Dynamical correlations and the direct summation method of evaluating infinite continued fractions

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The Mori-Lee formalism for solving the Liouville (or Heisenberg) equation of motion for Hermitian systems demonstrates that the Laplace-transformed dynamical correlations in canonical ensembles can be written as (in)finite continued fractions. We show that a model-independent direct summation method allows accurate numerical evaluation of *all* known classes of these (in)finite continued fractions that arise in dynamics problems and thus provides a powerful technique to study the dynamics of many-body and few-body systems. Some studies on dynamical correlations in $s = \frac{1}{2}$ quantum spin chains are cited as applications of the method presented.

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I. INTRODUCTION

There is currently a strong interest in studying dynamical phenomena in the physical and biological sciences [1–3]. Of key concern in most studies is the long-time behavior of dynamical correlations such as $\langle A(t)B(0)\rangle$, A, B being dynamical variables. For most interacting classical and quantum many-body and few-body systems, long-time simulation studies in canonical ensembles are seldom possible due to computational constraints [4–6]. Furthermore, time-evolution studies via simulations are more computationally intensive because of the two-point nature of the time correlations of interest. Therefore, in recent years, there has been a renewed interest in solving the Liouville (or Heisenberg) equation of motion for $A(t)$ in a canonical ensemble [7, 6, 8]. A formal way of solving the Liouville (or Heisenberg) equation of motion for Hermitian (i.e., nondissipative) systems with time-independent Hamiltonians is by using the continued-fraction (CF) formalism, originally due to Mori [9] and later developed by Lee [7]. This formalism allows one to study the dynamics of any Hermitian system whether ergodic or not within the context of a canonical ensemble [5].

Infinite continued fractions (ICF's) can seldom be exactly evaluated [8–11]. Therefore, historically, ICF's have posed a challenge to mathematicians and to theoreticians in physics and related disciplines. Often the usefulness of the CF formalism itself has been questioned [12]. The use of ICF's has either been avoided in favor of some other methods [13] of study (such as mean-field techniques, dynamic scaling or simulations) which do not rely on the CF representation or has been handled using a variety of *truncation functions* [14–17]. There have been two distinct approximation schemes used to evaluate these ICF's. One technique has centered on truncation with N poles (N being small, 3 being quite common) and replacing the $(\infty - N)$ poles via some ad hoc truncation function typically derived from some experimentally obtained spectra [4, 14–17]. In time it turned out that these N-pole approximation schemes were, at best, only of limited use. Recently, Hong and Lee [18] proposed a second, more general method, a perturbative approach for evaluating some ICF's when a closely related ICF is exactly soluble. This approach, while useful, suffers from the handicap that few exactly soluble cases exist. Fortunately, as we shall see later in this article, it turns out that many of the ICF's of interest in studying many-body relaxation phenomena can be approximated by a finite but large number of poles.

It may be noted that the ICF representations are also routinely used in density of states (DOS) studies as well as in studying diffusive properties of incompressible flows [19]. In these studies ICF's are often replaced by a few (say 10) poles. It may be noted that these calculations could become somewhat complicated in the presence of singularities in the DOS and require that the ICF's be approximated by as many as 20–30 poles [19]. DOS calculations, however, typically involve a tight-binding picture and hence a one-body approach. The kind of dynamical problems we are focusing upon here, on the other hand, involve interacting many body systems. Replacing an ICF by a 10-pole finite CF (FCF) almost always leads to extremely poor results for long-time relaxation functions in the real time domain in our systems of interest. The number of poles necessary for accurate evaluation of various classes of ICF's will be discussed at length in Sec. III of this article. Therefore, for the Mori-Lee for-

malism to be truly useful for studying the dynamics of a large variety of physical systems, it is essential to develop a theoretical framework for approximating ICF's which cannot be replaced by a few poles [8]. Thus ICF's in the CF formalism must be handled in a more general manner.

In this article we present an efficient and reliable method to evaluate numerically a large class of ICF's that are often encountered in studying dynamical correlations in many-body and one-body systems. We begin with a brief overview of the Mori-Lee formalism in Sec. II, followed in Sec. III by a discussion on the evaluation techniques of the ICF's using the direct summation method (DSM). Section IV presents several applications of the DSM to a variety of many-body dynamics problems. Section V summarizes this work.

II. OVERVIEW OF THE MORI-LEE FORMALISM

The Liouville (or Heisenberg) equation, as stated above, can be formally solved via the Mori-Lee formalism described as follows [7, 9]. In this formalism one attempts to construct satisfactory solutions to two recurrence relations (RR's). It turns out that the solution to these RR's are automatically solutions to the Liouville (or Heisenberg) equation for Hermitian (i.e., nondissipative) systems.

Consider a dynamical variable $A(t)$ in some d-dimensional vector space $\mathcal{S}$. Then $A(t)$ undergoes a sweeping motion in $\mathcal{S}$ governed by the Liouville (or Heisenberg) equation of motion. The space $\mathcal{S}$ is realized by a physically meaningful inner product, namely, the Kubo scalar product (KSP). The motion of A in $\mathcal{S}$ describes a trajectory which traces a hypersurface in $\mathcal{S}$. It turns out that the dimensionality d and the structure of this hypersurface completely characterize the time evolution problem for Hermitian Hamiltonians.

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

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

where L is the Liouville operator, i.e., it denotes a Poisson bracket $\{,H\}$ for a classical system and denotes a commutator bracket $(i/\hbar)[H,A]$ for a quantum system. Formally, for an operator $A(t)$ in $\mathcal{S}$ one can write down an orthogonal expansion

$$A(t) = \exp(iHt)A\exp(-iHt) = \sum_{n=0}^{d-1} a_n(t) f_n, \tag{2}$$

where $\{f_n\}$ is a complete set of orthogonal basis vectors that span $\mathcal{S}$. The inner product in $\mathcal{S}$ is the KSP 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 being the Boltzmann constant, T being the temperature, X and Y being vectors in $\mathcal{S}$, $X(\alpha) = \exp(-\alpha H)X\exp(\alpha H)$, and the angular brackets denote canonical ensemble averages. The individual terms in the right-hand side (RHS) 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 in the left-hand side (LHS) of Eq. (2) is temperature independent.

If $\mathcal{S}$ is realized by the KSP, then the orthogonal $\{f_n\}$ can be obtained via the following RR (referred to as RR I) for the basis vectors:

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

where $\Delta_n = (f_n, f_n)/(f_{n-1}, f_{n-1}) \equiv \| f_n \| \,/\, \| f_{n-1} \|$, $1 \le n \le d-1$ are the relative norms of the basis vectors referred to as *recurrants*.

Since Eq. (2) must satisfy Eq. (1), RR I leads to a second recurrence relation for the $a_n(t)$'s. This RR, i.e., RR II, is given below:

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

Thus, RR I and RR II completely determine $A(t)$, which satisfies the Liouville (or Heisenberg) equation of motion. If we choose f_0 as $A(0)$, then $a_0(t) = (A(t), A(0))/(A,A)$. Our choice renders $a_n(0) = 0$, $n \neq 0$. Note as a result that $da_0(0)/dt = 0$, which 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 [20].

Upon Laplace transformation RR II [see Eq. (5)] yields [7] the following expression for $a_0(z)$:

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

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. We shall return to a discussion on the nature of Δ_n's later in Secs. III and IV. Formally, if Δ_n's are known, the relaxation function $a_0(t)$ can be obtained. The evaluation of the ICF's of the form in Eq. (6) above will be the main topic of discussion in this article.

For some systems it is possible to obtain $\{\Delta_n\}$ exactly. However, it turns out that for most physical systems of interest one can obtain only the first few Δ_n's (typically, the first 5–30 depending upon the Hamiltonian). The remainder of the Δ_n's often have to be obtained through some extrapolation scheme. For most ergodic as well as nonergodic systems (a *completely* nonergodic system is one in which there rigorously is a finite number of Δ_n's only [5]) there are an infinite number of Δ_n's. We will return to a more elaborate discussion on Δ_n's in Sec. III. Perhaps not so surprisingly, even when $\{\Delta_n\}$ is given, evaluation of Eq. (6) is a challenge. As stated in Sec. I, various approximation schemes [15, 17] have been used to evaluate the ICF above with limited success.

III. THE DIRECT SUMMATION METHOD OF EVALUATING ICF'S

While using 3 or 5 poles with truncation functions for approximating ICF's yields satisfactory results for a few classes of ICF's [14], the form of the truncation function can usually be determined based on some ansatz. Typically, this ansatz depends on the properties of the ICF which is to be evaluated.

A better approximation for the ICF's is often possible using the Hong-Lee [18] dynamical convergence method. As mentioned in Sec. I, in this method one usually finds an exactly soluble ICF, $a_0^{(0)}(z)$, that is closely related to the ICF, $a_0(z)$, that needs to be solved. Suppose Δ_n's are the recurrants characterizing the $a_0(z)$ to be solved while Δ_n^0 are those characterizing $a_0^{(0)}(z)$. Let $\Delta_n \to \Delta_n^0$ for some large $n \geq L$. Then,

$$a_0(z) = \cfrac{1}{z + \cfrac{\Delta_1}{z + \cfrac{\Delta_2}{z + \cfrac{\Delta_3}{z + \cdots \cfrac{\Delta_L \alpha_L}{z}}}}}, \tag{7}$$

where $\alpha_L(z)$ is a function of Δ_n^0 with $n \geq L$ (see the Appendix). If the problem is such that $\Delta_L \to \Delta_L^0$ for small L, say, L=3, 4, or 5, etc., then the Hong-Lee scheme works very well [18]. If, on the other hand, $\Delta_L \to \Delta_L^0$ for larger L, say, $L > 10$ or so, this scheme leads to inaccurate results for $a_0(t)$. The reason for this inaccuracy lies in the fact that for $L > 10$ or so, $a_0(z) = N(z)/D(z)$ (see the Appendix) involves division between large numbers which most computers are unable to handle accurately. Indeed such problems are well known in the high-temperature-series-expansion literature [21].

It may be noted that the Hong-Lee scheme is especially well suited for the study of ICF's in which $\Delta_n = n^x$, $x > 2$. In such cases, the DSM converges slowly and becomes impractical to implement. However, such fast growth rates for Δ_n, as far as we are aware of, are almost never realized in many-body problems [22]. To summarize, in practice, the Hong-Lee scheme works well for $L < 10$. It turns out that there are physical many-body Hamiltonians in which one must go to $L \gg 10$ for reliable results. For such problems this scheme becomes increasingly difficult to implement on a computer. Of course, a major drawback of the Hong-Lee scheme lies in the fact that the scheme is of little use when a closely related soluble ICF is unavailable.

Thus one can argue that the effort one must spend on extracting a truncation function or in finding an appropriate soluble ICF to implement the Hong-Lee scheme is no less demanding than in evaluating the ICF itself via some other *computational* method. One such approach is to replace the ICF by a FCF. Thus we get $\alpha_L = 0$ in Eq. (7) for some large L in this scheme. How large L must be is sensitive to the properties of the ICF under study. Specifically, 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 availability of powerful computers, the evaluation of a FCF with as many as 10^5 poles ($\alpha_L = 0 \Rightarrow L$ poles) is readily possible. In fact, for some ICF's that appear in many-body dynamics problems [8], as few as 10^3 poles faithfully represent the relaxation function up to long enough times such that the asymptotic behavior of dynamical correlations can often be reliably extracted from the available information.

A. The sequence of Δ_n's

A standard problem in evaluating an ICF as an FCF with a large L lies in the determination of Δ_n itself. The determination of Δ_n is often the most difficult step in evaluating the ICF. It appears that for most interacting many-body problems it is practically impossible to obtain Δ_n for $n > 30$ or so, depending upon the spatial dimensionality of the problem and the nature of the interactions. One way of getting around this difficulty is to obtain some approximate form for the large-n behavior of Δ_n's through some acceptable extrapolation scheme.

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 [see Eq. (4)]. However, it turns out that for problems often encountered in many-body and one-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 long-time behavior of the relaxation function to be eventually calculated is not too sensitive to the exact values of the higher-order Δ_n's but rather depends instead more crucially upon certain general features of the higher-order Δ_n's, such as their n dependence.

So far the CF formalism has been used to study relaxation phenomena in a variety of simple many-body and one-body systems. A list of the major studies includes (i) density response in a quantum electron gas at $T = 0$ in the long-wavelength limit [18], (ii) two-spin relaxation function of the total spin operators in the Kittel-Shore model at all temperatures [23] and on-site dynamical spin relaxation in the one-dimensional XY and transverse Ising models at both $T = 0$ and at $T = \infty$ of [24–29], (iii) velocity autocorrelation function for a tagged mass in an infinite classical and quantum simple harmonic oscillator chain [30], and (iv) velocity autocorrelation functions of an oscillator in a single double-well, and in a quartic well (Duffing oscillator) at all temperatures [6].

In all these problems, Δ_n has been obtained for $1 \leq n < \infty$ either exactly or approximately. Many of the cases listed above can be described via ICF's that are exactly soluble. We have successfully compared our DSM calculations for those cases against the exact calculations. In cases where the exact results cannot be obtained, we have used extrapolation schemes to approximate large-n behavior of Δ_n's and have obtained reliable results.

The studies reveal that a general feature in most of these problems is that Δ_n can be generally described as $\Delta_n = n^x$ for large enough n where typically $0 < x <$

2. A second general feature is when $\Delta_{2n+1} = k^y$ and $\Delta_{2n} = k^{-y}$ where $y > 0$ say [24]. It turns out that the second case is easily soluble numerically and leads to oscillatory relaxation phenomena with the frequencies involved being sensitive to k and y. To see this behavior, observe that for $k > 1$ large k and/or y, $\Delta_{2n} \to 0$ even for small n and thus the ICF tends to naturally self-truncate thereby leading to oscillatory relaxation. We shall return to this simple behavior later.

For $\Delta_n = n^x$, $x < 0$, the ICF's again tend to self-truncate for large enough n and the relaxation phenomena exhibit oscillatory behavior. These ICF's can be accurately replaced by FCF's with less than 10^3 poles and yield accurate results. However, there are no physical systems that we know of which exhibit $x < 0$ behavior. One should note that the CF formalism of Mori and Lee, in its present form, is a recently introduced method. So far, relatively few physical systems have been studied using this scheme. Therefore it is quite plausible that $x < 0$ exists for some important and interesting class of physical problems.

The scenario $\Delta_n = n^x$, $0 < x < 2$ is, however, common in many-body as well as one-body relaxation studies. In these cases, $L = 10^\zeta$ typically has $3 \leq \zeta \leq 5$. The density response in a quantum electron gas at $T = 0$ in the long-wavelength limit is characterized by $x = 0$ behavior in two and three dimensions [18]. Relaxation of tagged two-spin correlations at $T = \infty$ in the semi-infinite quantum spin chain is characterized by $0 \leq x \leq 1$ depending upon the location of the spin. The surface spins exhibit $x = 0$ behavior while the bulk spin exhibits $x = 1$ behavior. The dynamics of the intermediate spins are characterized by $0 < x < 1$. The velocity autocorrelation function in an infinite classical simple harmonic oscillator chain is characterized by $x = 0$ behavior. There are some one-body and two-body problems in which the growth rates can be faster, say $2 < x < 3$ [22]. These are, however, rare and hence will not be addressed here. We have found that the DSM can handle $0 < x < 1$ very well. The calculations become computationally intensive but remain feasible for $1 < x < 2$. This method is no longer feasible for growth rates $x \geq 2$.

We will illustrate the use of DSM by applying it to some quantum spin chains. The choice of quantum spin chains is dictated by the fact that these strongly anharmonic systems have been rather extensively studied and are known to exhibit a rich variety of growth exponents in their Δ_n's.

B. Time regime for relaxation studies

The number of poles L needed to accurately evaluate an ICF using the DSM is sensitive to the time regime for which relaxation processes are being studied. For specificity we shall assume $0 \leq t^* \leq 100$, where t^* is t scaled by the appropriate coupling that sets the time scale for the dynamics of the system under study. Thus, in magnetic systems, $t^* = Jt$ where J is the coupling and for a harmonic oscillator $t^* = \mu t$ where $\mu = \sqrt{(\kappa/m)}$, κ being the spring constant and m being the oscillator mass. We shall drop the asterisk in t from now on for notational simplification.

First let us compare this simple truncation scheme with short-time expansion. One can show that [6] the short-time expansion of $a_0(t)$, obtained via inverse Laplace transform (ILT) of $a_0(z)$ is always an infinite series whether $a_0(z)$ in Eq. (7) is finite or infinite. Thus

$$a_0(t) = 1 - \Delta_1 t^2/2! + \Delta_1(\Delta_1 + \Delta_2)t^4/4! - \Delta_1[(\Delta_1 + \Delta_2)^2 + \Delta_2\Delta_3]t^6/6! + \Delta_1[(\Delta_1 + \Delta_2)^3 + \Delta_2\Delta_3(\Delta_1 + \Delta_2) + \Delta_2\Delta_3(\Delta_1 + \Delta_2 + \Delta_3 + \Delta_4)]t^8/8! - \cdots . \quad (8)$$

Observe that due to the two-point nature and time reversal invariance of $a_0(t)$, only terms with even powers of t appear in Eq. (8). We also observe that Δ_n's appear in such a way that they *persist* in terms of order t^m, $m > 2n$. Higher-order Δ_n's are unimportant if we are interested in short-time behavior. The accuracy of $a_0(t)$ obtained in DSM of order n is thus exact to $O(t^{2n})$ in the time domain and approximate beyond. This accuracy is, however, difficult to achieve if one carries out the same calculation in the time domain itself by expanding $a_0(t)$ directly without using CF representation of $a_0(z)$ and expanding the latter. The difficulties with accuracy in our CF approach arises when the time series is slowly convergent and when the cancellations between the coefficients of terms of $O(t^{2n})$, where n is a large number, in the power series in time in Eq. (8) introduce significant errors [8].

For noninteger x, it is typically not possible to calculate ICF's analytically. 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. In addition, one can and should also check whether the FCF is sensitive to L being 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*.

We have calculated $a_0(t)$ numerically for various values of x and L. The computation of the inverse Laplace transform is based on the paper of Crump [31], who uses 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

$$a_0(t) \approx \frac{\exp(bt)}{\tau}\left[\tfrac{1}{2}a_0(b) + \sum_{k=1}^{\infty}\left\{\mathrm{Re}a_0\left(b+\frac{ik\pi}{\tau}\right)\cos\left(\frac{k\pi t}{\tau}\right) - \mathrm{Im}a_0\left(b+\frac{ik\pi}{\tau}\right)\sin\left(\frac{k\pi t}{\tau}\right)\right\}\right], \quad (9)$$

where Re and Im denote real and imaginary parts, respectively, and b is a number bigger 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 Eq. (9) is carried out. $a_0(z)$ is calculated numerically using Eq. (7) for various values of x and L.

For ICF's with $\Delta_n = n^x$, we find that for $x < 0$, $2 \le \zeta \le 3$, where $\zeta = \log_{10} L$, is sufficient for evaluating Eqs. (7) and (8) *accurately* for $t \le 10^2$ where accuracy implies that there is no observable dependence within the accuracy of the calculations on the odd-even effect. For $0 \le x \le 1$, $3 \le \zeta \le 4$ is sufficient. We have numerically evaluated the exactly soluble cases of $x = 0$ and 1 up to $\tau = 10^2$. The former leads to $a_0(t) \propto 2J_1(\alpha t)/\alpha t$, where α is some scale factor ($\alpha = 1$ here) and J_1 is a first-order Bessel function while the latter leads to $a_0(t) \propto \exp(-\beta t^2/2)$, i.e., Gaussian decay with β being some scale factor ($\beta = 1$ here). In both of these cases our numerical evaluations are in excellent agreement with the exact solutions for the chosen time interval. In the former case, the oscillatory-algebraic decay of $t^{-3/2}\cos(t - 3\pi/4)$ is recovered at large t ($t \approx 10^2$) [8].

The numerical evaluation of Eqs. (6) and (9) via DSM becomes significantly more difficult when $x > 1$. Figure 1 shows the minimum truncation level L needed to obtain correct values of $a_0(t)$ as a function of t for various values of x. As x increases, it is more and more difficult for $a_0(t)$ to converge. For $x > 1.5$, it takes an extremely long CPU time to get the correct value of $a_0(t)$ for $t > 20$. The results cannot be significantly improved with larger L either, as shown in Fig. 2.

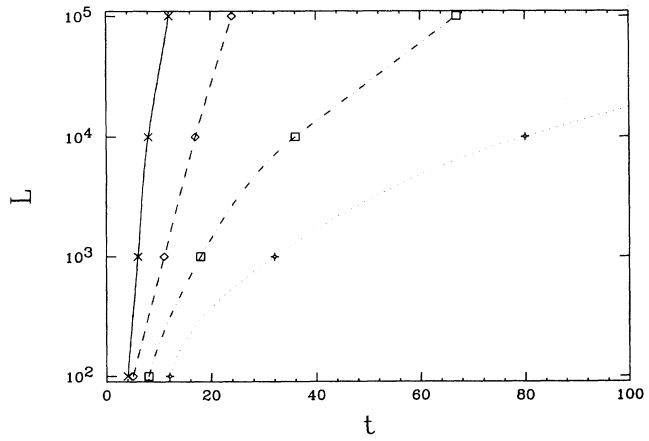

FIG. 1. The minimum truncation level L needed to obtain the correct value of $a_0(t)$ as a function of t for various values of x (which is defined in $\Delta_\mu = \mu^x$. $\times$ is for $x = 2$, $\diamond$ is for $x = 1.75$, $\square$ is for $x = 1.5$, and the cross is for $x = 1.25$. The lines are guides to the eye.

Figure 2 shows the $a_0(t)$ versus t curve for $\Delta_n = n^2$ obtained numerically for $L = 10\,000$ as compared to the exact solution $[a_0(t)|_{\text{exact}} = 1/\cosh(t)]$ [11]. The sharp spike in the numerically evaluated $a_0(t)$ reveals the strong dependence of the calculated FCF on the oddness or evenness of L. Clearly, the results obtained in this case are *not* convergent. As shown in Fig. 2, the agreement between exact and DSM results for $x = 2$ is accurate only up to $t = 10$ and cannot be improved much by increasing L by an order of magnitude. This example emphasizes that in the absence of exact results one should check for the odd-even effect to ensure the accuracy of $a_0(t)$.

IV. APPLICATIONS OF THE DSM TO PHYSICAL SYSTEMS

We present below two cases in which the DSM calculations lead to dynamical correlations in excellent agreement with exactly known results. The choice of the cases presented here is dictated by the fact that these pertain to studies of dynamical correlations in $s = \frac{1}{2}$ quantum spin chains which have been solved within the past few years.

A. Case 1: Dynamical correlations in a semi-infinite XY chain at $T = \infty$

Recently, we had published our calculations on the dynamic correlation functions of the surface spin $\langle S_j^x(t)S_j^x\rangle$ and the subsurface spin $\langle S_{j+1}^x(t)S_{j+1}^x\rangle$ in a semi-infinite spin-$\frac{1}{2}$ XY chain at infinite temperature, with $1 \le j \le \infty$

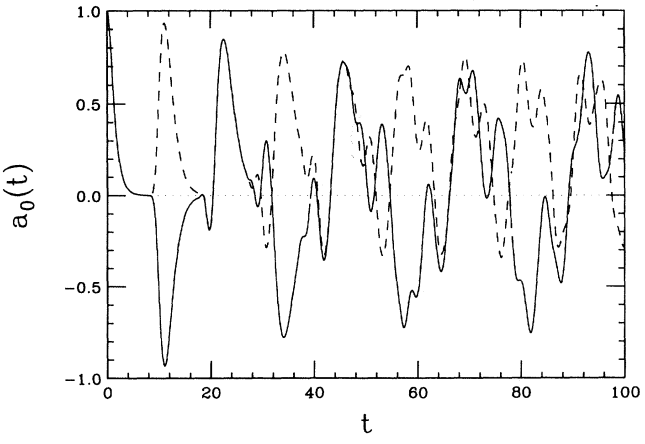

FIG. 2. $a_0(t)$ vs t for $\Delta_n = n^2$. The dotted line is the exact solution, the dashed line is the numerical result for $L = 10\,000$, the solid line is the numerical result for $L = 10\,001$. The differences between the dashed and solid lines illustrate the manifestations of the *odd-even effect.*

[24]. We were able to solve for the surface spin dynamics exactly. In fact, this case corresponds to $\Delta_n = \frac{1}{4}$ under appropriate scaling and leads to $a_0(t) = 2J_1(t)/t$. The subsurface spin, however, was much more difficult to solve. We calculated the first five Δ_n's exactly for that case. These were $\Delta_1 = \frac{1}{2}$, $\Delta_2 = \frac{7}{8}$, $\Delta_3 = \frac{67}{56}$, $\Delta_4 = \frac{1319}{938}$, and $\Delta_5 = \frac{90\,692\,374}{580\,257\,118}$. We then approximated the Δ_n's by a straight line extrapolation for $5 < n < \infty$ on the basis of the available results and given by $\Delta_n = (0.05)(n-4) + 1319/938$. We then summed up the resulting ICF using the direct summation scheme described here with $L = 10^4$. We have learned recently that using a different approach Stolze and co-workers [26] have obtained a closed form expression for the subsurface spin correlation function given as

$$a_0(t) = [J_0(t) + J_2(t)]\ \{[J_0(t) + J_2(t)][J_0(t) - J_4(t)] + [J_1(t) + J_3(t)]^3\}, \qquad (10)$$

where J_n's are Bessel functions of order n. The agreement between the Stolze formula and our approximate result is excellent as shown in Fig. 3. The impressive agreement between Stolze's result and ours can be readily attributed to the linear growth rate of the Δ_n's with n in this problem and hence the rapid convergence of the ICF under study. One should expect similar highly accurate results for all ICF's with effective growth rates that are less than quadratic in n. This successful prediction confirms that long-time behavior of strongly anharmonic systems can indeed be studied using this direct summation scheme for ICF's. Our earlier prediction that subsurface and inner spins rapidly go to bulk behavior (which is Gaussian decay), based on the numerical evaluation of ICF's using the direct summation scheme, is also confirmed by the analysis of Stolze.

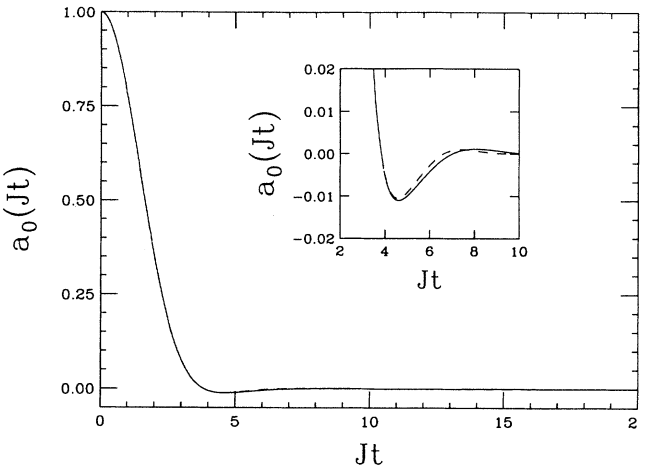

FIG. 3. $a_0(t)$ vs t for the subsurface spin of the semi-infinite XY chain at infinite temperature. The solid line is the result obtained using the formula of Stolze and co-workers [26]. The dashed line is the direct summation result [24]. The inset magnifies the regime where the two results differ the most.

B. Case 2: Dynamical correlations in a transverse Ising chain at $T = 0$

Recently [27], Lee and Kobayashi were able to solve for the relaxation function of the magnetization and the energy operators in a $s = \frac{1}{2}$ transverse Ising chain at $T = 0$. The calculations in [27] were performed for small σ, where $\sigma = -1/\ln|\epsilon|$, $\epsilon = (h - h_c)/h_c$, $h_c = J/2$, J and h being the Ising (between nearest-neighbor z components of the spin operators) and field couplings (along the x direction), respectively. It has been shown that the recurrants for the relaxation functions under study in this model are

$$\Delta_1 = (1+\epsilon)J^2\sigma/3, \qquad (11)$$

$$\Delta_{2n+1} = (1+\epsilon)J^2[2n(2n+1)/(4n+3)(4n+1)][1 + (4n+1)\sigma/2n(2n+1)], \qquad (12)$$

$$\Delta_{2n} = (1+\epsilon)J^2[2n(2n+1)/(4n+1)(4n-1)][1 - (4n+1)\sigma/2n(2n+1)], \quad n \geq 1 \qquad (13)$$

to $O(\sigma)$. The ICF corresponding to the Δ_n's above is solvable as shown in [27]. However, the result in [27] is not correctly linearized. The error can be trivially corrected by expanding the results in [27] to $O(\sigma)$ and is given by

$$a_0(z) = (z)^{-1}[1 - (\sigma/3)(J^2/z^2)F(1,1;5/2;-J^2/z^2)], \qquad (14)$$

$F(1,1;5/2;-J^2/z^2)$ being the hypergeometric function which when inverse Laplace transformed gives the relaxation function $a_0(t)$ given in Fig. 4. The rise in the magnitude of $a_0(t)$ at $t = 100$ in Fig. 4 is real and not an artifact of the calculations. Indeed it occurs in both the exact and the DSM results. Clearly then, the relaxation function has some oscillations even at $t = 100$ in this problem. The ICF characterized by the above Δ_n can be readily evaluated via DSM. The Laplace-transformed DSM result is plotted with that obtained via numerical inverse Laplace transform of $a_0(z)$ given above. The plot reveals remarkable agreement between the exact result obtained by plotting Eq. (14) and those using DSM results.

The above two cases demonstrate that the DSM leads to remarkably accurate results for many-body dynamical correlations. Since the spatial dimensionality of the problem under study does not enter into the DSM approach, we expect that this method will give equally good results for higher-dimensional problems.

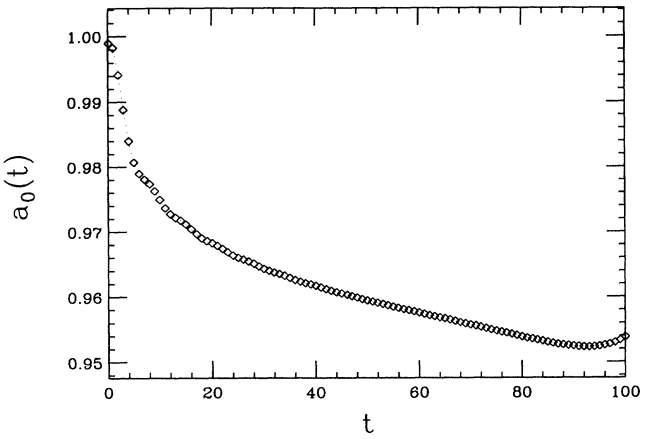

FIG. 4. Plot of $a_0(t)$ vs t for the transverse Ising chain at $T = 0$ using the exact result in Eq. (14) (dotted line) against the result obtained via DSM with $\zeta = 4$ (diamond). The difference between the two results is smaller than the line width in the figure.

V. SUMMARY

To summarize, we have presented a simple method of evaluating infinite continued fractions. We believe that this method is extremely useful for long-time dynamics studies of many-body and one-body systems in canonical ensembles. The *direct summation method* involves replacing an infinite continued fraction by a large finite continued fraction with $L = 10^{\zeta}$ poles with $3 \leq \zeta \leq 5$ poles. The ζ value necessary for accurate evaluation of dynamical correlations is determined by the nature of the recurrents which characterize the continued fraction and by the time regime in which the dynamical correlation is being studied (see Fig. 1). We have sketched several applications of the DSM to physical systems in this article (see Figs. 3 and 4).

We have included an appendix with this article, to generalize the Hong-Lee dynamical convergence scheme of evaluating ICF's for studying dynamical correlation functions in canonical ensembles. We believe that the general formulas can be readily included in a simple FORTRAN program for evaluating insoluble ICF's (i.e.,with quadratic or faster growth rates in Δ_n) when a closely related soluble ICF exists. We have pointed out that the only difficulty in implementing the generalized Hong-Lee scheme for large L values lies in one's ability to handle large roundoff errors when division between large numbers is involved. Until now, we have had limited success with the generalized Hong-Lee scheme [32]. We hope, however, that some of our readers will find the materials presented here to be insightful in understanding the behavior of ICF's and will perhaps be able to devise an accurate way to obtain higher-order Hong-Lee scheme calculations.

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APPENDIX

With reference to the discussions in Sec. III, one can approximate an insoluble ICF by writing it in terms of some soluble ICF beyond L levels. If L is sufficiently large and if the insoluble ICF is such that $\Delta_n \to \Delta_n^0$, where Δ_n^0's pertain to the recurrants of the soluble ICF, then the following simple expressions may be useful in evaluating the insoluble ICF. Let $a_0(z)$ and a_0^0 be the insoluble and the soluble ICF's, respectively, as given below,

$$a_0(z) = \cfrac{1}{z + \cfrac{\Delta_1}{z + \cfrac{\Delta_2}{z + \cfrac{\Delta_3}{z + \cdots \text{ to } \infty}}}}, \tag{A1}$$

$$a_0^{(0)}(z) = \cfrac{1}{z + \cfrac{\Delta_1^0}{z + \cfrac{\Delta_2^0}{z + \cfrac{\Delta_3^0}{z + \cdots \text{ to } \infty}}}}, \tag{A2}$$

where $\Delta_n = \Delta_n^0 + \epsilon_n$ and $\{\Delta_n^0\}$ and $\{\epsilon_n\}$ are known. Further, it is necessary to require that there exist some integer p $(0 < p < \infty)$ such that

$$\Delta_p^0 > \epsilon_p. \tag{A3}$$

Then for $L > p$

$$a_0^{(L)}(z) = \cfrac{1}{z + \cfrac{\Delta_1}{z + \cfrac{\Delta_2}{z + \cdots \cfrac{\Delta_p}{z + \cdots \cfrac{\Delta_L}{z + \cfrac{\Delta_{L+1}^0}{z + \cfrac{\Delta_{L+2}^0}{z + \cdots \text{ to } \infty}}}}}}}, \tag{A4}$$

where

$$\lim_{L \to \infty} a_0^{(L)}(z) = a_0(z). \tag{A5}$$

For finite L, the error E_L in Eq. (A4) can be estimated as follows:

$$E_L \equiv |a_0^{(L)}(z) - a_0^{(L+1)}(z)| / a_0^{(L)}(z). \tag{A6}$$

Now,

$$a_0^{(L)}(z) = \cfrac{1}{z + \cfrac{\Delta_1}{z + \cfrac{\Delta_2}{z + \cdots \cfrac{\Delta_p}{z + \cdots \cfrac{\Delta_L}{\alpha_L}}}}}, \tag{A7}$$

where

$$\alpha_L \equiv \cfrac{\Delta_{L+1}}{z + \cfrac{\Delta_{L+2}}{z + \cdots \text{ to } \infty}}. \tag{A8}$$

One can always show that

$$a_0^{(L)} = N^{(L)}(z)/D^{(L)}(z), \tag{A9}$$

where

$$N^{(L)}(z) = \sum_{n=0}^{L-1} z^n \Gamma_{L-1-n}^{(L)}, \tag{A10}$$

and

$$D^{(L)}(z) = \sum_{n=0}^{L} z^n \Lambda_{L-n}^{(L)}. \tag{A11}$$

The coefficients $\Gamma_{L-1-n}^{(L)}$ and $\Lambda_{L-n}^{(L)}$ are given as follows:

$$\Gamma_0^{(L)} = \Lambda_0^{(L)} = 1, \tag{A12}$$

$$\Gamma_1^{(L)} = \Lambda_1^{(L)} = \Delta_L \alpha_L, \tag{A13}$$

$$\Gamma_{2j}^{(L)} = \sum_{m_1=2j}^{L-1} \sum_{m_2=2(j-1)}^{m_1-2} \sum_{m_3=2(j-2)}^{m_2-2} \cdots \sum_{m_j=2}^{m_{j-1}-2} \Delta_{m_1} \Delta_{m_2} \Delta_{m_3} \cdots \Delta_{m_j}, \tag{A14}$$

$$\Gamma_{2j+1}^{L} \equiv \alpha_L \gamma_{2j+1}^{(L)} = \alpha_L \Delta_L \sum_{m_1=2j}^{L-2} \sum_{m_2=2(j-1)}^{m_1-2} \sum_{m_3=2(j-2)}^{m_2-2} \cdots \sum_{m_j=2}^{m_{j-1}-2} \Delta_{m_1} \Delta_{m_2} \Delta_{m_3} \cdots \Delta_{m_j}, \tag{A15}$$

$$\Lambda_{2j}^{(L)} = \sum_{m_1=2j-1}^{L-1} \sum_{m_2=2j-3}^{m_1-2} \sum_{m_3=2j-5}^{m_2-2} \cdots \sum_{m_j=1}^{m_{j-1}-2} \Delta_{m_1} \Delta_{m_2} \Delta_{m_3} \cdots \Delta_{m_j}, \tag{A16}$$

$$\Lambda_{2j+1}^{(L)} \equiv \alpha_L \lambda_{2j+1}^{(L)} = \alpha_L \Delta_L \sum_{m_1=2j-1}^{L-2} \sum_{m_2=2j-3}^{m_1-2} \sum_{m_3=2j-5}^{m_2-2} \cdots \sum_{m_j=1}^{m_{j-1}-2} \Delta_{m_1} \Delta_{m_2} \Delta_{m_3} \cdots \Delta_{m_j}. \tag{A17}$$

When L is odd the bounds on j in Eqs. (A14)–(A17) are, respectively,

$$1 \le j \le \frac{L-1}{2},$$

$$1 \le j \le \frac{L-3}{2},$$

$$1 \le j \le \frac{L-1}{2},$$

$$1 \le j \le \frac{L-1}{2}.$$

When L is even the bounds on j in Eqs. (A14)–(A17) are, respectively,

$$1 \le j \le \frac{L-2}{2},$$

$$1 \le j \le \frac{L-2}{2},$$

$$1 \le j \le \frac{L}{2},$$

$$1 \le j \le \frac{L-2}{2}.$$

Therefore, for odd and even L, α_L can be written, respectively, as

$$\alpha_L^{\rm odd} = \frac{a_0^{(0)}(z)[z_L\Lambda_0^{L(0)} + z^{L-2}\Lambda_2^{L(0)} + \cdots + z\Lambda_{L-1}^{L(0)}] - [z^{L-1}\Gamma_0^{L(0)} + z^{L-3}\Gamma_2^{L(0)} + \cdots + \Gamma_{L-1}^{L(0)}]}{[z^{L-2}\gamma_1^{L(0)} + z^{L-4}\gamma_3^{L(0)} + \cdots + z\gamma_{L-2}^{(L)}] - a_0^{(0)}(z)[z^{L-1}\lambda_1^{L(0)} + z^{L-3}\lambda_3^{L(0)} + \cdots + \lambda_L^{L(0)}]}, \tag{A18}$$

and

$$\alpha_L^{\rm even} = \frac{a_0^{(0)}(z)[z_L\Lambda_0^{L(0)} + z^{L-2}\Lambda_2^{L(0)} + \cdots + \Lambda_{L-1}^{L(0)}] - [z^{L-1}\Gamma_0^{L(0)} + z^{L-3}\Gamma_2^{L(0)} + \cdots + z\Gamma_{L-1}^{L(0)}]}{[z^{L-2}\gamma_1^{L(0)} + z^{L-4}\gamma_3^{L(0)} + \cdots + \gamma_{L-2}^{(L)}] - a_0^{(0)}(z)[z^{L-1}\lambda_1^{L(0)} + z^{L-3}\lambda_3^{L(0)} + \cdots + z\lambda_L^{L(0)}]}, \tag{A19}$$

where the superscript (0) implies Δ_n^0's instead of Δ_n's are involved in the evaluation of Γ's and Λ's.

It may be noted that the formulas in Eqs. (A18) and (A19) above may be used to evaluate ICF's with fast growth rates, i.e., when $x > 2$. Unfortunately, as mentioned earlier, it is computationally challenging to carry out the approach presented here. The primary reason for the difficulty lies in the fact that for $L > 10$ or so, the evaluation of α_L involves division between two large numbers, which contributes to large roundoff errors in the computation. However, we feel that, should there be some convenient algorithm to accurately carry out division between large numbers [21], the reader can benefit from these general formulas and incorporate them in a computer code to calculate ICF's with rapidly growing Δ_n's.

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