{n^{1+\sigma}} . \qquad (9)$$

The problem with the above expression is that the sum diverges as $N^{|\sigma|}$ for $\sigma < 0$. Thus, in order to have a thermodynamic limit for the correlation functions, we either have to divide J by $N^{|\sigma|}$ or have to consider temperatures that are proportional to $N^{|\sigma|}$. Since only the ratio $J/k_B T$ enters the expressions, the two routes are equivalent. Introducing $\theta = T_c(N)/T$ and $\bar{\theta} = (1-m^2)\theta$, where $T_c(N)$ is defined through the sum in (9) without taking the $N \to \infty$ limit, we obtain the spatial correlation function from the inverse Fourier transform of (8):

$$C_l = \frac{1-m^2}{2N+1} \left\{ \frac{1}{1-\bar{\theta}} + 2 \sum_{n=1}^{N} \frac{\cos\left(\frac{2\pi n}{2N+1} l\right)}{1 - \bar{\theta} Q_N(n)} \right\} , \qquad (10)$$

where $Q_N(n)$ is given by

$$Q_N(n) = \sum_{j=1}^{N} \frac{\cos\left(\frac{2\pi j}{2N+1} n\right)}{j^{1+\sigma}} \bigg/ \sum_{j=1}^{N} \frac{1}{j^{1+\sigma}} . \qquad (11)$$

One can see that correlations in the low- and high-temperature phases are simply related by rescaling the temperature and the amplitude by $1 - m^2$ [15]. For this reason we shall consider only the high-temperature phase and the critical point and thus set $m = 0$ and $\bar{\theta} = \theta$.

Equations (10) and (11) can be easily evaluated numerically and the mean-field results can be compared to Monte Carlo (MC) simulations (see Sec. III). First, however, we shall discuss the analytic properties of C_l in the "thermodynamic limit" where $N \to \infty$. As can be seen from (10), the average of C_l over l is given by $[(2N+1)(1-\theta)]^{-1}$ and is negligible for $\theta \ne 1$. The part of C_l that remains after subtracting the average also diminishes, but with a smaller exponent. It is of the order of N^σ and thus no spatial correlations remain in the $N \to \infty$ limit for $\sigma < 0$. It turns out, however, that the correlation function has an interesting singular behavior for small $x = l/(2N+1)$, which can be well observed in finite-size systems. We shall investigate this spatial dependence by amplifying it through subtracting the average part of C_l and multiplying the result by $2N + 1$:

$$\Phi_N(x) \equiv (2N+1)C_l - \frac{1}{1-\theta} = 2\sum_{n=1}^{N} \frac{\cos(2\pi nx)}{1 - \theta Q_N(n)} \quad .$$
(12)

The function $Q_N(n)$ is finite and can be evaluated exactly in the $N \to \infty$ limit

$$\lim_{N\to\infty} Q_N(n) = \frac{\pi^\sigma \Gamma(1-\sigma)\cos\frac{\sigma\pi}{2}}{n^{|\sigma|}} \equiv \frac{D_\sigma}{n^{|\sigma|}} \quad , \quad (13)$$

where $\Gamma(z)$ denotes the gamma function. Thus we can take the upper limit of the sum in (12) to infinity and find a scaling function $\Phi(x)$, which is independent of N. The singular part of $\Phi(x)$ in the limit $x \to 0$ is calculated by first noting that the identity $2\sum_{n=1}^{N}\cos(2\pi nx) = -1$ is valid for any x that can be written as $l/(2N+1)$, where l is an integer not divisible by $2N+1$. Using this identity, the sum in (12) can be rewritten so that it contains the expression $(1 - \theta D_\sigma/n^{|\sigma|})^{-1} - 1$. This expression is then expanded in θ and, finally, the sums over n are changed into integrals. The number of singular terms obtained in this way depends on σ and, for $(j+1)^{-1} < |\sigma| < j^{-1}$, where j is an integer, we find

$$\Phi_{\text{sing}}(x) = \theta\frac{A_1(\sigma)}{x^{1+\sigma}} + \theta^2\frac{A_2(\sigma)}{x^{1+2\sigma}} + \cdots + \theta^j\frac{A_j(\sigma)}{x^{1+j\sigma}} \quad . \quad (14)$$

The coefficients $A_n(\sigma)$ can be calculated explicitly. For example, the coefficient of the strongest singularity A_1 is given by

$$A_1(\sigma) = 2^{-1-\sigma}|\sigma| \quad . \quad (15)$$

If $|\sigma| = 1/j$ then the last term in (14) changes from power-law singularity into a term of logarithmic singularity, $A_j \ln(x)$. For example, the case $\sigma = -1/2$ yields the singular part

$$\Phi_{\text{sing}}(x) = \frac{\theta}{\sqrt{8x}} + \frac{\theta^2}{4}\ln(x) \quad . \quad (16)$$

One can compare $\Phi_N(x)$ calculated for $\sigma = -0.5$ and $\theta = 0.5$ from the exact sum with, e.g., $2N+1 = 801$ and $\Phi_{\text{sing}}(x)$ obtained from (16). One then finds that $\Phi_N(x) - \Phi_{\text{sing}}(x)$ is constant ($A = -2.35$) to an accuracy of the order of 1%. Thus the singular part plus a constant represents the exact solution to a very good accuracy over the entire range $0 < x < 0.5$, which is relevant physically. We checked the "singular-terms-plus-constant" description for other values of σ and found that the accuracy decreases as σ decreases. For example, in order to achieve a 1% accuracy at $\sigma = -0.75$ and $\theta = 1$, one must also include an additional term and write $\Phi(x) \approx A_1 x^{-1/4}(1 + Bx) + C$.

Next, we turn to the calculation of $\Phi(x)$ at the critical point ($\theta = 1$). In systems with short-range interactions, the decay of correlations changes from exponential to power-law as the critical point is reached. Systems with long-range, integrable interactions ($\sigma > 0$) have power-law correlations already in the high-temperature phase and the change that occurs in these systems when T_c is approached is that the exponent of the power-law decay changes (becomes smaller at T_c). For example, in

the exactly solvable spherical model [16], $C_l \sim l^{-d-\sigma}$ for $T > T_c$ and $C_l \sim l^{-d+\sigma}$ at T_c. As we shall see below, the nonintegrable systems are different from the cases discussed above in the sense that the singular structure of C_l does not change when $\theta = 1$ is reached. The scaling function $\Phi_{\text{sing}}(x)$ at criticality is obtained by just setting $\theta = 1$ in Eq. (14).

The first question that arises when the $\theta = 1$ case is considered is the infinity of the $1/(1-\theta)$ term, which has been subtracted from $(2N+1)C_l$ in the definition of Φ [see (12)]. Since this term is the sum of the correlation function, it is equal to the magnetization fluctuation

$$\frac{1}{1-\theta} = C(k=0) = \frac{\langle M^2\rangle}{2N+1} \quad , \quad (17)$$

where $M = \sum_i s_i$ is the total magnetization of the system. Thus, at the critical point, $(1-\theta)^{-1}$ does not diverge in a finite-size system; it just changes from a quantity of $O(1)$ to $O(N^\rho)$, where $\rho = 1/2$ in the mean-field theory. The apparent singularity of $1/(1-\theta)$ is the result of effectively linearizing Eq. (5) when using Eq. (4) for calculating the correlation function. For our purpose of calculating Φ, the real or apparent singularity of $C(k=0)$ does not pose a difficulty since Φ is defined after subtracting $C(k=0)$ from the correlation function. Note that $\Phi(x)$ is well defined physically: it is the correlation function after the average has been subtracted.

The second question that has to be answered for $\theta = 1$ is whether any of the terms in the sum (12) defining Φ becomes singular in the $\theta \to 1$ limit. [After all, $1/(1-\theta)$ was a term in this sum before being treated separately and, in general, one may expect long-wavelength singularities at the critical point.] The answer to this question is no and the reason for the absence of singularities is that long-range interactions develop a gap in the "fluctuation spectrum" of the system. In order to see how this happen and why nonintegrable interactions are different from the short-range ones, let us examine the denominator of the terms in the sum in Eq. (10). For short-range, e.g., nearest-neighbor, interactions one finds in the long-wavelength limit

$$1 - \theta Q_N(n) = 1 - \theta\cos\left(\frac{2\pi}{2N+1}n\right)$$
$$\approx 1 - \theta + \frac{\theta}{2}\left(\frac{2\pi n}{2N+1}\right)^2 . \quad (18)$$

One can see that the above expression is nonzero for $\theta < 1$ while it goes to zero at $\theta = 1$ as the square of the wave number (for $N \to \infty$). This is the origin of the exponential (power-law) decay of *large-distance* correlations at $\theta < 1$ ($\theta = 1$).

The structure of the denominator changes for nonintegrable potentials ($\sigma < 0$). It becomes independent of N for $N \to \infty$ and, using (13), one finds

$$1 - \theta Q_N(n) \approx 1 - \theta\frac{\pi^\sigma \Gamma(1-\sigma)\cos\frac{\sigma\pi}{2}}{n^{|\sigma|}} \quad . \quad (19)$$

Since $D_\sigma \equiv \pi^\sigma \Gamma(1-\sigma)\cos\frac{\sigma\pi}{2} < 1$ for $-1 < \sigma < 0$ ($D_\sigma \to 1$ only for $\sigma \to 0$), the denominator in (19) is

nonzero even for the smallest $n = 1$ at $\theta \leq 1$. Thus there is a gap in the spectrum of magnetization fluctuations for all wave numbers and the singularity of the scaling function $\Phi(x)$ at *small* arguments (small distances) comes from the nonanalytic structure of the denominator at large wave numbers. It should be noted that the above argument also holds in the low-temperature phase after replacing θ by $\bar{\theta}$ and using the fact that $0 \leq \bar{\theta} \leq 1$ [15].

It is clear from the above discussion that $\theta = 1$ can be set in the sum (12) for evaluating $\Phi(x)$ and it is also clear that the result for the singular part Φ_{sing} is given by Eq. (14) with $\theta = 1$. One can again compare Φ_{sing} and Φ, the latter evaluated for large but finite systems, and one again finds 1% accuracy with the Φ_{sing}+const description at $\sigma = -0.5$. The trends with the accuracy of the singular-part description is also the same for $\theta = 1$ as in the case of $\theta < 1$ discussed above.

III. MONTE CARLO SIMULATIONS

In this section, we describe the results of addressing the following question: Do the results of the mean-field calculation remain valid when fluctuations are included? Since no exact solutions are available, we studied the problem by performing MC simulations on the long-range Ising model described at the beginning of Sec. II. We considered cases of $\sigma = -0.50$ and -0.25 at both $\theta = 0.5$ and 1.0. Single-spin flip dynamics with Metropolis flip rates was used and we studied systems of sizes $2N + 1 = 201, 401, 801,$ and 1601. After an initial estimate of the relaxation times, we let the system equilibrate and the equilibrium correlations were calculated and analyzed.

Apart from the usual difficulties of simulating a system with long-range interactions (calculating the energy changes is time consuming and no cluster algorithms can

FIG. 2. Scaling of data in Fig. 1 after subtracting the average of C_l over l and multiplying the results by $2N + 1$, i.e., plotting $\Phi_N(x)$ defined in Eq. (12) against $x = l/(2N + 1)$. For clarity, only 40 points are included from each data set.

be used to reduce critical slowing down), there is one extra problem when a $\sigma < 0$ system is simulated. Namely, the definition of the $\theta = 1$ critical point is not quite obvious. The mean field $T_c^{\text{MF}}(N)$ defined in (9) has the right asymptotics for $N \to \infty$ but for a finite N, T_c has corrections due to fluctuations. For a sequence of systems of increasing size, one can, in principle, use any sequence of $T_c(N)$ that approaches $T_c^{\text{MF}}(N)$ in the thermodynamic limit. In practice, we defined $T_c(N)$ as the temperature where the macroscopic magnetization fluctuations have the large-N behavior that follows from mean-field theory, namely, $\langle M^2 \rangle/(2N + 1) \approx 1.17 \ldots \times (2N + 1)^{1/2}$.
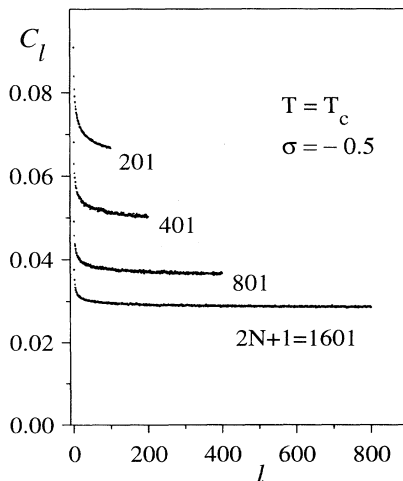

FIG. 1. Raw data from the MC simulation of an Ising chain of length $2N + 1$ at the critical temperature $T = T_c$ with the long-range parameter set to $\sigma = -0.5$. The correlation function C_l is plotted against l.
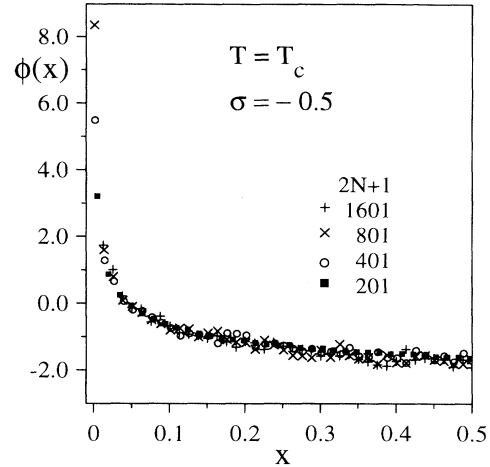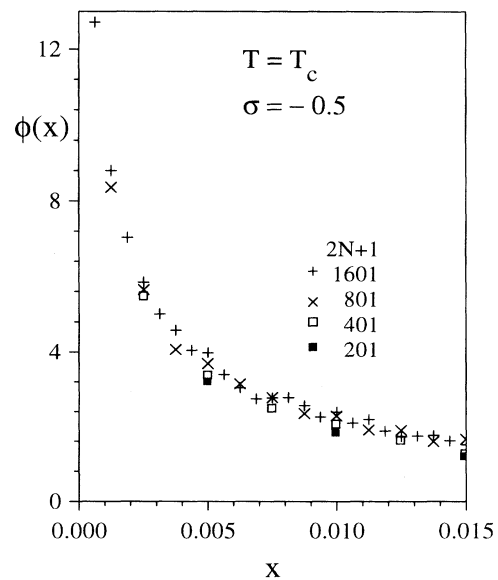

FIG. 3. Blowup of the small-x region of Fig. 2. All data points in the given x interval are included.
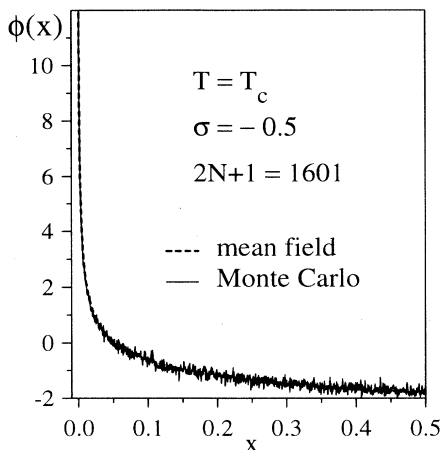
FIG. 4. Comparison of the scaled MC data (Fig. 2) and the mean-field results for the $2N + 1 = 1601$ data.

FIG. 5. Comparison of the scaled MC data and the mean-field results for $\sigma = -0.5$ and $T = 2T_c$.

Since $\langle M^2 \rangle/(2N + 1) = 1/(1 - \theta)$, the above choice means that we approach the $\theta_c = 1$ critical point as $\theta_c(N) = 1 - [1.17\ldots \times (2N + 1)]^{-1/2}$. The same correction can also be made in the mean-field calculation. This correction, however, is small and would not be visible in the figures discussed below.

Figure 1 displays the raw data for the correlation function C_l at $\sigma = -0.5$ and $\theta_c(N)$. After subtracting the average correlation and multiplying the result by $2N + 1$ (i.e., calculating Φ) we obtain a collapse of data (Fig. 2) if Φ is plotted against $x = l/(2N + 1)$. A blowup of the small-x region is shown in Fig. 3.

In Fig. 4, the MC data are compared with $\Phi(x)$ calculated from the mean-field theory of Sec. II and we observe excellent agreement between simulations and theory. In Fig. 5 we can see similar agreement away from the critical point ($\theta = 0.5$) for the case of $\sigma = -0.5$. We have also performed simulations with $\sigma = -0.25$ at both $\theta = 0.5$ and $\theta_c(N)$ and we again observed both the scaling of the data when $\Phi(x)$ vs x was plotted as well as the agreement between MC and mean-field results. Thus we conclude that the mean-field theory presented in Sec. II correctly describes the correlations of Ising models in which the interactions are of long-range, power-law form $J_l \sim l^{-1-\sigma}$ with $-1 < \sigma < 0$.
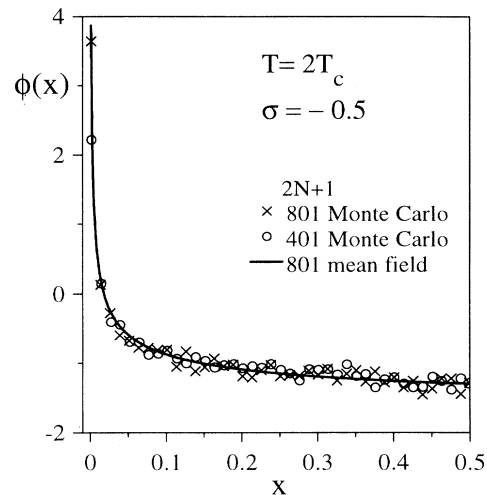
IV. FINAL REMARKS

The main conclusions of our work are that (i) the mean-field theory provides us with explicit expressions for the correlation function in case of nonintegrable interactions and (ii) the singularity of the correlations for a given σ has the same structure at all temperatures. The results appear to be unaffected by fluctuations as indicated by Monte Carlo simulations for particular values of σ and T.

We expect that the mean-field theory is also correct for higher-dimensional systems where the fluctuations play an even smaller role. This problem is currently being investigated.

ACKNOWLEDGMENTS

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