Finite-size scaling of the Glauber model of critical dynamics

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We obtain the exact critical relaxation time $\tau_L(\xi)$, where ξ is the bulk correlation length, for the Glauber kinetic Ising model of spins on a one-dimensional lattice of finite length L for both periodic and free boundary conditions (BC's). We show that, independent of the BC's, the dynamic critical exponent has the well-known value $z=2$, and we comment on a recent claim that $z=1$ for this model. The ratio $\tau_L(\xi)/\tau_\infty(\xi)$, in the double limit $L,\xi\to\infty$ for fixed $x=L/\xi$, approaches a limiting functional form, $f_\tau(L/\xi)$, the finite-size scaling function. For free BC's we derive the exact scaling function $f_\tau(x)=[1+(\omega(x)/x)^2]^{-1}$, where $\omega(x)$ is the smallest root of the transcendental equation $\omega\tan(\omega/2)=x$. We provide expansions of $\omega(x)$ in powers of x and x^{-1} for the regimes of small and large x, respectively, and establish their radii of convergence. The scaling function shows anomalous behavior at small x, $f_\tau(x)\approx x$, instead of the usual $f_\tau(x)\approx x^z$, as $x\to 0$. This is because, even for finite L, the lifetime of the slowest dynamical mode diverges for $T\to$ 0 K. For periodic BC's, with the exception of one system, τ_L is independent of L, and hence $f_\tau=1$. The exceptional system, that with an odd number of spins and antiferromagnetic couplings, exhibits frustration at $T=0$ K, and the scaling function is given by $f_\tau(x)=[1+(\pi/x)^2]^{-1}$. [S1063-651X(96)07306-0]

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I. INTRODUCTION

The finite-size scaling (FSS) method [1] is a powerful technique for studying critical phenomena that is used [2,3] to extrapolate to the thermodynamic limit information obtained from systems of finite linear size L. Provided that the "bulk," thermodynamic limit $L\to\infty$ has been taken [4], as the temperature T approaches the critical temperature T_C the correlation length $\xi(T)$ diverges and thermodynamic quantities become singular. The bulk-system relaxation time $\tau_\infty(\xi)$ diverges in the critical region as ξ^z, where z is the dynamic critical exponent [5]. Adopting L and ξ as the basic thermodynamic variables, the FSS theory predicts that, for L and ξ sufficiently large compared to the lattice spacing d, the relaxation time $\tau_L(\xi)$ obtained for a finite system is related to $\tau_\infty(\xi)$ by

$$\tau_L(\xi)/\tau_\infty(\xi)=f_\tau(L/\xi), \tag{1.1}$$

where f_τ is the FSS function. According to (1.1), for a sequence of systems which differ in their individual values of L and ξ, but which have a common value of the *ratio* L/ξ, the corresponding ratios $\tau_L(\xi)/\tau_\infty(\xi)$ are also equal. One can thus identify the scaling function with the limiting value of $\tau_L(\xi)/\tau_\infty(\xi)$ for $L,\xi\to\infty$, subject to the constraint that the ratio $x\equiv L/\xi$ remains fixed. The scaling function f_τ is universal in the sense that it does not depend upon irrelevant operators (in the language of renormalization-group theory), but may depend on boundary conditions [6] (BC's). We note, however, that while the scaling function provides the *leading* behavior of $\tau_L(\xi)/\tau_\infty(\xi)$ when both L and ξ are sufficiently large compared to d, there are numerous correction terms involving d/L and d/ξ that are not included in (1.1). [See, for example, (2.25) and the discussion in Sec. II E.]

In numerical simulations it is often difficult to achieve the large-size regime necessary to extract reliable information about critical phenomena. Predictions could be made using (1.1) if one knew the form of the FSS function; however, it is rare that one has the exact form of the FSS function. The two cases $x\ll 1$ and $x\gg 1$ clearly correspond to vastly different physical regimes. The analytic form of f_τ will thus be quite different in these two regimes. Frequently, one's limited knowledge of f_τ is represented by the first few terms of separate expansions in an appropriate small quantity for either large or small x. The radius of convergence of each such expansion is determined by the singularities of f_τ in the complex x plane, which reflect global analytic properties of f_τ. Typically, some or even all of these singularities have little direct connection to the physics of the model, yet vitally determine the domain of validity of the series expansion representation of f_τ for regions of either small or large, real, positive x. This will be amply demonstrated in Sec. II C for the present model. Extrapolations to one regime of $f_\tau(x)$ based on a limited number of expansion terms appropriate to a second regime may thus prove problematic. It is of interest to note, therefore, that recently it has been demonstrated [3] for several model systems that FSS may be used to extrapolate Monte Carlo simulation data from the regime of relatively small systems, $x<1$, to the desired large-size regime, $x>1$, a point that we will discuss further in Sec. III.

In this paper we derive the exact FSS function f_τ associated with the critical relaxation time $\tau_L(\xi)$ for the Glauber [7] kinetic Ising model of spins on a one-dimensional (1D) lattice for both periodic and free BC's. This is an analytically tractable model of critical dynamics, and it is of considerable interest to have an exact expression for f_τ, since it can provide a testing ground or reference system for theories of the FSS function. We note that f_τ is conventionally taken [6] to have the following two *a priori* asymptotic limits: (i) $f_\tau(x)\to 1$ for $x\to\infty$, which follows simply from the definition of f_τ; and (ii) $f_\tau(x)\approx x^z$ for $x\to 0$. The latter result is based [6] on the assumption that, for finite L, the lifetime τ_L remains *finite* as $\xi\to\infty$, and in particular that $\tau_L(\infty)\approx L^z$. As we will show, however, this assumption does not usually hold for the 1D Glauber model for which $T_C=0$ K, since in most cases the dynamics stops (''freezes'') in this limit *independent of the size of the system*, and hence $\tau_L(\infty)$ is infinitely large *even if L is finite*. The single exceptional case, where $\tau_L(\infty)$ remains finite for finite L, features frustration at zero temperature.

In Sec. II we present the basic equation of motion satisfied by nonequilibrium single-spin averages in the 1D Glauber model. We then derive the exact spectrum of relaxation rates for the finite-size Glauber model. We first obtain the spectrum in the case where one assumes periodic BC's, i.e., where the system is given as a ring of spins. After that we obtain the spectrum for the more difficult case of free BC's, defined by (2.3), chosen in accord with the requirement of detailed balance. We remark that the finite ring of spins was explicitly treated in Glauber's original article [7]; the spectrum associated with free BC's is presented here for the first time to the best of our knowledge. Of key interest of course is λ_1, defined as the *smallest* relaxation rate allowed by the BC's, since this quantity controls the long-time critical response. We present detailed expressions for λ_1 for both periodic and free BC's. These results then enable us to establish the *exact* form of $f_\tau(x)$, and to consider the issue of extrapolation of results derived for $x<1$ to the regime $x>1$.

For periodic BC's, many properties of the Glauber model are well known [8,9], in particular that the bulk-system dynamic critical exponent z has the value $z=2$. As we will show, for periodic BC's one obtains, with one exception, that $\tau_L\sim\xi^2$, *independent of* L, and is thus *divergent* for $\xi\to\infty$. For these systems, then, the scaling function is trivial, $f_\tau\equiv 1$, since τ_L is independent of L. The exceptional case is the system with antiferromagnetic couplings and an *odd* number of spins. This system does not ''freeze'' at low temperature but instead exhibits frustration, with the consequence that the lifetime of the slowest dynamical mode remains finite, where we find that $\tau_L\sim L^2$ as $\xi\to\infty$. This is what may be termed ''normal'' scaling behavior: τ_L finite as $\xi\to\infty$, which, we recall, is the behavior in systems with $T_C\neq 0$. The anomalous behavior of τ_L for the other instances of the 1D Glauber model with periodic BC's arises because these systems do not exhibit frustration and simply freeze at low temperatures. In Sec. II C, we present the only nontrivial FSS function for periodic BC's, that for the frustrated system.

For free BC's, we find in all cases anomalous behavior of τ_L, again due to the lack of an opportunity to develop frustration at low temperature. For these BC's, however, we find, for fixed $L,\tau_L\sim\xi$ for $\xi\to\infty$, as opposed to $\tau_L\sim\xi^2$ for periodic BC's. In Sec. II C we obtain, in the double limit $L,\ \xi\to\infty$ for fixed $x=L/\xi$, the exact form of the FSS function for the system with free BC's, with the result

$$f_\tau(x)=(1+[\omega(x)/x]^2)^{-1}, \tag{1.2}$$

where $\omega(x)$ denotes the smallest real positive root of the transcendental equation

$$\omega\tan(\omega/2)=x. \tag{1.3}$$

The FSS function (1.2) applies for both ferromagnetic and antiferromagnetic couplings, and whether the number of spins is even or odd. We provide convergent power series expansions of $\omega(x)$ in powers of x and x^{-1} for the regimes of small and large x, respectively, and establish the radii of convergence of these expansions. We note that the one nontrivial FSS function for periodic BC's is of the form of (1.2), but with $\omega(x)=\pi$ for all x.

At first sight, the anomalous behavior of the relaxation time for free BC's appears to bear on the question of the dynamic critical exponent for this system. In Ref. [10], it was recently claimed that $z=1$ for this system, based on just this fact, that for finite $L,\tau_L\sim\xi$ as $\xi\to\infty$. We believe this claim is not warranted, for the following reason. The regime $L\ll\xi$ is not characterized by critical fluctuations; rather, this limit corresponds to the low-temperature, ''frozen'' regime of the finite system, and thus we believe it inappropriate to infer that $z=1$. In fact, we show in Sec. II D that in the *opposite* regime, $L\gg\xi\gg 1$, which *is* characterized by critical fluctuations, one actually obtains $\tau_L\sim\xi^2$ for free BC's. Additionally, an erroneous claim made in Ref. [10] is that one recovers $z=2$ only for the *infinite* system, $L\to\infty$, whereas in actuality $z=2$ for the finite system when $L\gg\xi$. In short, the dynamic critical exponent is independent of the BC's when the system is large enough for critical phenomena to manifest. A detailed discussion of this and other claims made in Ref. [10] is provided in Sec II E.

Our discussion in Sec. II D on the dynamic critical exponent is based on our explicit, exact results for the relaxation time, $\tau_L=\lambda_1^{-1}$. The broader, *qualitative* conclusion, however, that the dynamic critical exponent is independent of the BC's, can also be established on general grounds from the form of the equation of motion using well-known theorems of matrix analysis, without having to solve for the actual spectrum of relaxation rates. These general arguments concerning the influence of the BC's on the spectrum of relaxation rates are presented in Sec. II F.

Finally, in Sec. III we summarize our major conclusions and discuss the problematics of extrapolating the first *finite* number of terms of the expansion appropriate to the regime $x<1$ to the opposite regime $x>1$.

II. FINITE-SIZE GLAUBER MODEL

In this section we obtain the exact spectrum of relaxation rates associated with free and periodic BC's for the finite-size 1D Glauber kinetic Ising model. Of particular interest is the smallest relaxation rate λ_1, since that controls the long-time critical response. With these results, we then derive the exact FSS functions associated with each of the two BC's. Finally, we discuss the dynamic critical properties of this model in detail.

A. Equation of motion

We consider a 1D lattice of N Ising spins, $\sigma_n=\pm 1, 1\leqslant n\leqslant N$. The Ising model for free BC's is defined by the Hamiltonian,

$$H[\sigma]=-J\sum_{n=1}^{N-1}\sigma_n\sigma_{n+1}, \quad (2.1)$$

where J is exchange interaction energy. If instead we adopt periodic BC's, the upper limit of summation in (2.1) should be N with $\sigma_{N+1}\equiv\sigma_1$. Taking the lattice constant to be unity, the length L of the N-spin system is given by $L=N-1$ for the case of free BC's, whereas $L=N$ for periodic BC's. All equilibrium thermodynamic properties of this model can be obtained exactly, for both free and periodic BC's [11]. For our purposes we note the following. The infinite system ($L\to\infty$) has a critical point at $T_C=0$. The correlation length ξ is given by $\xi^{-1}=\ln[\coth(|K|)]$, independent of L and independent of the BC's, where $K\equiv J/k_BT$, and k_B is Boltzmann's constant. Note that the spin couplings are (anti)ferromagnetic for $K>(<)0$. In the critical region, ($|K|\to\infty$), ξ diverges as $\xi\sim\frac{1}{2}\exp(2|K|)$.

In the 1D Glauber mode [7] the basic equation of motion satisfied by single-spin, time-dependent nonequilibrium averages $s_n(t)$ is given by

$$-\frac{ds_n}{dt}=s_n-\frac{\gamma}{2}(s_{n-1}+s_{n+1}), \quad (2.2)$$

where $\gamma\equiv\tanh(2K)$ and $s_k(t)=\langle\sigma_k\rangle_t$, with the angular brackets denoting an average with respect to a nonequilibrium ensemble. Equation (2.2) defines, for $1\leqslant n\leqslant N$, the dynamical evolution of the system when periodic BC's are employed, i.e., $s_0\equiv s_N$ and $s_{N+1}\equiv s_1$. The equation of motion (2.2) is derived from the assumption that the nonequilibrium probability distribution satisfies a Markovian master equation satisfying detailed balance.

For free BC's, (2.2) applies for the interior spins, s_n, $2\leqslant n\leqslant N-1$, whereas additional dynamical equations must be posited for the ''end'' spins s_1 and s_N. In Ref. [10] these auxiliary dynamical equations were derived from the requirement of detailed balance, and are given by

$$-\frac{ds_1}{dt}=s_1-\beta s_2 \quad (2.3a)$$

and

$$-\frac{ds_N}{dt}=-\beta s_{N-1}+s_N, \quad (2.3b)$$

where $\beta\equiv\tanh(K)$. The form of (2.3) differs from that of (2.2) in that an end spin is coupled to only one nearest neighbor, whereas in the interior of the lattice a spin is coupled to its two nearest neighbors. Dynamical equations similar to (2.3) have been derived previously for the 1D Glauber model with anisotropic spin couplings [8], and in the context of a real-space renormalization-group analysis [9].

B. Eigenvalue spectrum

The eigenvalues and eigenvectors of the equation of motion can be found by means of the substitution

$$s_n=[A\exp(in\theta)+B\exp(-in\theta)]\exp(-\lambda t), \quad (2.4)$$

where A and B are constants and the eigenvalue λ is real and positive from general theorems pertaining to Markovian master equations satisfying detailed balance [12]. Using (2.4) in conjunction with (2.2), one obtains the dispersion relation

$$\lambda(\theta)=1-\gamma\cos\theta. \quad (2.5)$$

We can then restrict θ to be real, so that λ remains real, and to lie in the interval $[-\pi,\pi]$. The specific allowed values of θ within this interval are yet to be determined by the BC's. From (2.5), however, we can see that, even before we impose the BC's, the eigenvalue spectrum $\lambda(\theta)$ will be bounded between $1-|\gamma|$ and $1+|\gamma|$. We will find in all cases that the smallest eigenvalue λ_1 is either given by $1-|\gamma|$ for all finite L, or converges to it in the thermodynamic limit.

1. Periodic boundary conditions

It is easily shown that the assumption of periodic BC's leads to the requirement that the allowed values of θ in (2.5) are determined as the solutions of the equation $\cos(L\theta)=1$. This simple equation has N roots, $\theta=2\pi p/L$, for integer $p=0,1,\ldots,L-1$. In particular, for this choice of BC's, the allowed values of θ are independent of the temperature. Further, if θ satisfies $\cos(L\theta)=1$, then so does $2\pi-\theta$; hence the spectrum is symmetric about $\theta=\pi$. For ferromagnetic couplings $(\gamma>0)$, the smallest eigenvalue $\lambda_1=1-\gamma$ occurs for the root $p=0$, which is attained *independently* of the value of L. For antiferromagnetic couplings $(\gamma<0)$, the smallest eigenvalue $\lambda_1=1-|\gamma|$ occurs for $\theta=\pi$, i.e., $p=L/2$, which is attained for any *even* value of L. For these two cases, then, the value $\lambda_1=1-|\gamma|$ *is independent* of L, and hence the FSS function is trivial, $f_\tau\equiv1$.

For $\gamma<0$ and L *odd*, however, it is easily seen that $\lambda_1=1-|\gamma|\cos(\pi/L)$, which is achieved for both $p=(L\pm1)/2$. We will examine the form of f_τ for this exceptional case in Sec. II C1.

2. Free boundary conditions

For free BC's, the allowed values of θ are determined by requiring that the equations of motion (2.3) for the end spins be satisfied as well as that for the interior spins, (2.2). After some algebra, it can be shown that θ must satisfy the transcendental equation

$$\tan(L\theta)=\frac{-2\tilde{\xi}\tan\theta}{1-\tilde{\xi}^2\tan^2\theta}, \quad (2.6)$$

where $\tilde{\xi}\equiv\coth(\xi^{-1})$, with $\xi^{-1}=\ln[\coth(|K|)]$ the exact correlation length given above. It is easy to see that $\tilde{\xi}=\xi+(3\xi)^{-1}+O(\xi^{-2})$. To our knowledge, this is the first derivation of (2.6).

It can readily be shown that there are N nontrivial roots [13] of (2.6) in the open interval $0<\theta<\pi$. Furthermore, if θ is a root of (2.6), then so is $\pi-\theta$; the spectrum of roots of (2.6) is therefore symmetric about $\theta=\pi/2$. Using this fact, it follows that $\lambda_1=1-|\gamma|\cos\theta_1$, where θ_1 is the smallest root of (2.6), independent of the sign of K.

C. Exact scaling functions

We now determine the FSS function f_τ associated with the relaxation time $\tau_L = \lambda_1^{-1}$, where λ_1 is the smallest of the eigenvalues (2.5) consistent with the specified BC's. For periodic BC's the analysis is quite simple. However, as we see below, for free BC's the full analysis becomes somewhat intricate.

1. Periodic boundary conditions

We have seen in Sec. II B 1 that for periodic BC's we have $\lambda_1 = 1 - |\gamma|$, with the one exception that for antiferromagnetic interactions and an odd number of spins, $\lambda_1 = 1 - |\gamma|\cos(\pi/L)$. Clearly, for all cases we have

$$\tau_\infty = (1 - |\gamma|)^{-1}, \tag{2.7}$$

and it follows that, except for the ring with an odd number of spins and antiferromagnetic couplings, $\tau_L/\tau_\infty = 1$, independent of L, and thus $f_\tau \equiv 1$.

For the exceptional system, which as discussed in Sec. I exhibits frustration at low temperature, we may write

$$\tau_L/\tau_\infty = \left[1 + \sin^2(\theta_1/2)\sinh^{-2}\left(\frac{1}{2\xi}\right)\right]^{-1}, \tag{2.8}$$

where $\theta_1 = \pi/L$. In writing (2.8) we have used the fact that

$$\frac{1-|\gamma|}{2|\gamma|} = \sinh^2\left(\frac{1}{2\xi}\right). \tag{2.9}$$

Note from (2.8) that τ_L/τ_∞ is *not* in general of the form asserted by the FSS theory, (1.1). Strictly speaking, τ_L/τ_∞ is a function of the single variable x *only* for the double limit, $L, \xi \to \infty$, subject to the constraint that $x = L/\xi$ is kept fixed, and we have

$$f_\tau(x) = [1 + (\pi/x)^2]^{-1}. \tag{2.10}$$

However if both $L > 5$ and $\xi > 5$, we may approximate (2.8) by (2.10). Note that (2.10) displays the ''normal'' behavior discussed in Sec. I, namely $f_\tau(x) \to x^z$ as $x \to 0$, with $z = 2$.

2. Free boundary conditions

For the case of free BC's, one finds that (2.8) continues to apply; however, θ_1 now denotes the smallest root of the transcendental equation (2.6) in the open [13] interval $(0,\pi)$. We can simplify our task of determining θ_1 by noting, using double-angle formulas, that the complete set of roots of (2.6) in the above interval coincide with the combined set of roots obtained by separately solving

$$\tanh(\xi^{-1})\cot(L\theta/2) = \tan\theta \tag{2.11}$$

and

$$\tanh(\xi^{-1})\tan(L\theta/2) = -\tan\theta, \tag{2.12}$$

again for values of θ in the interval $(0,\pi)$. However, for determining θ_1, only (2.11) is of relevance. This is because the smallest root of (2.11) necessarily lies in the θ interval $(0,\pi/L)$, since for this interval the cotangent function spans the range $(0,\infty)$ while the right-hand side of the equation remains positive. By contrast, for this same θ interval (2.12) has no solution since the left-hand side is positive whereas the right-hand side is negative. We now introduce the variable $\omega(x,L) \equiv L\theta_1$, where, from (2.11), ω is to be found as the root of the equivalent equation

$$\tan(\omega/L)\tan(\omega/2) = \tanh(\xi^{-1}) \tag{2.13}$$

in the interval $(0,\pi)$. The corresponding formula for τ_L/τ_∞ is given by

$$(\tau_L/\tau_\infty)^{-1} = 1 + \sinh^{-2}\left(\frac{1}{2\xi}\right)\sin^2\left(\frac{\omega}{2L}\right), \tag{2.8$'$}$$

which is formally similar to (2.8).

Clearly, for arbitrary *finite* values of L and ξ, the root ω of (2.13) is a function of both independent variables, and not solely a function of their ratio. The same remark thus applies to τ_L/τ_∞. However, when we apply the double limit $L, \xi \to \infty$ with x remaining fixed, (2.8′) becomes

$$f_\tau(x) = (1 + [\omega(x)/x]^2)^{-1}, \tag{2.14}$$

and (2.13) yields $\omega(x) \equiv \omega(x,\infty)$, a function of the single variable x, as the root of the transcendental equation

$$\omega\tan(\omega/2) = x. \tag{2.15}$$

Equations (2.14) and (2.15) should provide excellent approximations to τ_L/τ_∞ and $\omega(x,L)$ as long as $L > 5$ and $\xi > 5$. Using Eq. (2.15) one may also write f_τ as

$$f_\tau(x) = \tfrac{1}{2}[1 - \cos\omega(x)]. \tag{2.14$'$}$$

In Fig. 1, we show results for the root $\omega(x,L)$ of (2.13) for $L = 5$ and 10, respectively, as well as for the infinite system, obtained by solving (2.15) numerically. In accord with our previous discussion, the root $\omega(x,5)$ is barely distinguishable from $\omega(x)$ for $x < 1$ $(\xi > 5)$. The same holds for $\omega(x,10)$ as long as $x < 2$.

Equations (2.14) and (2.15) provide the *exact* FSS function for the 1D Glauber model with free BC's. We remark

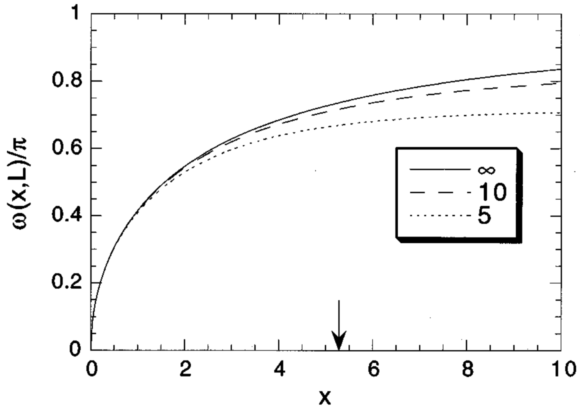

FIG. 1. The solid curve is the auxiliary function $\omega(x)$ for free boundary conditions in the double limit $L, \xi \to \infty$, for fixed $x = L/\xi$, as obtained by solving (2.15) using numerical methods. The finite-size scaling function $f_\tau(x)$ is given in terms of $\omega(x)$ according to (2.14). The arrow indicates the radius of convergence, $R = 5.2794\ldots$, of the series expansion (2.18) in ascending powers of x. Similarly, expansion (2.23), in ascending powers of x^{-1}, converges for $|x| > R$. Also shown are the roots $\omega(x,L)$ vs x for systems of length $L = 5$ and 10, respectively.

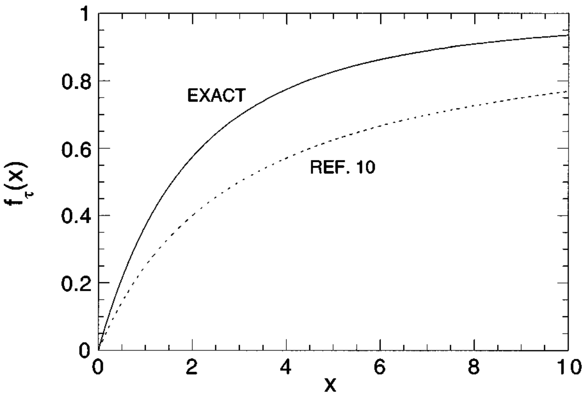

FIG. 2. The exact finite-size scaling function $f_\tau(x)$ vs $x=L/\xi$ for free boundary conditions, given by (2.14) in conjunction with (2.15), shown as the solid curve. The dashed curve is the corresponding result given in Ref. [10].

that this result applies for an even or odd number of spins and regardless of whether the interactions are ferromagnetic or antiferromagnetic. Note that (2.10), the only nontrivial scaling function for periodic BC's, is of the form of (2.14), but with $\omega(x)=\pi$ for all x. For free BC's we must first solve (2.15) for the root $\omega(x)$ before $f_\tau(x)$ is fully specified. Analytically, it is straightforward to develop the leading terms

$$\omega(x)\to\sqrt{2x}\quad (x\ll 1) \tag{2.16}$$

and

$$\omega(x)\to\pi\quad (x\gg 1). \tag{2.17}$$

For intermediate values of x we provide power-series expansions for $\omega(x)$ below. Combining (2.16) with (2.14), it can be seen that $f_\tau(x)\to x$ as $x\to 0$, and thus the FSS function associated with free BC's does not exhibit the conventional limiting behavior $f_\tau\to x^z$. As discussed in Sec. I, this anomalous behavior of f_τ is related to the freezing of the system at low temperature.

A plot of the resulting scaling function $f_\tau(x)$ from (2.14), having used our numerical data for $\omega(x)$, is shown in Fig. 2. In Fig. 2 we also display the results of Ref. [10]. The latter deviates significantly from our exact results. As we discuss in Sec. II E, the results of Ref. [10] were obtained through an unjustified extrapolation of a series expansion result outside its domain of validity. This underscores the need to carefully establish the radius of convergence of series expansions of $\omega(x)$. In the following, we derive expansions of $\omega(x)$ in powers of x and x^{-1} for the regimes of small and large x, respectively, and establish their radii of convergence. These expansions are superfluous for the purpose of creating the data shown in Fig. 2. However, in the course of deriving these expansions we will obtain considerable information concerning the analytic properties of $\omega(x)$ in the complex x plane. As discussed in Sec. III, the analytic properties of $\omega(x)$ are of crucial importance to any effort to extrapolate results obtained for the regime of small x to that of large x (or vice versa).

a. Power series in x. We have utilized the MAPLE computer algebra system to develop an expansion of the root ω of (2.15) about the point $x=0$. Our procedure consisted of substituting in (2.15) an arbitrary number of terms of the series expansion of $\tan(\omega/2)$ in powers of ω, and then reverting the equation so as to obtain ω as a function of x. In this manner we arrived at

$$\omega(x)=\sqrt{2x}\left[1-\tfrac{1}{12}x+\tfrac{11}{1440}x^2-\tfrac{17}{40\,320}x^3-\tfrac{281}{9\,676\,800}x^4+\tfrac{44\,029}{3\,832\,012\,800}x^5+\cdots\right]. \tag{2.18}$$

Here we list only the first six terms, although in practice we have generated a large number of additional terms.

The most efficient method for determining the radius of convergence, R, of the power series in (2.18) is to note that this quantity can be identified with the smallest value of $|x|$, other than $x=0$, that corresponds to a singularity of $\omega(x)$ in the complex x plane. To determine the singularities of $\omega(x)$ we first define the function $\Omega(\omega)\equiv\omega\tan(\omega/2)$, so that, using (2.15), $d\omega/dx=1/\Omega'(\omega)$. It follows that the singularities of $\omega(x)$, branch points, are those values of x associated with the zeros of $\Omega'(\omega)$. Now $\Omega'(\omega)=0$ if $\omega+\sin\omega=0$. With the exclusion of $\omega=0$, all roots of the latter equation are complex. Moreover, if $\omega=\rho+i\sigma$ is a zero of $\Omega'(\omega)$, where ρ and σ are real and positive, then so are $\rho-i\sigma, -\rho+i\sigma$, and $-\rho-i\sigma$. Furthermore, these four zeros of $\Omega'(\omega)$ correspond to complex-conjugate pair values of x, the singularities of $\omega(x)$, namely $\Omega(\omega)$ and $[\Omega(\omega)]^*$, since $\Omega(-\omega)=\Omega(\omega)$ and $\Omega(\omega^*)=[\Omega(\omega)]^*$. Clearly it is sufficient to search for the zeros of Ω' in the first quadrant of the ω plane. Note also that upon using (2.14′) we have $df_\tau/dx=\frac{1}{2}(\sin\omega)d\omega/dx$. Hence the singularities of $f_\tau(x)$ coincide with those of $\omega(x)$.

We may summarize as follows: Excluding $\omega=0$, which corresponds to $x=0$, in the following the quantity ω_n will denote the nth zero of $\Omega'(\omega)$ in the first quadrant in the ω plane, and the corresponding branch point singularity of $\omega(x)$, to be denoted by x_n, is given by $x_n=\Omega(\omega_n)$. Our task thus consists of determining the ω_n and the corresponding x_n, and then noting that $R=\min(|x_n|)$.

MAPLE proved extremely useful for carrying out the actual numerical calculations; however, it was necessary to provide suitable input information concerning the approximate location of the roots ω_n. A straightforward analysis shows that the equations determining ω_n, for $n=0,1,2\ldots$, are given by

$$\omega_n=(2n+1)\pi+r_n+i\sigma_n, \tag{2.19}$$

where both r_n and σ_n are real and positive and satisfy the coupled nonlinear equations

$$r_n=\cos^{-1}(\sigma_n/\sinh\sigma_n), \tag{2.20}$$

and

$$\sigma_n=\cosh^{-1}\left[\frac{(2n+1)\pi+r_n}{\sin r_n}\right]. \tag{2.21}$$

Note that $0<r_n<\pi/2$. In particular, there are an *infinite* number of roots ω_n in the first quadrant, and each of these corresponds to a singularity $x_n=\Omega(\omega_n)$ of $\omega(x)$. It turns out that the (symmetric) pair of singularities lying closest to the origin of the x plane occur for $n=0$, and these are given by x_0 and x_0^*, where $x_0=-3.301\,222\,589+i4.119\,962\,917$.

Thus, $R=|x_0|=5.279\,409\,5$. The corresponding value of ω_0 is given by $\omega_0=4.212\,392\,238+i2.250\,728\,636$.

The fact that the singularities in the x plane are removed from both the real and imaginary axes is responsible for the absence of any hint in both Figs. 1 and 2 that the series (2.14) and (2.18) converge only $|x|<R$. This is also the cause of the irregular pattern in the variation in the signs of the expansion coefficients in (2.18), especially those not listed but which we have generated using MAPLE. Clearly there is no obvious direct connection between the physics of this system and the value of the radius of convergence. The latter reflect global analytic properties of the function $\omega(x)$ throughout the complex x plane, whereas the FSS function uses the solution of (2.15) only for real positive x. We will comment on the broader implication of these results in Sec. III.

b. Power series in x^{-1}. Inspecting (2.15), and as noted in (2.17), for large positive values of x, the function $\omega(x)$ approaches the value π from below. To develop an expansion of $\omega(x)$ in powers of x^{-1}, we first rewrite (2.15) as

$$\frac{\tan[(\pi-\omega)/2]}{\pi-(\pi-\omega)}=\frac{1}{x}, \tag{2.22}$$

and use MAPLE to expand the left-hand side in powers of the small quantity $\pi-\omega$, and then revert so as to obtain the latter quantity in powers of the small quantity x^{-1}. The final result is

$$\frac{\omega}{\pi}=1-2x^{-1}+4x^{-2}-\tfrac{2}{3}(12-\pi^2)x^{-3}-\tfrac{16}{3}(\pi^2-3)x^{-4} -\tfrac{2}{15}(3\pi^4-200\pi^2+240)x^{-5}+\cdots. \tag{2.23}$$

Determination of the radius of convergence of this series provided a serious challenge. General theorems [14] relating to Lagrange's method of series reversion proved insufficient because of the fact that ω is a multivalued function of x possessing an infinite number of branches. These theorems relate to the *totality* of branches of $\omega(x)$, rather than to any individual branch. More specifically, in principle the above branch of $\omega(x)$, which equals π as one approaches the origin of the x^{-1} plane, could have singularities at any of the points x_n^{-1}, where the x_n were introduced in Sec. II C 2 a. Now the sequence of values $|x_n|$ grows without bound for $n\to\infty$. Hence, *in principle*, the radius of convergence of the expansion (2.23) might be identically zero. In practice, however, R might be as large as $|x_0^{-1}|$, if the other values of $|x_n^{-1}|$ are not singular points of the given branch. One can put the question as follows: What is the location of the singularity, lying closest to the origin in the x^{-1} plane, of the specific branch of interest? To our knowledge, general theorems in the mathematical literature do not address this question.

What ultimately proved successful for us was to explicitly determine, using graphical techniques offered by MAPLE, the domain of the conformal mapping of a family of concentric circles and the corresponding family of orthogonal, diverging rays with respect to the point $\omega=\pi$ using (2.22). In this empirical manner, we found that the pair of points lying closest to the origin in the x^{-1} plane for which the mapping (2.22) is *not* conformal are approximately given by $-0.12\pm i0.15$. These numerical values allow us to identify this closest pair of singularities with x_0^{-1} and $(x_0^{-1})^*$. We may therefore conclude that the power series (2.23) converges if $|x|>5.279\,410$. We have no doubt that our finding, based on graphical methods, could be confirmed by an elegant and rigorous proof, even though we did not succeed in our attempts to do so.

D. Dynamic critical exponent

The dynamic scaling hypothesis [5] states that, *in the critical region*, the smallest relaxation rate λ_1 vanishes with the correlation length ξ as $\lambda_1\sim\xi^{-z}$. We identify the critical region as satisfying the inequalities $L\gg\xi\gg1$. We will find that $z=2$ for the Glauber model, independent of the BC's. In Sec. II E we comment on a recent claim [10] that $z=1$ for this model with free BC's.

1. Periodic boundary conditions

As we have seen in Sec. II B 1, with the exception of the ring with an odd number of spins and antiferromagnetic interactions, $\lambda_1=1-|\gamma|$ independent of L. We can rewrite this using (2.9), with the result $\lambda_1=\tanh[(2\xi)^{-1}]\tanh(\xi^{-1})$. Hence, in the critical region, $\lambda_1\sim\frac{1}{2}\xi^{-2}$, independent of the size of the ring, and we have $z=2$.

For the one exceptional case, we found previously that $\lambda_1=1-|\gamma|\cos(\pi/L)$. In the regime where both L and ξ are large compared to the lattice constant, we have, to leading order, $\lambda_1\approx\frac{1}{2}(\xi^{-2}+\pi^2L^{-2})$. Obviously, for $L\gg\xi,\lambda_1\approx\frac{1}{2}\xi^{-2}[1+(\pi\xi/L)^2]$, and so $z=2$. Hence we obtain the result $z=2$ for *all* cases of periodic BC's. We note that, for the opposite regime, $\xi\gg L,\lambda_1\approx\frac{1}{2}L^{-2}[\pi^2+(L/\xi)^2]$. As we have stated previously, this is the one instance of the 1D Glauber model that exhibits "normal" scaling behavior, where, for finite L, $\lambda_1\sim L^{-z}$ as $\xi\to\infty$.

2. Free boundary conditions

We found in Sec. II B 2 that, independent of the sign of the coupling constant, $\lambda_1=1-|\gamma|\cos\theta_1$, where θ_1 is the smallest root of (2.6). We then showed in Sec. II C that θ_1 is equivalent to the root ω of (2.13) in the interval $(0,\pi)$, where $\omega=L\theta_1$. An alternate, exact expression for λ_1 can thus be given in terms of ω,

$$\lambda_1(L,\xi)=\tanh\left(\frac{1}{2\xi}\right)\tanh\left(\frac{1}{\xi}\right)\left[1+\sinh^{-2}\left(\frac{1}{2\xi}\right)\sin^2\left(\frac{\omega}{2L}\right)\right]. \tag{2.24}$$

In the critical regime, $L\gg\xi\gg1$, it suffices to use (2.23) and in particular to replace ω by π, even though that equation was derived under the assumption that $L,\xi\to\infty$ for a fixed value of L/ξ. We find, to leading order, $\lambda_1\approx\frac{1}{2}\xi^{-2}[1+(\pi\xi/L)^2]$. Once again we conclude that $z=2$, just as we obtained for periodic BC's.

E. Comparison with Ref. [10]

In this section we compare our results with those obtained in Ref. [10] for the case of free BC's. We will show that the major conclusions of that work are flawed, since they are based on an unjustified extrapolation of results valid exclusively in the regime $L \ll \xi$, to *all* values of L/ξ. This includes the unwarranted conclusion that the dynamic critical exponent is given by $z=1$, contradicting our result $z=2$ given in Sec. II D, as well as an erroneous form for the FSS function listed below (see also Fig. 2).

We have found that for sufficiently small values of $x=L/\xi$, the quantity $\lambda_1(L,\xi)$ may be expanded as

$$\lambda_1(L,\xi)=L^{-2}\sum_{n=0}^{\infty} P_n(L^{-2})x^{n+1}, \tag{2.25}$$

where $P_n(u)$ is a polynomial of degree n in the variable u. We list here the first five polynomials P_n, which we have obtained using MAPLE,

$$P_0(u)=1,\ P_1(u)=(2-5u)/6,\ P_2(u)=(2-40u+53u^2)/90,$$

$$P_3(u)=-(16+924u-3276u^2+2651u^3)/7560, \tag{2.26}$$

$$P_4(u)=(8-1360u+20\,664u^2-37\,640u^3+19\,273u^4)/113\,400.$$

Equations (2.25) and (2.26) were derived by first developing $\omega(x,L)$, the solution of (2.13) for finite L, as an expansion in L/ξ, substituting that expansion in (2.24), and then expanding (2.24) as a power series in x. A useful check on the polynomials $P_n(u)$ can be had by noting that $P_n(1)=(-1)^n/(n+1)!$, which follows from the fact that $\lambda_1(1,\xi)=1-\exp(\xi^{-1})$, as can easily be shown. A further consistency check can be had if we use (2.25) to consider $\lambda_1(L,\xi)/\lambda_1(\infty,\xi)$ in the double limit $L,\xi\to\infty$ for a fixed, but sufficiently small value of $x=L/\xi$. Using $\lambda_1(\infty,\xi)$ from (2.24), and comparing with (2.14), the following result must hold, again for sufficiently small x:

$$2\sum_{n=0}^{\infty} P_n(0)x^{n-1}=1+[\omega(x)/x]^2. \tag{2.27}$$

Using the expansion (2.18) for $\omega(x)$, we have used MAPLE to verify this relation between the values of $P_n(0)$ and the values of the expansion coefficients in (2.18). Equation (2.27) therefore holds for $|x|<R=5.297\ldots$, the radius of convergence of (2.18).

We now discuss in detail the procedures invoked in Ref. [10]. In that work, the first two terms of (2.25) are correctly given; no further terms are listed, however. Even though it is stressed in Ref. [10] that these are but the first two terms of an expansion for $\lambda_1(L,\xi)$, arrived at by considering $L\ll\xi$, these terms are nonetheless (erroneously) extrapolated to the thermodynamic limit, $L\to\infty$, for fixed finite ξ. Let us consider the consequences of this extrapolation procedure. Based on just the first two terms of (2.25), one might conclude, along with Ref. [10], that to leading order $\lambda_1(\infty,\xi)=\frac{1}{3}\xi^{-2}$. We note, however, that this seemingly sensible result for λ_1 is actually invalid, since it lies outside the allowed spectrum of relaxation rates for the Glauber model (2.5), i.e., $\frac{1}{3}\xi^{-2}<1-|\gamma|\approx\frac{1}{2}\xi^{-2}$. Moreover, to be consistent, if we were to extrapolate the third, fourth, and all further terms in (2.25), it is readily seen that this procedure yields the patently nonsensical result $\lambda_1(\infty,\xi)=\infty$, in contradiction with the correct result, $\lambda_1(\infty,\xi)\approx\frac{1}{2}\xi^{-2}$, appropriate to the critical regime $L\gg\xi\gg1$. Of course the origin of this incorrect, divergent result for $\lambda_1(\infty,\xi)$ is the invalid procedure utilized in Ref. [10] of extrapolating $L\to\infty$, since (2.25) is only valid for the opposite limit $L\ll\xi$. As we have seen in Sec. II C 2, entirely different expansions [see (2.18) and (2.23)] apply for the two regimes $L\ll\xi$ and $L\gg\xi$.

In Ref. [10], the first two terms of (2.25) were also used to construct their version of the FSS function, $f_\tau(x)$ for *arbitrary* values of x, with the result $f_\tau(x)=x/(3+x)$. Note that even for the regime $L\ll\xi$, the result of Ref. [10] ($f_\tau\to x/3$) disagrees with the correct limiting form $f_\tau\to x/2$ that we obtain from our exact result (2.14) in the small-x regime. This discrepancy is due to the use in Ref. [10] of the incorrect value $\lambda_1(\infty,\xi)=\frac{1}{3}\xi^{-2}$. Moreover, for all other, larger values of x there is significant disagreement between our exact result for $f_\tau(x)$ and that given in Ref. [10], as can be seen in Fig. 2.

Finally, returning to (2.25), we have to leading order, $\lambda_1\approx(L\xi)^{-1}$ when $L\ll\xi$. This fact was used in Ref. [10] to conclude, incorrectly, that $z=1$. That conclusion is specious since, as we have stressed above, it is misleading to associate critical phenomena with this regime. The dynamic critical exponent can be inferred only by studying the behavior of λ_1 in the opposite regime, $L\gg\xi\gg1$, where (2.25) no longer applies. As we have seen in Sec. II D, the analysis for that regime yields $z=2$.

F. Role of boundary conditions

In the preceding we have shown, using our explicit results for λ_1, that the dynamic critical exponent is given by $z=2$ for both periodic and free BC's. It is of interest to show that the same *qualitative* conclusion, that the dynamic critical exponent is independent of the BC's, can be obtained without explicitly calculating λ_1, by invoking a powerful theorem of Ledermann [15] for Hermitian matrices that is well known in the theory of lattice dynamics.

Our starting point is to note that the equations of motion (2.2), together with the periodic BC's, are equivalent to the matrix equation

$$\frac{d}{dt}S=-\mathbf{M}\cdot S, \tag{2.28}$$

where S is the N-dimensional vector $S=(s_1,\ldots,s_N)$, and $\mathbf{M}$ is the real symmetric NxN matrix, whose only nonzero elements are given by $M_{k,k}=1$ along the diagonal, $1\leqslant k\leqslant N$, $M_{k,k+1}=M_{k+1,k}=-\gamma/2$ along the super diagonals and subdiagonals, $1\leqslant k\leqslant N-1$, and $M_{1,N}=M_{N,1}=-\gamma/2$ in the "corners" of the matrix. The eigenvalue spectrum was given in Sec. II B 1 as $\lambda=1-\cos(2\pi p/N)$ for integer p, $0\leqslant p\leqslant N-1$. Note that for very large N, this spectrum is dense throughout the interval $[1-|\gamma|,1+|\gamma|]$.

For free BC's, (2.28) continues to apply, except that $\mathbf{M}$ is replaced by an $N\times N$ real tridiagonal matrix $\mathbf{M}'$, identical to $\mathbf{M}$, except that $M'_{1,2}=M'_{N,N-1}=-\beta$ and the corner elements $M'_{1,N}=M'_{N,1}=0$. Note that $\mathbf{M}'$ is not symmetric as it stands; in fact it is a real "quasisymmetric" tridiagonal matrix. As such, $\mathbf{M}'$ can be cast into symmetric form using a similarity transformation given in Ref. [16], $\mathbf{M}'\rightarrow\bar{\mathbf{M}}'=\mathbf{PM}'\mathbf{P}^{-1}$. The matrix $\bar{\mathbf{M}}'$ is identical to $\mathbf{M}'$, except for the four elements $\bar{M}'_{1,2}=\bar{M}'_{2,1}=\bar{M}'_{N-1,N}=\bar{M}'_{N,N-1}=-\alpha$, where $\alpha=\beta/\sqrt{1+\beta^2}$.

Now the key point is that the pair of Hermitian matrices $\mathbf{M}$ and $\bar{\mathbf{M}}'$, corresponding, respectively, to periodic and free BC's, differ by only four rows, the top two and bottom two; otherwise they are identical. As applied to the present situation, the Ledermann theorem states that within any interval of the real line, the number of eigenvalues of $\mathbf{M}$ can differ by at most eight (twice the number of differing rows) from those of $\bar{\mathbf{M}}'$. This has the immediate consequence that in the limit of large N, the smallest eigenvalue of $\bar{\mathbf{M}}',\lambda_1'$, cannot be separated by an interval of *finite* width from the smallest eigenvalue of $\mathbf{M}$, namely $\lambda_1=1-|\gamma|$. These considerations prove that as $N\rightarrow\infty$ the smallest eigenvalue for the case of free BC's coincides with the smallest eigenvalue for the case of periodic BC's, and hence that the dynamic critical exponent is independent of the BC's in the thermodynamic limit.

III. SUMMARY

In this paper we have investigated the finite-size scaling behavior of the critical relaxation time $\tau_L(\xi)$ for the Glauber kinetic Ising model of spins on a 1D lattice of finite length L, where ξ is the bulk correlation length, for both periodic and free BC's and for ferromagnetic and antiferromagnetic interactions. We have seen that the ratio $\tau_L(\xi)/\tau_\infty(\xi)$ becomes a function f_τ of the single variable L/ξ in the double limit $L,\xi\rightarrow\infty$, with the ratio $x=L/\xi$ held fixed, and we have determined the exact form of $f_\tau(x)$ for each choice of BC's in Sec. II. Having established f_τ for all x, it follows that (1.1) provides a good approximation to $\tau_L(\xi)$ when both of the inequalities $L/d>5$ and $\xi/d>5$ apply, where d is the lattice constant. We are not familiar with any other model of critical dynamics for which the exact form of the FSS function has been determined.

The dynamic scaling hypothesis [5] states that the *bulk* relaxation time $\tau_\infty(\xi)$ scales as ξ^z for large ξ, where z is the dynamic critical exponent. In Sec. II we have emphasized that the nominal critical region for the *finite* system should be identified with the regime $L\gg\xi\gg d$. In this regime one can expect that $\tau_L(\xi)$ also scales as ξ^z. We have explicitly confirmed that, for the 1D Glauber model, in the regime $L\gg\xi\gg d$, $\tau_L(\xi)$ scales as ξ^2, independent of the BC's and independent of the sign of the coupling constant, yielding $z=2$, the well-known value of the dynamic critical exponent for the bulk system. In Sec. II F we have used a well-known theorem from the theory of lattice dynamics to provide an explanation for the fact that $\tau_L(\xi)$ scales as ξ^2 irrespective of the specific BC employed. In particular, we showed that in the thermodynamic limit the smallest relaxation rate, and hence the dynamic critical exponent, is unaffected by a change in BC's. In Sec. II E we discussed in detail the results of Ref. [10], and in particular the claim that $z=1$ for this model. We showed that this conclusion is inappropriate since it was arrived at for the *opposite* regime, $L\ll\xi$, which is not the nominal critical region for a finite system.

The FSS function $f_\tau(x)$ is conventionally expected to vanish as x^z in the small-x limit [6]. That is, $\tau_L(\xi)$ is assumed to scale as L^z for finite L in the regime $L\ll\xi$. This expectation, however, is not generally fulfilled for the present model. For periodic BC's we find, with one exception, that for fixed, finite L, $\tau_L\sim 2\xi^2$ as $\xi\rightarrow\infty$, whereas for free BC's we find, again for fixed L, that $\tau_L\sim L\xi$ as $\xi\rightarrow\infty$. This anomalous behavior, of $\tau_L(\xi)$ becoming divergent as $\xi\rightarrow\infty$ for *finite* L, is related to the fact that the critical temperature $T_C=0$ for this system. Even for finite L, the dynamics stops in the low-temperature limit, and $\tau_L(\xi)$ diverges as $\xi\rightarrow\infty$. Note that this low-temperature ''freezing'' of the dynamics for the finite system is not a critical effect. The dynamics stops in this limit because the finite system can attain its lowest-energy ground state, and hence the single-spin relaxation time diverges. The one exceptional system (that with periodic BC's, antiferromagnetic interactions, and an odd number of spins) cannot attain a ground-state configuration. This system exhibits frustration as $T\rightarrow 0$ K, and the lifetime of the slowest mode remains finite as $\xi\rightarrow\infty$. Indeed, for this one system we have $\tau_L\sim L^2$ as $\xi\rightarrow\infty$, in agreement with the conventional expectation.

The form of the FSS function is rather intricate in the case of free BC's. In particular, the result of (2.14) involves the function $\omega(x)$, which is a solution of the transcendental equation (2.15). As shown in Sec. II C 2, this function possesses an infinite number of branch points in the complex x plane. As a result of these singularities, the series expansion (2.18) in powers of x converges only for $|x|<R=5.2794\ldots$, whereas the expansion (2.23) in powers of x^{-1} converges only for $|x|>R$.

These considerations hint of a potentially serious lesson that can be inferred for the FSS for other specific model systems. In essence, FSS implicitly provides a hopeful message, that knowledge of the properties of a system for $\xi\gg L\gg d$ can be used to infer properties in the regime $L\gg\xi\gg d$. This message is warranted as long as one can establish the major properties of the FSS function throughout the complex x plane. In particular, the presence of mathematical singularities, such as those manifested for the 1D Glauber model with free BC's, must be expected to play an important role in any efforts to extrapolate to the regime $x\gg 1$ results derived for the opposite regime, $x\ll 1$. To use the present model as a specific example, suppose that one is informed about (2.14) and the six terms displayed in (2.18) derived for the regime $\xi\gg L\gg d$, but that one is unaware of (2.15) and the expansion (2.23). *With such limited information, to what extent can one make useful inferences for this model regarding the behavior of* $\tau_L(\xi)$ *for the opposite regime* $L\gg\xi\gg d$? (As discussed in Sec. II E, it was precisely this, unjustified, extrapolation of the first few terms of an expansion appropriate to the regime $\zeta\gg L\gg d$ to the regime $L\gg\zeta\gg d$ that led in Ref. [10] to incorrect results for the dynamic explicit exponent of the FSS function.) Unfortunately, without a comprehensive study the correct answer to this question is, virtually nothing. Elsewhere [17] we present just such a study for the present model in the context of Padé approximants. More generally, the global analytic properties of the FSS function must be carefully considered and accounted for before any proposal for extrapolation to large values of x can be regarded as credible.

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