Relaxation in $S=1/2$ quantum spin chains: The role of second neighbor interactions

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Most of the existing dynamical studies in one dimension on magnetic insulators have considered the simplest spin models with nearest-neighbor interactions. In *real* systems, however, it is possible that longer range interactions are not entirely negligible. It is expected that the inclusion of next-nearest-neighbor interactions between spins in one-dimensional spin models will introduce a multitude of *new* frequencies in addition to the ones already present in the dynamics that arises due to nearest-neighbor interactions. We first present an *exact solution* for the dynamical xx-spin-pair correlations in an Ising chain with both nearest- and next-nearest-neighbor interactions to confirm our expectation. We next show, via an approximate analytical calculation, that the dynamical zz-spin-pair correlations in the next-nearest-neighbor transverse Ising chain when plotted as a function of time is noticeably different with respect to the exactly solvable nearest-neighbor transverse Ising chain at $T\to\infty$ when the next-nearest-neighbor interaction is $>\frac{1}{2}$ of the magnitude of the nearest-neighbor interaction. The effects could be fairly subtle in the time domain representation and in the spectral function when these additional interactions are weak (i.e., $<\frac{1}{2}$ of the nearest-neighbor interaction magnitude). The general conclusions reached in this work are expected to be valid for other simple quantum spin models such as the XY and XXZ models in one dimension.

I. INTRODUCTION

The study of the time-dependent behavior of simple quantum spin systems, especially in one dimension, has seen considerable progress within the past couple of decades.[1–4] A significant amount of literature consisting of experimental[5,6] and theoretical work now exists on the dynamical behavior of the transverse Ising model which is regarded as one of the simplest quantum spin systems with nontrivial spin dynamics.[7–13] The dynamical correlations in the $s=1/2$ XY (Refs. 14–17) and XXZ models[18–23] have also been studied in much detail at $T=0$ and at $T=\infty$. In addition, there also exists a handful of *exact* results that are available for the transverse Ising and XY models[8,9,14–17] in one dimension. Very little, however, is known about the dynamical spin-pair correlations in two and three dimensions.[10–13,23,24] All of the theoretical studies mentioned above have been carried out for quantum spin Hamiltonians with nearest-neighbor interactions. In this work we shall focus our attention on the extent to which spin dynamics is sensitive to the inclusion of next-nearest-neighbor interactions in one-dimensional systems.

In *real* magnetic systems it is quite possible that the spin-spin interactions may not be precisely nearest neighbor in nature. While the nearest-neighbor interaction may be the dominant interaction the second- and third-neighbor interactions may be weak but non-negligible. While ignoring these weak longer-range interactions may be adequate for studying the equilibrium critical properties of quantum spin models,[25] it does not necessarily follow that the same would be true for their dynamical behavior as well at all temperatures. In fact, it turns out that the existence of longer-range interactions may lead to the presence of frequencies that characterize the dynamical behavior of the spin system under study.[26] Thus, the dynamical spin-pair correlations and the dynamical structure factors of these systems could differ visibly when these additional interactions are taken into account.

The study of quantum spin dynamics is a challenging subject. It is seldom possible to carry out calculations of the dynamical correlations exactly. However, the simple spin systems among others can often be studied approximately and rather reliably using certain recently developed techniques. We therefore explore the question of the role of next-nearest-neighbor interactions in affecting the system dynamics using the following approach.

We first study the transverse (i.e., xx-) dynamical spin-pair correlations in an Ising chain with a transverse field that is switched off at some time $t=0$ (for related work the reader may find Refs. 27–43 useful). We assume that both nearest- and next-nearest-neighbor interactions are present in this Ising chain. For this simple spin chain one can *exactly* determine the dynamical spin-pair correlations at all temperatures. We show that the inclusion of the next-nearest-neighbor interactions leads to the presence of frequencies in the relaxation process in this model.

We then consider a richer system, namely, the transverse Ising model, that is, one in which the transverse field is present at all t, with both nearest- and next-nearest-neighbor interactions. We carry out an approximate analytical calculation of the dynamical zz correlations for this system in the high-temperature limit. The reason why we choose to perform our calculations in this limit is as follows. The dynami-

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cal spin-pair correlations can be described in terms of static multipoint correlations. These correlations are, in general, extremely difficult to calculate for most systems. However, the calculations become more manageable in the limit the temperature $T\rightarrow\infty$ when the traces over the Pauli matrices that constitute the multipoint correlations become trivial to calculate. For simple spin systems it may turn out that the behavior of the dynamical correlations at $T=\infty$ is not very different from that at any finite temperature above T_c.[13] Hence the results often are adequate for providing significant insights into the nature of the spin dynamics at $T>T_c$.

We find that our results for the dynamical spin-pair correlations for the transverse Ising model with both nearest- and next-nearest-neighbor interactions differ from the one with only a nearest-neighbor interaction in a well-defined way. This is a significant finding in view of the fact that the presence of the next-nearest-neighbor interactions affect the time-dependent correlations in a noticeable fashion as we shall see. For weak next-nearest-neighbor interactions the character of the frequency spectrum remains almost unchanged with respect to the nearest-neighbor system. Differences with respect to the spectrum of the nearest-neighbor system become readily visible upon strengthening the next-nearest-neighbor interaction strength to some $\frac{1}{2}$ of the nearest-neighbor interaction strength or greater.

II. CONTINUED FRACTION FORMALISM

A. Fundamentals

We carry out our studies using the continued fraction formalism. This is sketched below. The Liouville (or Heisenberg) equation can be formally solved via this formalism which was originally due to Mori[44] and Dupuis[45] and later extensively developed by Lee, Grigolini, and others.[46–51] In this formalism one attempts to construct satisfactory solutions to two recurrence relations. It turns out that the solution to these recurrence relations are automatically solutions to the Liouville (or Heisenberg) equation for Hermitian (i.e., nondissipative) systems. The subject of continued fractions enters from the fact that one of the key recurrence relations can be expressed in a continued fraction representation upon a Laplace transformation. This continued fraction is often much easier to work with than the recurrence relation itself.

Consider a dynamical variable $A(t)$ in some d-dimensional vector space $\mathscr{S}$. Then $A(t)$ undergoes a sweeping motion in $\mathscr{S}$ governed by the Liouville (or Heisenberg) equation of motion. The space $\mathscr{S}$ is realized by a physically meaningful inner product; typically this is the Kubo scalar product.[46] The motion of A in $\mathscr{S}$ describes a trajectory which traces a hypersurface in $\mathscr{S}$. It turns out that the dimensionality d and the structure of this hypersurface σ completely characterize the time evolution problem for Hermitian Hamiltonians. As will become evident below, $d<\infty$ completely characterizes nonergodic systems,[52] while $d\rightarrow\infty$ characterizes ergodic and partially ergodic systems.[52,53] In Sec. III we shall present calculations that will describe the dynamics of a nonergodic system. In Sec. IV we shall address the dynamics of an ergodic system. These latter systems are by far more common in the study of the dynamical response of quantum spin systems.

The time evolution of $A(t)$ is described by the Liouville (or Heisenberg) equation of motion

$$dA(t)/dt=LA(t), \tag{1}$$

where L is the Liouville operator; i.e., it denotes a commutator bracket $(i/\hbar)[H,A]$ for a quantum system. From now on we shall set $\hbar\equiv1$. Formally, for an operator $A(t)$ in $\mathscr{S}$ one can write down an orthogonal expansion (as opposed to a Taylor expansion in which one must worry about convergence properties)

$$A(t)=\exp(iHt)A\exp(-iHt)=\sum_{n=1}^{d-1}a_n(t)f_n, \tag{2}$$

where $\{f_n\}$ is a complete set of orthogonal basis vectors that span $\mathscr{S}$. The inner product in $\mathscr{S}$ is the Kubo scalar product defined by

$$(X,Y)=(\beta)^{-1}\int_0^\beta d\alpha\langle X(\alpha)Y^\dagger\rangle-\langle X\rangle\langle Y^\dagger\rangle, \tag{3}$$

where $\beta=1/kT$, k is the Boltzmann constant, X and Y are vectors in $\mathscr{S}$, $X(\alpha)=\exp(-\alpha H)X\exp(\alpha H)$, and the angular brackets denote canonical ensemble averages. Observe that at the $\beta\rightarrow0$ limit, Eq. (3) above can be replaced by the usual fluctuation formula. The individual terms on the right-hand side of Eq. (2), i.e., the f_n's and the $a_n(t)$'s, are therefore temperature dependent in such a way that their sum on the left-hand side of Eq. (2) is temperature independent.

If $\mathscr{S}$ is realized by the Kubo scalar product,[46] then the orthogonal $\{f_n\}$ can be obtained via the following recurrence relation (referred to as RR I) for the basis vectors:

$$f_{n+1}=Lf_n+\Delta_n f_{n-1}, \quad 0\leqslant n\leqslant d-1, \tag{4}$$

where $\Delta_n=(f_n,f_n)/(f_{n-1},f_{n-1})\equiv\|f_n\|/\|f_{n-1}\|, 1\leqslant n\leqslant d-1$ are the relative norms of the basis vectors referred to as *recurrants*. These recurrants play a crucial role in describing the dynamical spin correlations.

Since Eq. (4) must satisfy Eq. (1), RR I leads to a second recurrence relation for the $a_n(t)$'s, i.e., the autocorrelation functions. This recurrence relation, i.e., RR II, is

$$\Delta_{n+1}a_{n+1}(t)=-da_n(t)/dt+a_{n-1}(t). \tag{5}$$

Thus, RR I and RR II completely determine $A(t)$, which satisfies the Liouville (or Heisenberg) equation of motion. Observe that $da_0(0)/dt=0$ is a consequence of RR II and gives a condition which excludes the exponential function as a relaxation function from the class of admissible solutions for Hermitian Hamiltonians.[54]

Upon Laplace transformation RR II [see Eq. (5)] yields[46] the following continued fraction expression for $a_0(z)$:

$$a_0(z)=\cfrac{1}{z+\cfrac{\Delta_1}{z+\cfrac{\Delta_2}{z+\cfrac{\Delta_3}{z+\text{to } \infty}}}}, \tag{6}$$

where Δ_n's introduced above are static quantities, involving static correlations, that, in general, depend upon temperature, wave vector, system size, interaction strength, and other system parameters. Formally, if Δ_n's are known, the relaxation function $a_0(t)$ can be obtained. Observe that for $d<\infty$ the continued fraction in Eq. (6) truncates naturally and hence can be expressed in terms of a finite number of poles, which implies that the inverse Laplace transform of Eq. (6), i.e., the relaxation function, can be expressed as a collection of cosine terms with appropriate amplitudes. Thus, for $d<\infty$ the system never relaxes and hence is a completely nonergodic system.[52,54] As alluded to above, this case will be realized in the relaxation processes associated with the Ising system in Sec. III. For most interacting many-body systems, however, $d\to\infty$ which can lead to relaxation at $t\to\infty$ (note that $d\to\infty$ is not a sufficient condition for ergodicity but a necessary one[52]). As we shall see in Sec. IV, $d\to\infty$ for the transverse Ising chain. Often, however, the infinite continued fractions are not exactly solvable. We (Ref. 55 and the work of Sen *et al.* in Ref. 9) have recently developed a reliable approximation technique to estimate unsolvable infinite continued fractions. This technique will be used to perform calculations in Sec. IV below. In what follows, we briefly describe the method of approximating unsolvable infinite continued fractions.[55–59]

B. Estimating unsolvable infinite continued fractions

In the past various groups have truncated infinite continued fractions using a finite number of levels and an *ad hoc* truncation function. While using three or five poles with truncation functions for approximating infinite continued fractions such as in Eq. (6) yields satisfactory results for a few classes of infinite continued fractions,[60] the form of the truncation function can only be determined based on some ansatz or another. Typically, this ansatz is strongly dependent on the properties of the system under study.

One can argue that the effort one must spend in extracting a truncation function is no less demanding than in evaluating the infinite continued fraction itself via some other *brute force* method. One such approach is to replace the infinite continued fraction by a finite continued fraction. In this approach one sets $\Delta_L=0$ in Eq. (6) for some large L. How large L must be is sensitive to the properties of the infinite continued fraction under study, in particular to the n dependence of Δ_n. It turns out that an infinite continued fraction can be readily replaced by a finite continued fraction as long as the overall growth rate of $\Delta_n=n^x$, where $x<2$,[55,56] which is rather common in the systems that have been studied until now. For faster growth rates in Δ_n, more sophisticated truncation procedures may work better.[55–59] Therefore, L is determined by (i) the sequence Δ_n, and (ii) by the maximum time τ up to which the relaxation function is to be studied. It turns out that with the ready availability of powerful computers, the evaluation of a finite continued fraction with as many as 10^6 poles and subsequent estimation of the relaxation function $a_0(t)$ up to $t=\tau=10^2$ are readily possible. In fact, for many typical infinite continued fractions that appear in many-body dynamics problems, as few as 10^3 poles may be sufficient to faithfully represent the relaxation function up to long enough times such that the asymptotic behavior of dynamical correlations can sometimes be reliably extracted from the available information.

The approximate form of Δ_n for large n is often motivated by the physical content of the lower order f_n's and Δ_n's. However, it turns out that for problems often encountered in many-body canonical ensemble dynamics studies it may be sufficient to know the first few Δ_n's (say, the first 5–30 or so depending upon the nature of the Hamiltonian, as stated above) accurately and the rest approximately. It turns out that often the intermediate- or even long-time behavior of the relaxation function to be eventually calculated is not too sensitive to the accuracy of the higher order Δ_n's but rather depends instead more crucially upon the general features of the higher-order Δ_n's.[55–59]

As stated earlier, most infinite continued fractions are not exactly solvable. For these cases, the results obtained with a large value of truncation level L can be used to compare with the results obtained using a slightly smaller L for fixed x and τ. In addition, one should also check whether the finite continued fraction is sensitive to whether L is an odd or an even number. A stable and convergent result is insensitive to the oddness or evenness of L. This dependence on the oddness and the evenness of L is commonly referred to as the *odd-even effect*.[55,56]

$a_0(t)$ can be calculated numerically for various values of x $(0<x<2)$ and L in this method which is often referred to in the literature as the direct summation method.[55,56] The computation of the inverse Laplace transform is based on the paper of Crump,[61] who used a Fourier series approximation. For a given complex-valued function $a_0(z)$, we can obtain an approximation of its inverse Laplace transform $a_0(t)$ by computing the partial sums of

$$a_0(t)\approx\frac{\exp(bt)}{\tau}\left[\frac{1}{2}a_0(b)+\sum_{k=1}^{\infty}\left\{\mathrm{Re}\,a_0\left(b+\frac{ik\pi}{\tau}\right)\cos\left(\frac{k\pi t}{\tau}\right)-\mathrm{Im}\,a_0\left(b+\frac{ik\pi}{\tau}\right)\sin\left(\frac{k\pi t}{\tau}\right)\right\}\right], \tag{7}$$

where Re and Im denote real and imaginary parts, respectively, b is a number larger than the maximum of the real parts of the singularities of $a_0(z)$, and $1/\tau$ is the step in which the summation in the equation above is carried out.

III. RELAXATION IN THE NEXT-NEAREST-NEIGHBOR ISING CHAIN

A. Relaxation in the nearest-neighbor Ising chain

We consider the $s=1/2$ next-nearest-neighbor Ising chain described by the Hamiltonian

$$H=-\sum_{i=1}^{N} J_1 S_i^z (S_{i+1}^z + J_2/J_1 S_{i+2}^z), \qquad (8)$$

where the spin at site i interacts with its nearest neighbors and next-nearest neighbors with interaction strengths J_1 and J_2, respectively, the spin operators S_i^α, $\alpha=\{x,y,z\}$, at site i are given by the Pauli spin matrices σ_i^α, and $S_i^\alpha=(\hbar/2)\sigma_i^\alpha$. We also assume periodic boundary conditions for our Ising chain. To study the nonequilibrium behavior of this system we consider any spin S_k^z in the system. Since S_k^z commutes with the Hamiltonian in Eq. (8), it is a constant of motion. Let us now assume that one uses a transverse magnetic field to "turn" this spin to S_k^x and the field is then switched off at $t=0$. S_k^x is no longer in a stationary state and must evolve in time according to the Heisenberg equation of motion [Eq. (1)].

One might interpret the resulting dynamical process as follows. Let us first focus on the Ising chain with nearest-neighbor interactions only, i.e., $J_2=0$. The transverse spin S_k^x in an effort to relax to its stationary state now tries to transfer its excess energy to its nearest neighbors to which it is coupled by J_1. However, the neighbors, being in their stationary states, cannot accept this energy, which must thus remain on the original site. Therefore, there is no delocalization of the excitation energy in this problem. Hence, no spins other than S_k^x and its two nearest neighbors, S_{k-1}^z and S_{k+1}^z, can be involved in the time evolution process (in this connection see Refs. 29 and 26).

It turns out that the time evolution in the Ising chain can be characterized by two distinct excitation frequencies. This implies that the Hilbert space of $S_k^x(t)$ has a dimensionality $d=3$. The first one is of zero frequency. It corresponds to the antiparallel state formed by the two nearest-neighbor spins. The second frequency has magnitude unity and corresponds to the parallel state formed by the two nearest-neighbor spins. Observe that the lowest frequency is unrelated to the lowest-energy state of the system. The transverse dynamics of an Ising model is, therefore, a rigorously nonergodic process in which the time average of an operator will *not* equal its ensemble average.[26,52]

Choosing $f_0=S_k^x$ and using Eq. (2) one finds

$$f_1=J_1 S_k^y (S_{k-1}^z + S_{k+1}^z) \qquad (9)$$

and

$$\Delta_1=(f_1,f_1)/(f_0,f_0)=(J_1^2/2)(1+4\xi), \qquad (10)$$

where $\xi=(S_k^y, S_k^y S_{k-1}^z S_{k+1}^z)/\chi$, with $\chi\equiv(S_k^x,S_k^x)$. χ is often referred to in the literature as perpendicular or transverse susceptibility (see Ref. 39 and references therein). The equilibrium quantities ξ and χ may be assumed to be known for our purposes here. The calculation of f_2 is straightforward. Using Eqs. (8) and (4) one obtains

$$f_2=2J_1^2(\xi S_k^x - S_{k-1}^z S_k^x S_{k+1}^z), \qquad (11)$$

where

$$\Delta_2=(f_2,f_2)/(f_1,f_1)=(J_1^2/2)(1-4\xi). \qquad (12)$$

It turns out that $f_3=0$ in this problem, which gives us a Hilbert space with $d=3$ for the $q=2$ Ising model, q being the coordination number. This result suggests the possibility of a general relation for the class of Ising dynamics problems. This relation is $d=q+1$. It can be shown[26,43] that this relation indeed holds true.

Given Δ_1 and Δ_2, Eq. (6) is readily solvable. It turns out that

$$a_0(t)=(1/2)[(1-4\xi)+(1+4\xi)\cos(\omega t)], \qquad (13)$$

where $\omega^2\equiv\Delta_1+\Delta_2=J_1^2$. The other relaxation functions are

$$a_1(t)=(1/J_1)\sin(\omega t), \qquad (14)$$

$$a_2(t)=(1/J_1^2)[1-\cos(\omega t)]. \qquad (15)$$

All the higher relaxation functions vanish in this problem. We have therefore demonstrated that the transverse dynamics of the Ising model is characterized by two frequencies, a zero frequency mode and a unit frequency mode, the origin of these two modes being in the antiparallel and parallel orientations of the nearest-neighbor spins of site k and these modes are unaffected by the sign of J_1, i.e., by whether we have a ferromagnetic or an antiferromagnetic exchange interaction between the Ising spins.

B. Δ_n's for the next-nearest-neighbor Ising chain

Let us now work out the dynamical problem when $J_2\neq 0$. To keep the algebra somewhat tractable let us focus on the simpler case in which $J_1=J_2\equiv J$. The first basis vector $f_0=S_k^x$. Thus, via RR I,

$$f_1=JS_k^y\{S_1\} \qquad (16)$$

and

$$\Delta_1=J^2\langle(1/4)S_1^2\rangle=J^2(1+\Lambda), \qquad (17)$$

where

$$S_1\equiv S_{k-1}^z+S_{k+1}^z+S_{k-2}^z+S_{k+2}^z \qquad (18)$$

and

$$\Lambda\equiv 2\langle S_2+\hat{S}_2\rangle, \qquad (19)$$

with

$$S_2=S_{k-1}^z S_{k-2}^z+S_{k-1}^z S_{k+2}^z+S_{k+1}^z S_{k-2}^z+S_{k+1}^z S_{k+2}^z, \qquad (20)$$

$$\hat{S}_2 = S^z_{k-1}S^z_{k+1} + S^z_{k-2}S^z_{k+2}. \tag{21}$$

Applying RR I again to f_1 one obtains f_2 which is

$$f_2 = J^2 S^x_k\{\Lambda - 2(S_2 + \hat{S}_2)\} \tag{22}$$

and

$$\Delta_2 = J^4(\Gamma - 2\Lambda + \Lambda^2)/(1+\Lambda), \tag{23}$$

where

$$\Gamma \equiv (3/2 + 24\gamma), \tag{24}$$

$$\gamma \equiv \langle S_3 \rangle, \tag{25}$$

$$S_3 = S^z_{k-1}S^z_{k+1}S^z_{k-2} + S^z_{k-1}S^z_{k+1}S^z_{k+2} + S^z_{k-2}S^z_{k+2}S^z_{k-1} + S^z_{k-2}S^z_{k+2}S^z_{k+1}. \tag{26}$$

Continuing in this fashion one finds

$$f_3 = J^3 S^y_k\left\{ \frac{(\Gamma + 3\Lambda/2 - 3/2)}{(1+\Lambda)} S_1 - 6S_3 \right\}, \tag{27}$$

$$\Delta_3 = J^2 \frac{(3\Gamma + \Lambda)(3-\Lambda)}{(1+\Lambda)(\Lambda + 2\Gamma - \Gamma^2)}, \tag{28}$$

$$f_4 = J^4 S^x_k\left\{ \left[3/2 - \frac{(\Lambda + 3\Gamma)(\Lambda - \Gamma)}{(\Lambda - 2\Gamma - \Gamma^2)} \right] + 2\frac{\Gamma(\Lambda - 3)}{(\Gamma + 2\Lambda - \Lambda^2)}(S_2 + \hat{S}_2) + 24 S_4 \right\}, \tag{29}$$

where

$$S_4 = S^z_{k-1}S^z_{k+1}S^z_{k-2}S^z_{k+2}, \tag{30}$$

$$\Delta_4 = J^2 \frac{(1+\Lambda)(\Gamma - \Lambda)}{(\Gamma - 2\Lambda - \Lambda^2)}, \tag{31}$$

and finally it turns out that

$$f_5 = 0, \tag{32}$$

and hence

$$\Delta_5 = 0. \tag{33}$$

Given that $\Delta_5 = 0$, it implies that $d = 5$ in this problem in accordance with our expectation that $d = q + 1$, where q equals the number of spins that interact with site j, which here is 4. Thus, the excitation is completely localized at site j and the relaxation is characterized completely by a finite number of frequencies as in the nearest-neighbor case. The Δ_i's satisfy the identities

$$\sum_{i=1}^{5} \Delta_i = 5J^2 \tag{34}$$

and

$$\Delta_1(\Delta_3 + \Delta_4) + \Delta_2\Delta_4 = 4J^4. \tag{35}$$

Given all these equations one can readily calculate the dynamical transverse spin-pair correlation function which is described in the following subsection.

C. Calculation of the relaxation function

Using Eq. (6) one can write,

$$a_0(z) = \frac{z^4 + \alpha_1 z^2 + \alpha_2}{z(z^4 + 5z^2 + 4)}, \tag{36}$$

where

$$\alpha_1 = (4 - \Lambda) \tag{37}$$

and

$$\alpha_2 = (\Gamma - \Lambda). \tag{38}$$

The poles of $a_0(z)$ lie at $0, \pm i, \pm 2i$. Since $\omega = J$ we get

$$a_0(t) = \frac{\Gamma - \Lambda}{4} + \frac{3-\Gamma}{3}\cos Jt + \frac{3\Lambda + \Gamma}{12}\cos 2Jt, \tag{39}$$

where the zero frequency or translation mode describes the dynamics when there is an equal number of up and down orientations of the nearest and next-nearest neighbors. The higher relaxation functions $a_1(t)$–$a_4(t)$ can also be obtained via RR II and are listed below for the sake of completeness:

$$a_1(t) = \frac{1}{3J(1+\Lambda)}\left[(3-\Gamma)\sin Jt + \frac{3\Lambda + \Gamma}{2}\sin 2Jt \right], \tag{40}$$

$$a_2(t) = \frac{1}{J^2(\Gamma + 2\Lambda - \Lambda^2)}\left[\frac{(\Gamma - \Lambda)(1+\Lambda)}{4} + \frac{\Lambda(3-\Gamma)}{3}\cos Jt + \frac{(\Lambda - 3)(3\Lambda + \Gamma)}{12}\cos 2Jt \right], \tag{41}$$

$$a_3(t)=\frac{1}{J^3}\left\{\sin Jt-\frac{1}{3}\sin 3Jt\right\}, \tag{42}$$

$$a_4(t)=\frac{1}{4}-\frac{1}{3}\cos Jt+\frac{1}{12}\cos 2Jt. \tag{43}$$

IV. RELAXATION IN NEXT-NEAREST-NEIGHBOR TRANSVERSE ISING CHAIN

A. Calculation of Δ_n's

The equilibrium properties of the transverse Ising model and its realization in physical systems have been addressed by several authors.[62–66] The Hamiltonian for our model which includes *competing* interactions is given by

$$H=-\sum_{i=1}^{N}(J_1S_i^zS_{i+1}^z-J_2S_i^zS_{i+2}^z)-h\sum_{i=1}^{N}S_i^x, \tag{44}$$

where $J_1(>0)$ is the nearest-neighbor ferromagnetic exchange while $J_2(>0)$ is the next-nearest-neighbor antiferromagnetic exchange and h denotes the strength of the transverse field. We assume periodic boundary conditions and work in the thermodynamic limit. The on-site dynamical spin-pair correlations of a bulk spin, say, S_k^z, can be written as $\langle S_k^z(t)S_k^z(0)\rangle/\langle S_k^zS_k^z\rangle$, where the angular brackets denote canonical ensemble averages. The calculation of the above-mentioned dynamical correlation function is the main focus of this work. As mentioned above, it turns out that for $J_2=0$ in Eq. (44), the dynamical zz correlations are exactly solvable[8,9] at $T=\infty$ and are given by

$$\langle S_k^z(t)S_k^z\rangle/\langle(S_k^z)^2\rangle=\sqrt{\pi/2K}\,\Theta_3(\pi t/2K,q)\exp[-(1/2)(1-E/K)t^2],\quad \alpha<1, \tag{45}$$

$$\langle S_k^z(t)S_k^z\rangle/\langle(S_k^z)^2\rangle=\exp[-(1/2)t^2],\quad \alpha=1, \tag{46}$$

$$\langle S_k^z(t)S_k^z\rangle/\langle(S_k^z)^2\rangle=\sqrt{\pi\alpha/2K}\,\Theta_2(\pi\alpha t/2K,q)\exp[1(1/2)(1-E/K)\alpha^2t^2],\quad \alpha>1, \tag{47}$$

where $\alpha\equiv h/J_1$, K and E are complete elliptic integrals[67] of the first and second kinds of argument α (when $\alpha<1$) and $1/\alpha$ (when $\alpha>1$), and q is the nome defined as $q\equiv\exp(-\pi K'/K)$, where K' is the elliptic integral of complementary argument.[67] Time is measured in units of $t=2J_1t_{\rm real}$. The functions Θ_2 and Θ_3 are Jacobi theta functions, which have the expansion[67]

$$\Theta_2(z,q)=2\sum_{n=0}^{\infty}q^{(n+1/2)^2}\cos[(2n+1)z], \tag{48}$$

$$\Theta_3(z,q)=1+2\sum_{n=1}^{\infty}q^{n^2}\cos(2nz). \tag{49}$$

To study the dynamical zz spin-pair correlations for the next-nearest-neighbor transverse Ising chain using the continued fraction formalism we proceed as follows. We choose the first basis vector f_0 in Eq. (4) to be the dynamical variable of interest, namely, $S_k^z(t=0)\equiv S_k^z$. This choice implies that the dynamical correlation function $a_0(t)=\langle S_k^z(t)S_k^z\rangle/\langle(S_k^z)^2\rangle$, the Laplace transform of which has the continued fraction representation in Eq. (6) above. Given f_0 and RR I one may now obtain the entire set $\{f_n\}$, which in this case, turns out to be an infinite set. Of course, in the absence of an exact solution, it is impossible to obtain the entire set $\{f_n\}$. Typically, the best one can do is to obtain as many f_n's as possible and get an estimate of n dependence of Δ_n's therefrom. The basis vectors, i.e., the f_n's, contain valuable information on how the perturbation imparted to $S_k^z(t=0)$ propagates through the chain which is dictated by the nature of the spin-spin interactions in the Hamiltonian. Hence it is important and interesting to study the structure of these basis vectors, the first five of which, calculated at $T=\infty$, are detailed below. Obviously, in principle, one *can* obtain more than the ones given here. The procedure involved in doing so is straightforward but extremely tedious.

We base our calculations of the relaxation function $a_0(t)$ on the rigorous knowledge of the first five basis vectors and the first five Δ_n's. The rest of the Δ_n's that enter into the structure of the continued fraction in Eq. (6) are estimated on the basis of simple extrapolation schemes which are discussed below. Thus, we believe that the short-time dynamics of the system obtained by us is highly accurate. The results for longer times are dependent upon the extrapolation of Δ_n's and hence should be accepted as good estimates. The dynamical spin-pair correlations appear to decay to zero rather rapidly in this problem.

The rigorously known basis vectors and the corresponding Δ_n's are as follows:

$$f_1=-hS_k^y, \tag{50}$$

$$\Delta_1=h^2, \tag{51}$$

$$f_2=hS_k^x\{J_1(S_{k-1}^z+S_{k+1}^z)-J_2(S_{k-2}^z+S_{k+2}^z)\}, \tag{52}$$

$$\Delta_2 = \frac{1}{2}(J_1^2 + J_2^2), \tag{53}$$

$$f_3 = 2hS_k^y\{J_1^2 S_{k-1}^z S_{k+1}^z - J_1 J_2 (S_{k-1}^z S_{k-2}^z + S_{k-1}^z S_{k+2}^z + S_{k+1}^z S_{k-2}^z + S_{k+1}^z S_{k+2}^z + J_2^2 S_{k-2}^z S_{k+2}^z\} - h^2 S_k^x \{J_1 (S_{k-1}^y + S_{k+1}^y) - J_2 (S_{k-2}^y + S_{k+2}^y)\}, \tag{54}$$

$$\Delta_3 = h^2 + \frac{1}{2}(J_1^2 + J_2^2) + \frac{J_1^2 J_2^2}{(J_1^2 + J_2^2)}, \tag{55}$$

$$f_4 = \frac{hJ_1 J_2 (J_1^2 + J_2^2) S_k^x}{2(J_1^2 + J_2^2)}\{J_2(S_{k-1}^z + S_{k+1}^z) + J_1(S_{k-2}^z + S_{k+2}^z)\} + 6hJ_1 J_2 S_k^x \{J_1 S_{k-1}^z S_{k+1}^z (S_{k-2}^z + S_{k+2}^z) - J_2 S_{k-2}^z S_{k+2}^z (S_{k-1}^z + S_{k+1}^z)\} - 3h^2 S_k^y \{J_1^2 (S_{k-1}^z S_{k+1}^y + S_{k-1}^y S_{k+1}^z) - J_1 J_2 (S_{k-2}^z S_{k-1}^y + S_{k-2}^y S_{k-1}^z + S_{k-2}^z S_{k+1}^y + S_{k-2}^y S_{k+1}^z + S_{k+2}^z S_{k-1}^y + S_{k+2}^y S_{k-1}^z + S_{k+2}^z S_{k+1}^y + S_{k+2}^y S_{k+1}^z) + J_2^2 (S_{k-2}^z S_{k+2}^y + S_{k-2}^y S_{k+2}^z)\} + 2h^2 S_k^z \{J_1^2 S_{k-1}^z S_{k+1}^z - J_1 J_2 (S_{k-1}^z S_{k+2}^z + S_{k+1}^z S_{k-2}^z + S_{k+1}^z S_{k+2}^z) + J_2^2 S_{k-2}^z S_{k+2}^z\} + h^2 S_k^x \{J_1^2 (S_{k-2}^z S_{k-1}^x + S_{k+2}^z S_{k+1}^x) - J_1 J_2 (S_{k-3}^z S_{k-2}^x + S_{k-3}^z S_{k-1}^x + S_{k+3}^z S_{k+2}^x + S_{k+3}^z S_{k+1}^x + S_{k_1}^z S_{k+1}^x + S_{k-1}^z S_{k-2}^x + S_{k+1}^z S_{k-1}^x + S_{k+1}^z S_{k+2}^x) + J_2^2 (S_{k-4}^z S_{k-2}^x + S_{k+4}^z S_{k+2}^x)\}, \tag{56}$$

$$\Delta_4 = \mathscr{N}_4 / \mathscr{D}_4, \tag{57}$$

$$\mathscr{N}_4 = 6h^2 J_1^6 + 5J_1^6 J_2^2 + 30h^2 J_1^4 J_2^2 + 8J_1^4 J_2^4 + 30h^2 J_1^2 J_2^4 + 5J_1^2 J_2^6 + 6h^2 J_2^6,$$

$$\mathscr{D}_4 = (J_1^2 + J_2^2)(J_1^4 + 2h^2 J_1^2 + 4J_1^2 J_2^2 + 2h^2 J_2^2 + J_2^4), \tag{58}$$

$$f_5 = -24J_1^2 J_2^2 S_k^y \{S_{k-1}^z S_{k+1}^z S_{k-2}^z S_{k+2}^z\} - 4h^2 J_1^2 J_2 S_k^y \{S_{k-2}^x (S_{k-3}^z S_{k-1}^z + S_{k-1}^z S_{k+1}^z + S_{k-3}^z S_{k+1}^z) + S_{k-1}^x (S_{k-3}^z S_{k+1}^z + S_{k-2}^z S_{k+2}^z) + S_{k+1}^x (S_{k-2}^z S_{k+2}^z + S_{k-1}^z S_{k+3}^z) + S_{k+2}^x (S_{k-1}^z S_{k+3}^z + S_{k-1}^z S_{k+1}^z + S_{k+1}^z S_{k+3}^z)\} + 4h^2 J_1 (J_1^2 + J_2^2) S_k^y \{S_{k-2}^z S_{k-1}^x S_{k+1}^z + S_{k-1}^z S_{k+1}^x S_{k+2}^z\} - 4h^2 J_2^3 S_k^y \{S_{k-4}^z S_{k-2}^x S_{k+2}^z + S_{k-2}^z S_{k+2}^x S_{k+4}^z\} + 4h^2 J_1 J_2^2 S_k^y \{S_{k-2}^x (S_{k-4}^z S_{k-1}^z + S^z k - 4 S_{k+1}^z + S_{k+2}^z S_{k-1}^z + S_{k+2}^z S_{k-3}^z) + S_{k-1}^x (S_{k+2}^z S_{k-3}^z + S_{k+2}^z S_{k+1}^z + S_{k-3}^z S_{k_2}^z) + S_{k+1}^x (S_{k+2}^z S_{k+3}^z + S_{k-2}^z S_{k-1}^z + S_{k+3}^z S_{k-2}^z) + S_{k+2}^x (S_{k+3}^z S_{k-2}^z + S_{k+1}^z S_{k-2}^z + S_{k-1}^z S_{k+4}^z + S_{k+1}^z S_{k+4}^z)\} - 14h^2 J_1^2 J_2 S_k^x \{S_{k-2}^z S_{k-1}^y S_{k+1}^z + S_{k-1}^z S_{k+1}^y S_{k+2}^z\} - 12h^2 J_1^2 J_2 S_k^x \{S_{k-1}^z S_{k-2}^y S_{k+1}^z + S_{k+1}^z S_{k-1}^y S_{k+2}^z + S_{k-2}^z S_{k+1}^y S_{k-1}^z + S_{k-1}^z S_{k+2}^y S_{k+1}^z\} + 12h^2 J_1 J_2^2 S_k^x \{S_{k-2}^y S_{k+2}^z (S_{k-1}^z + S_{k+1}^z) + S_{k-2}^z S_{k+2}^z (S_{k-1}^y + S_{k+1}^y) + S_{k-2}^z S_{k+2}^z (S_{k-1}^z + S_{k+1}^z)\} - 2h^2 J_1^2 J_2 S_k^x \{S_{k-1}^z S_{k-2}^y S_{k-3}^z + S_{k-3}^z S_{k-1}^y S_{k-2}^z + S_{k+2}^z S_{k+1}^y S_{k+3}^z + S_{k+3}^z S_{k+2}^y S_{k+1}^z\} + 2h^2 J_1 J_2^2 S_k^x \{S_{k-4}^z S_{k-2}^y (S_{k-3}^z + S_{k-1}^z) + S_{k-3}^z S_{k-1}^y S_{k+1}^z + S_{k-1}^z S_{k+1}^y S_{k+3}^z + S_{k+2}^y S_{k+4}^z (S_{k+1}^z + S_{k+3}^z)\} - h^3 J_1^2 S_k^x \{S_{k-2}^y S_{k_1}^x + S_{k+2}^y S_{k+1}^x\} + h^3 J_1 J_2 S_k^x \{S_{k-3}^y (S_{k-2}^x + S_{k-1}^x) + S_{k-1}^y (S_{k-2}^x + S_{k+1}^x) + S_{k+1}^y (S_{k+2}^x + S_{k_1}^x) + S_{k+3}^y (S_{k+2}^x + S_{k+1}^x)\}, - h^3 J_2^2 S_k^x \{S_{k-4}^y S_{k-2}^x + S_{k+4}^y S_{k+2}^x\} - 5h^3 J_1^2 S_k^z \{S_{k-1}^y S_{k+1}^z + S_{k-1}^z S_{k+1}^y\} + 5h^3 J_1 J_2 S_k^z \{S_{k-2}^y (S_{k-1}^z + S_{k+1}^z) + S_{k-1}^y (S_{k-2}^z + S_{k+2}^z) + S_{k+1}^y (S_{k-2}^z + S_{k+2}^z) + S_{k+2}^y (S_{k-1}^z + S_{k+1}^z)\} - 5h^3 J_2^2 S_k^z \{S_{k-2}^y S_{k+2}^z + S_{k-2}^z S_{k+2}^y\} + 6h^3 J_1^2 S_k^y \{S_{k-1}^y S_{k+1}^y\} - 6h^3 J_1 J_2 S_k^y \{S_{k-2}^y S_{k-1}^y + S_{k-2}^y S_{k+1}^y + S_{k+2}^y S_{k-1}^y + S_{k+2}^y S_{k+1}^y\} + 6h^3 J_2^2 S_k^y \{S_{k-2}^y S_{k+2}^y\} - 2h^2 J_1^2 J_2 S_k^y \{S_{k-1}^x + S_{k+1}^x\} - h^2 J_1^2 J_2 S_k^y \{S_{k-2}^x + S_{k+2}^x\} - (\alpha_1 / 2\rho) S_k^x \{S_{k-2}^y + S_{k+2}^y\} + (\alpha_2 / 2\rho) S_k^x \{S_{k-1}^y + S_{k+1}^y\} + (\alpha_3 / \rho) S_k^y \{S_{k-1}^z S_{k+1}^z\} + (\alpha_4 / \rho) S_k^y \{S_{k-2}^z S_{k-1}^z + S_{k-2}^z S_{k+1}^z + S_{k+2}^z S_{k-1}^z + S_{k+2}^z S_{k+1}^z\} - (\alpha_5 / \rho) S_k^y \{S_{k-2}^z S_{k+2}^z\}, \tag{59}$$

$$\Delta_5 = \mathscr{N}_5 / \mathscr{D}_5, \tag{60}$$

$$\mathscr{N}_5 = (J_1^2 + J_2^2)(4h^2 J_1^{10} + 4J_1^{10} J_2^2 + 10h^4 J_1^8 + 108h^2 J_1^8 J_2^2 + 5J_1^8 J_2^4 + 76h^6 J_1^6 + 312h^4 J_1^6 J_2^2 + 444h^2 J_1^6 J_2^4 + 380h^6 J_1^4 J_2^2 + 532h^4 J_1^4 J_2^4 + 36J_1^6 J_2^6 + 380h^6 J_1^2 J_2^4 + 402h^2 J_1^4 J_2^6 + 284h^4 J_1^2 J_2^6 + 76h^6 J_2^6 + 5J_1^4 J_2^8 + 94h^2 J_1^2 J_2^8 + 10h^4 J_2^8 + 4J_1^2 J_2^{10} + 4h^2 J_2^{10}), \tag{61}$$

$$\mathscr{D}_5 = (J_1^4 + 2h^2 J_1^2 + 4J_1^2 J_2^2 + 2h^2 J_2^2 + J_2^4)(6h^2 J_1^6 + 5J_1^6 J_2^2 + 30h^2 J_1^4 J_2^2 + 8J_1^4 J_2^4 + 30h^2 J_1^2 J_2^4 + 5J_1^2 J_2^6 + 6h^2 J_2^6), \tag{62}$$

where

$$\alpha_1=h^2J_2(5J_1^6-2h^2J_1^4+10J_1^4J_2^2-38h^2J_1^2J_2^4+J_1^2J_2^4-8h^2J_2^4+2J_2^6),$$

$$\alpha_2=h^2J_1(2J_1^6-8h^2J_1^4+J_1^4J_2^2-38h^2J_1^2J_2^2+10J_1^2J_2^4-2h^2J_2^4+5J_2^6),$$

$$\alpha_3=4hJ_1^2(h^2J_1^4+2J_1^4J_2^2-4h^4J_1^2+3h^2J_1^2J_2^2-4h^4J_2^2-J_1^2J_2^4-h^2J_2^4-J_2^6),$$

$$\alpha_4=2hJ_1J_2(J_1^6-J_1^4J_2^2+8h^4J_1^2-6h^2J_1^2J_2^2+8h^4J_2^2-J_1^2J_2^4+J_2^6),$$

and

$$\alpha_5=4hJ_2^2(J_1^6+h^2J_1^4+J_1^4J_2^2+4h^4J_1^2-3h^2J_1^2J_2^2+4h^4J_2^2-2J_1^2J_2^4-h^2J_2^4), \quad \text{while } \rho=J_1^4+2h^2J_1^2+4J_1^2J_2^2+2h^2J_2^2+J_2^4).$$

The reader may recall that dynamical correlations for the nearest-neighbor transverse Ising model are exactly solvable in the limit $T\rightarrow\infty$. Thus, by setting $J_2=0$ in the above expressions for f_n and Δ_n one immediately recovers the corresponding expressions in Ref. 8, and the simple linear behavior of Δ_n's. In addition to checking our results for the $J_2=0$ case, we have also checked the orthogonality that must be satisfied by the individual f_n's, i.e., $\langle f_n f_m\rangle=0$ for $n\neq m$. The f_n's given above satisfy the orthogonality criteria, which leads us to believe that the expressions given above are algebraically correct.

An interesting feature of the Δ_n's above is that up to Δ_4 the expressions remain invariant upon interchange of J_1 and J_2. This symmetry is broken at Δ_5 and above, where interchanging of J_1 and J_2 leads to the incorrect expression for Δ_n's. It turns out, however, that the invariance under exchange of J_1 and J_2 in the expressions for the f_n's is broken already at f_2, which is expected from the fact that the excitations propagate farther out from site k compared to what would have been the case if $J_2=0$ due to the next-nearest-neighbor interaction. This breakdown of symmetry simply does not show up in the Δ_n's for $n\leqslant 4$. This is so because the Δ_n's are the ratios of the length squared of the basis vectors, and hence they contain thermally averaged information (with all the energy states being equally weighted in the $T\rightarrow\infty$ limit) on the microscopic details of the propagation of a perturbation from k to its neighborhood in real space. However, f_5 is constructed out of the commutation between the Hamiltonian in Eq. (44) and f_4 and f_3 contain cubic terms in the field strength h with asymmetric couplings with J_1 and J_2 [observe the last two sets of terms involving h^3 in Eq. (59)]. As a consequence, the level of complexity of f_5 is significantly higher than the lower-order f_n's.

B. Calculation of the relaxation function

The behavior of Δ_n as a function of n is rather complicated for $J_2\neq 0$. The behavior of Δ_n versus n for $1\leqslant n\leqslant 5$ is shown in Fig. 1 for $0\leqslant J_2\leqslant J_1=2$. Δ_n increases linearly with n for $J_2=0$ (i.e., for the nearest-neighbor transverse Ising model) and very nearly linearly with n for $J_2=J_1=2$. In the intermediate regime for $J_2=\frac{1}{4},\frac{1}{2},1$ cases it turns out that Δ_n's behave in a superlinear fashion with n for small n. It is not clear from the completed calculations (i.e., up to Δ_5) as to how Δ_n would behave for $n>>5$ for $J_2=\frac{1}{4},\frac{1}{2},1$. Based upon the formulas in Eqs. (51), (53), (55), (57)–(59), and (60)–(62) and the visible trends in the growth of Δ_n versus n we assume that eventually Δ_n behaves linearly with respect to n and more importantly that there are no intersections between the curves for Δ_n for different magnitudes of J_2 for $J_2\leqslant J_1$. This assumption can be defended on somewhat intuitive grounds as follows.

If the plots of Δ_n versus n for two distinct values of J_2 were to intersect, then, almost inevitably, such behavior would have manifested itself in terms of certain frequency peak(s) in the spectral function corresponding to the zz dynamical spin-pair correlation function for the next-nearest-neighbor transverse Ising model.[68] Physically, such a drastic effect is unexpected when the next-nearest-neighbor interaction is weak, i.e., $J_2<J_1$. After all, the magnitude of J_2 is weaker than that of J_1 and hence its effect should be corrective with regard to the spectral function one obtains for the nearest-neighbor model, not a drastically different one.

Very different physical behavior of the relaxation process can occur if, however, $J_2>J_1$. Such a scenario would be interesting from a theoretical standpoint for the following reasons. First, the rate of growth of Δ_n's with respect to n could be very different from linear behavior. This is evident from the results for $J_2=4$ in Fig. 2. Second, there exists the possibility of finding well-defined peaks and/or dips in the growth profile of Δ_n versus n as in the $J_2=6$ case of Fig. 2. What these mean is that one can obtain systems with a very different dynamical response if $J_2>J_1$. Such a response could be characterized by well-defined peaks and a rich variety of high- and low-frequency behavior of the spectral function. Interestingly, in the regime $J_2/J_1\rightarrow\infty$ one will

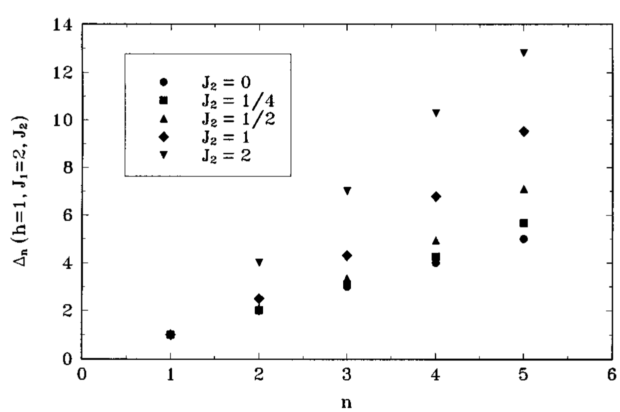

FIG. 1. Plot of Δ_n versus n for $J_2\leqslant J_1=2$ with $h\equiv 1$. Observe that the growth of Δ_n is linear for $J_2=0$ and is very nearly linear (with slight oscillations about linearity) for $n>3$ for $J_2=J_1=2$.

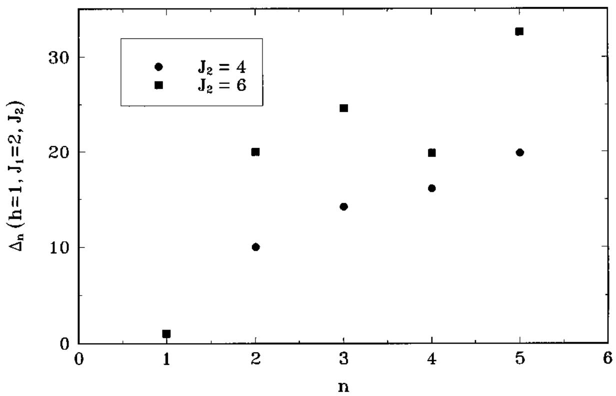

FIG. 2. Plot of Δ_n versus n for $J_2 > J_1$ with $h \equiv 1$. Observe the dip in the growth of Δ_n for $J_2 = 6 = 3J_1$ at $n = 4$. See the discussion in the text for more on such features in the growth of Δ_n's.

again recover the small linear growth rate of Δ_n versus n. Due to the lack of knowledge of higher Δ_n's for the $J_2 > J_1$ case we do not carry out any approximate analysis of the relaxation function for these cases. In what follows, we return to our approximate calculations of the relaxation and spectral functions for the $J_2 \leqslant J_1$ cases discussed in Fig. 1.

To estimate the relaxation function $a_0(t) \equiv \langle S_k^z(t) S_k^z(0)\rangle / \langle (S_k^z)^2 \rangle$ for the next-nearest-neighbor transverse Ising model at $T \to \infty$ it is imperative to have some knowledge of the higher Δ_n's for various J_2's. Given that $J_2 = 0$ is exactly known, we focus upon the cases with $J_2 < J_1$ in this study. We assume that for $J_2 = \frac{1}{4}, \frac{1}{2}, 1$, the superlinear behavior of Δ_n with respect to n will eventually become linear in n for $n >> 5$. Such linearity also appears for the case $J_2 = J_1 = 2$. On the basis of our calculations of $\Delta_1 - \Delta_5$ we find that the following simple extrapolation schemes are reasonable estimates for Δ_n for $n > 5$. The extrapolation schemes invoked here are based upon the magnitudes of Δ_4 and Δ_5 for $J_2 = \frac{1}{4}, \frac{1}{2}, 1$ cases and of Δ_3, Δ_4, and Δ_5 for the $J_2 = 2$ case. These are as follows.

Thus, for $J_2 = \frac{1}{4}$,

$$\Delta_n = 1.42181(n-4) + 4.26086, \quad n \geqslant 5, \tag{63}$$

for $J_2 = \frac{1}{2}$,

$$\Delta_n = 2.15384(n-4) + 4.94195, \quad n \geqslant 5, \tag{64}$$

for $J_2 = 1$,

$$\Delta_n = 2.75445(n-4) + 6.78139, \quad n \geqslant 5, \tag{65}$$

and for $J_2 = 2$,

$$\Delta_n = 3(n-3) + 7, \quad n \geqslant 6. \tag{66}$$

Using these extrapolation schemes we obtain $a_0(t)$ via the direct summation method discussed in Sec. II B with 10 000 poles in the calculation of $a_0(t)$ for each chosen J_2. We have tested our results for sensitivity to truncation of the continued fraction at odd and at even levels and found no odd-even effect within the accuracy of our calculations. Our results are essentially invariant upon changes of a few percent in the parameters mentioned in the above extrapolation schemes.

Obviously, by definition, $a_0(t) \to 1$ as $t \to 0$. This is indeed the case in all our calculations. In Fig. 3 we show our results for $a_0(t)$ for $2 \leqslant t \leqslant 10$, which appears to be the more interesting time regime in this problem. Let us briefly discuss the relaxation processes depicted in this figure.

The solid line in Fig. 3 describes the relaxation process for the exactly solvable limit in which $J_2 = 0$ and $a_0(t)$ is a Gaussian function [see Eq. (46)]. The dot-dashed line with the deepest minima at $t \approx 4.4$ is for the case $J_2 = \frac{1}{4}$. The minima becomes slightly shallower and occurs at $t \approx 4.2$ for $J_2 = \frac{1}{2}$ as shown using the second dot-dashed line. The dip mentioned above disappears for $J_2 = 1$ which seems to exhibit slower relaxation than for the $J_2 = 0$ case as shown in the dotted curve. Not surprisingly, the relaxation process slows down further as J_2 is tuned up to 2, i.e., when $J_1 = J_2$. The time domain results demonstrate the sensitivity of $a_0(t)$ to small changes in J_2 much better than the frequency domain results. This is typically the case in many calculations. This is because a certain degree of inaccuracy

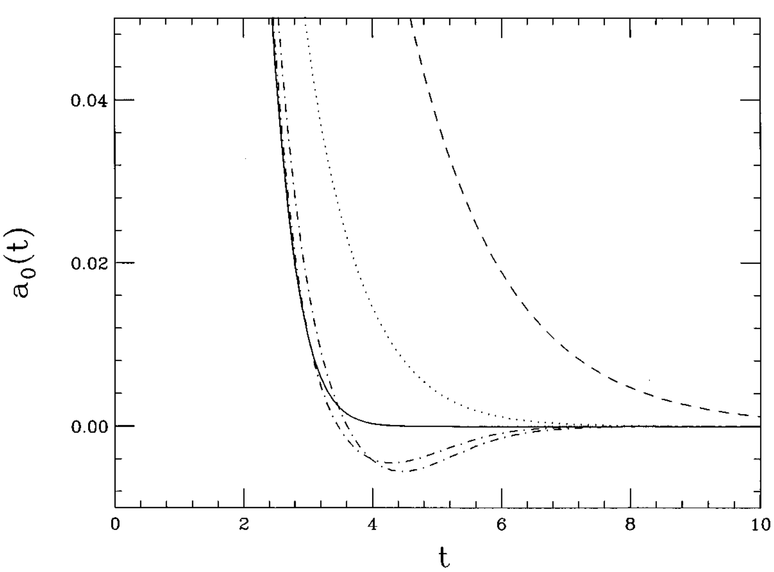

FIG. 3. Plot of the dynamical spin-pair correlation function for the next-nearest-neighbor transverse Ising model with $J_1 = 2$, $h = 1$ at $T = \infty$. The solid line represents the $J_2 = 0$ case for which $a_0(t)$ is a Gaussian. The dot-dashed line with a minimum at $t \approx 4.4$ and the same with a minimum at $t \approx 4.2$ represent $J_2 = \frac{1}{4}$ and $J_2 = \frac{1}{2}$ cases, respectively. The dotted line is for $J_2 = 1$ while the dashed line is for $J_2 = 2$.

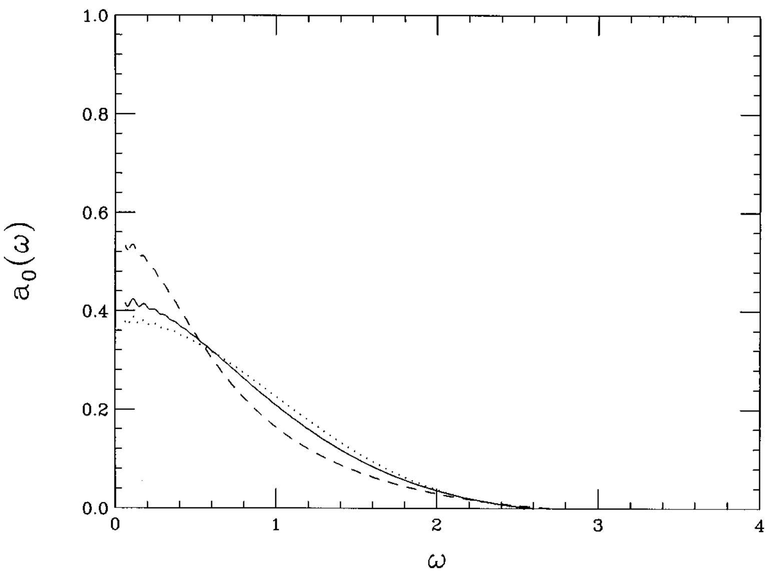

FIG. 4. Plot of the spectral functions of the quantities in Fig. 3. We do not show the plots for $J_2=\frac{1}{4}$ and $\frac{1}{2}$ cases because it is very difficult to resolve the differences between these cases and the $J_2=0$ case when obtaining their spectral functions. The dotted line is for $J_2=0$, the solid line is for $J_2=1$ and the dashed line is for $J_2=2$. Observe that the central peak increases in weight as J_2 is increased, thus implying that slower dynamics emerged as $J_2 \to J_1$.

inevitably creeps in from the numerical calculation that is involved in obtaining the frequency domain result.

In Fig. 4 we present the spectral function corresponding to $a_0(t)$ presented in Fig. 3. The dotted line represents the spectral function for the $J_2=0$ case. The solid line represents the same for the $J_2=1$ case and the dashed line shows the $J_2=2$ case. It is obvious from Fig. 4 that the system exhibits progressively slower dynamics as J_2 is tuned up from $J_2=0$ to $J_2=J_1=2$ as expected from the results in Fig. 3. This is manifested via the central peak in $a_0(\omega)$ becoming progressively dominant, thus showing that low frequency and hence longer time relaxation processes are becoming more and more important as J_2 competes in magnitude with J_1. The reader may note that the small oscillations in $a_0(\omega)$ in Fig. 4 enter from numerical errors in computing $a_0(\omega)$ and have no physical significance.

V. SUMMARY

In this work we have discussed the effects of incorporating second-nearest-neighbor interactions on the relaxation processes in simple $s=\frac{1}{2}$ spin chains. To begin with, we have demonstrated via an exact calculation that the introduction of next-nearest-neighbor interactions results in the entry of a multitude of frequencies in the characterization of the dynamical process. This point becomes especially clear when one considers a nonergodic dynamical system such as the transverse dynamics of the Ising model (see Sec. III) which is characterized by a finite number of frequencies.

We next consider the dynamics of one of the simplest quantum spin chains, namely, the $s=\frac{1}{2}$ transverse Ising chain, and consider relaxation processes in this system in the presence of next-nearest-neighbor interactions. We show that for this ergodic system, the relaxation processes are significantly affected at intermediate and at long times (see Fig. 3). The effects are rather distinct when one considers the spectral function corresponding to the relaxation functions studied (see Fig. 4).

The results presented in this paper are valid for the temperature regime $T\to\infty$. The effects of incorporating second-nearest-neighbor interactions are not obvious in the study of low-T dynamics from our work. One might expect that if the ground state and the low-lying states of the system are strongly affected by a competitive J_2 the low-temperature dynamics will be significantly altered with respect to the nearest-neighbor model. Also, the calculations discussed in this article strongly suggest that similar behavior of relaxation processes is expected for other simple quantum spin chains such as the XY and XXZ chains. The effect of including the next-nearest-neighbor interactions on relaxation processes in ergodic systems is unknown in systems[26] with lattice dimension greater than 1.

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