Asymptotic behavior of dynamical correlations via perturbative analysis of infinite continued fractions

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The continued-fraction formalism demonstrates that the Laplace-transformed dynamical correlations can be expressed as infinite continued fractions (ICF's). We propose a generalization of the dynamical convergence method (GDCM) of J. Hong and M. H. Lee [Phys. Rev. Lett. **55**, 2375 (1985)] of perturbatively evaluating insoluble ICF's when a closely related ICF is exactly soluble. The proposed method overcomes an existing limitation of the dynamical convergence method which involves accurate computing of ratios of small numbers. The limitations are surmounted by exploiting an "inversion" property of ICF's. The GDCM allows computationally fast and simple perturbative evaluation of insoluble ICF's with up to 10^{ξ}, $\xi \leq 6$, levels of the insoluble ICF when a related ICF is soluble. The method appears to be appropriate for studies of asymptotic behavior of dynamical correlations described by *slowly converging and nonconverging* ICF's, which are otherwise insoluble, when closely related soluble ICF's exist. The desirable feature of the GDCM is that the computation times required to solve the ICF's are unrelated to the details of the convergence properties. The method has been applied to recalculate the dynamical-spin pair correlation of a recently studied classical XX spin cluster. This application is described in this work.

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I. INTRODUCTION

An understanding of dynamical correlations such as $\langle A(t)B \rangle$, A and B being dynamical variables, is central to the study of nonequilibrium processes in physical systems which are slightly removed from equilibrium. For most interacting anharmonic classical and quantum systems dynamical correlations are a challenge to evaluate [1]. While simulational techniques can be useful for studying dynamical correlations [2], such approaches are often computationally intensive and hence unsuitable for extensive long-time studies. Therefore, it has become increasingly important to develop techniques which are geared to solve the Liouville equation of motion as accurately as possible to extract long-time dynamics [3].

A formal way of solving the Liouville (or Heisenberg) equation of motion is by using the continued-fraction formalism [4,5]. Using this formalism, one can express the Laplace transform of a dynamical correlation such as $\langle A(t)B \rangle$ as an infinite continued fraction (ICF) of the following form:

$$\mathcal{L}[\langle A(t)B \rangle] = 1/[z+\Delta_1/(z+\Delta_2/(z+\Delta_3/(z+\Delta_4/(z+\cdots))))] = N(z)/D(z) , \quad (1)$$

where Δ_n's are equilibrium quantities which are functions of the static correlations, $\mathcal{L}$ denotes a Laplace transform, and $N(z)$ and $D(z)$ provide an alternative way to express the ICF in Eq. (1) [see the Appendix in Ref. [5] for a detailed discussion of $N(z)$ and $D(z)$]. In general, most anharmonic systems, one obtains an infinite number of Δ_n's [5]. Typically, $\Delta_n = n^{\phi}$, $0 \leq \phi \leq 2$ being common [3]. The ICF's can be accurately approximated by a large but finite number of poles, typically of the order of a few hundred thousand to a million poles and hence via a finite continued fraction (FCF), when $\phi < 2$ [3]. In other words, the ICF's are convergent when $\phi < 2$. In most cases long-time dynamics can be studied with such FCF's and even asymptotic behavior of dynamical correlations may be occasionally estimable as in the case of two-spin dynamical correlations in the $s = 1/2$ Heisenberg and XXZ chains [5,6]. The estimation of an ICF by a FCF, however, becomes intractable when $\phi \to 2$ [3,5]. Given that quadratic growth of the Δ_n's is the limit of convergence of the ICF's of interest, this is hardly surprising [7]. For such ϕ's the ICF's can no longer be replaced by FCF's for purposes of long-time studies as shown recently in [3]. Even a FCF with 10^6 poles turns out to be grossly inadequate for long-time studies in such cases [3,5].

It turns out that $\phi \approx 2$ has been found in recent years in the study of canonical-ensemble dynamical-spin pair correlations in some classical spin clusters [8,9]. It was not possible to evaluate the ICF accurately to compute the dynamical-spin pair correlation in a recent study of a classical two-spin XX cluster [8]. Comparable growth rates have also been obtained for the canonical ensemble velocity autocorrelation function of a particle in a multiple-well potential which will be discussed in forth-

coming publications [10]. Given the current interest in cluster physics and in the dynamics of anharmonic oscillators, it is imperative that a different approach than truncation of ICF's is needed for studying the dynamical properties of clusters via the continued-fraction formalism. That is precisely the focus of this work.

This work is arranged as follows. Section II presents a brief sketch of the formalism. Section III discusses the generalized dynamical convergence method (GDCM) of approximately evaluating insoluble ICF's. Section IV describes the application of the GDCM to the study of the spin dynamics of a classical two-spin XX cluster and Sec. V closes with a summary of the work described here.

II. SKETCH OF THE FORMALISM

In this formalism, one writes [11]

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

where f_n's are time-independent bases in a Hilbert space defined by the following inner product (the following choice being motivated by the Kubo formula for susceptibility), i.e.,

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

where $\langle\ \rangle$ implies a canonical ensemble average and $X(\lambda)\equiv \exp(\lambda H) X \exp(-\lambda H)$, where H is the Hamiltonian and λ is a dummy variable for inverse temperature β, describes the "temperature evolution" of X [11]. Choosing f_0 and using the above formula to orthogonalize f_n's in the Hilbert space of f_n's one finds the following two recurrence relations which completely determine $\{f_n\}$ and $\{a_n(t)\}$ in Eq. (2) and hence completely solve the Heisenberg equation of motion. These recurrence relations are

$$f_{n+1}=i[H,f_n]+\Delta_n f_{n-1} \ , \tag{4}$$

where $\hbar\equiv 1$, $\Delta_n \equiv (f_n,f_n)/(f_{n-1},f_{n-1})$, and

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

for all $n>1$ and the last term on the right-hand side of Eq. (5) is absent for the $n=0$ case. As noted, the choice of the first basis vector f_0 is arbitrary when defining a Hilbert space. In this case, $f_0=A(0)$, turns out to be an appropriate choice and one can generate the rest of the f_n's and the $a_n(t)$'s for our problem using this choice of f_0 and using Eqs. (4) and (5). The Laplace-transformed equation (5) can be expressed as an ICF as follows [11]:

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

where the ICF above is, in general, infinite [12]. The relaxation function $a_0(t)$ can then be determined as in Eq. (1) and the higher relaxation functions then follow from Eq. (5). Evaluation of the ICF in Eq. (6) amounts to solving the second recurrence relation in Eq. (5) which, in general, is extremely difficult to solve. Nevertheless, the ICF representation of a dynamical correlation is a powerful and convenient one. While the exact solution of Eq. (6) is often not possible, approximate solutions may be obtained. An approximate estimation of Eq. (6) is therefore important.

III. GENERALIZED DYNAMICAL CONVERGENCE METHOD

In the dynamical convergence method (DCM) an insoluble ICF is approximated by substituting the insoluble ICF with a soluble ICF beyond a certain level of the ICF [13]. In the Hong-Lee DCM work [13], it turned out that it was difficult to carry out a perturbative evaluation of an insoluble ICF accurately when, typically, more than fifth-level corrections to some closely related exactly soluble continued fraction to approximate the insoluble ICF was necessary. The numerical errors in the computation of the ICF for all the z values, especially the smaller z values, became especially significant when, approximately, tenth-level corrections were to be made [5]. The primary reason for this limitation lies in the fact that the computation of the insoluble ICF as a perturbation of the soluble ICF can be viewed as a calculation of a ratio of two polynomials which typically involve division between small numbers [5]. Such problems are often encountered in high-temperature series-expansion studies in physics for instance [14]. The numerical accuracy therefore becomes difficult when the ratio of small numbers can be a large number and hence the difficulties concerning the practical implementation of the DCM.

The GDCM under discussion here solves the difficulty of doing the DCM with a large number of levels. In fact, the GDCM allows one to construct an ICF with little effort when some related ICF is known with as many as 10^6 corrected levels. Calculations with as many as a million poles is possible in a mini supercomputer. We expect that this huge improvement in the ability to do DCM calculations for evaluation of dynamical correlations will be of much use in realistic calculations. It appears that the study of cluster dynamics is one of the areas in which the GDCM approach might yield reliable results for dynami-

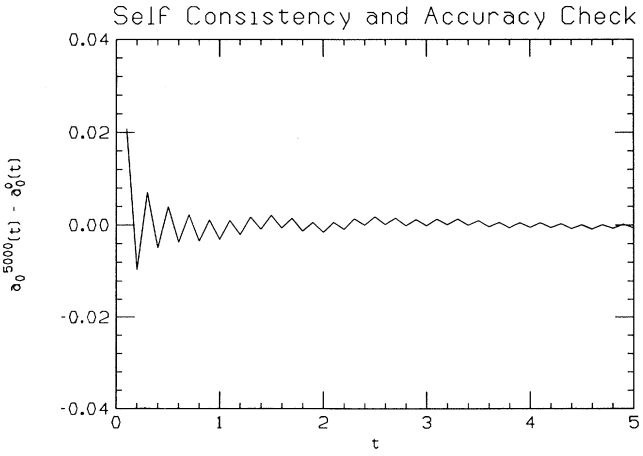

FIG. 1. Self-consistency check for $a_0^L(t)$ obtained via the inversion lemma. Observe improved accuracy at larger times. Time and frequency are scaled by $J(=1)$ in all the plots.

cal correlations. This would indeed be interesting because clusters can exhibit slow relaxation processes and can therefore, possibly, be associated with a rich variety of relaxation processes.

Formally, the GDCM can be described as follows. Let $a_0(z)$ and $a_0^0(z)$ [Eq. (6)] be, respectively, the insoluble and the soluble ICF's. Let the soluble case be given as

$$a_0^0(z)=1/[z+\Delta_1^0/(z+\Delta_2^0/(z+\Delta_3^0/(z+\cdots)))]\ , \tag{7}$$

and let $\Delta_n \to \Delta_n^0$ for large n, where Δ_n's define the insoluble ICF to be evaluated. Let $\Delta_n=\Delta_n^0+\epsilon_n$. If there exists, for all practical purposes, some regime in which $\Delta_p^0 \gg \epsilon_p$ then for $L \approx p$ we can approximate $a_0(z)$ faithfully by

$$a_0^L(z)=\cfrac{1}{z+\cfrac{\Delta_1}{z+\cfrac{\Delta_2}{z+\cfrac{\vdots}{z+\cfrac{\Delta_{L-1}}{z+\cfrac{\Delta_L}{z+\cfrac{\Delta_{L+1}^0}{z+\cfrac{\Delta_{L+2}^0}{z+\ddots}}}}}}}}=\cfrac{1}{z+\cfrac{\Delta_1}{z+\cfrac{\Delta_2}{z+\cfrac{\vdots}{z+\cfrac{\Delta_{L-1}}{z+\cfrac{\Delta_L}{\alpha_L(z)}}}}}}\ , \tag{8}$$

where we let

$$\alpha_L(z)=z+\cfrac{\Delta_{L+1}^0}{z+\cfrac{\Delta_{L+2}^0}{z+\cfrac{\Delta_{L+3}^0}{z+\ddots}}}\ . \tag{9}$$

While it is always possible to express $\alpha_L(z)$ as a quotient of polynomials in z and $a_0^0(z)$ [5], the coefficients are tedious to compute. Furthermore, the calculations of $a_0(z)$ via that approach typically involves division between small numbers which might lead to a large number as alluded to earlier. The latter is often difficult to perform accurately as is well documented in the physics and applied-mathematics literature [14]. In fact, this is precisely the drawback of doing the DCM directly to any desired high order as mentioned above. Fortunately, it is possible to express $\alpha_L(z)$ more simply as an "effectively" finite continued fraction (FCF) with L levels as below. The expression for this FCF can be obtained via an *inversion lemma* which is presented below. The "effective" FCF's can be easily calculated as demonstrated in [3,5] and no longer present any computational difficulties.

The main result of this inversion lemma is

$$\alpha_L(z)=\cfrac{-\Delta_L^0}{z+\cfrac{\Delta_{L-1}^0}{z+\cfrac{\Delta_{L-2}^0}{z+\cfrac{\vdots}{z+\cfrac{\Delta_2^0}{z+\cfrac{\Delta_1^0}{z-\cfrac{1}{z_0^0(z)}}}}}}} \tag{10}$$

Proof of the inversion lemma. Let us recall that

$$a_0^0(z)=\cfrac{1}{z+\cfrac{\Delta_1^0}{z+\cfrac{\Delta_2^0}{z+\cfrac{\Delta_3^0}{z+\ddots}}}} \tag{11}$$

and

$$\alpha_L(z)=z+\cfrac{\Delta_{L+1}^0}{z+\cfrac{\Delta_{L+2}^0}{z+\cfrac{\Delta_{L+3}^0}{z+\ddots}}}(L\geq 0)\ . \tag{12}$$

Observe that this makes $\alpha_0(z)=1/a_0^0(z)$. Therefore, it follows that

$$\alpha_L(z)=z+\cfrac{\Delta_{L+1}^0}{\alpha_{L+1}(z)}\ . \tag{13}$$

and therefore

$$\alpha_{L+1}(z)=\cfrac{\Delta_{L+1}^0}{\alpha_L(z)-z}\ . \tag{14}$$

It follows then that $\alpha_L(z)$ can be written as

$$\alpha_L(z)=\cfrac{\Delta_L^0}{\cfrac{\Delta_{L-1}^0}{\cfrac{\Delta_{L-2}^0}{\cfrac{\vdots}{\cfrac{\Delta_2^0}{\cfrac{\Delta_1^0}{\cfrac{1}{a_0^0(z)}-z}-z}-z}-z}-z}-z}=-\cfrac{\Delta_L^0}{z+\cfrac{\Delta_{L-1}^0}{z+\cfrac{\Delta_{L-2}^0}{z+\cfrac{\vdots}{z+\cfrac{\Delta_2^0}{z+\cfrac{\Delta_1^0}{z-\cfrac{1}{a_0^0(z)}}}}}}} \tag{15}$$

Q.E.D. The right-hand side of Eq. (15) is the same as that of Eq. (10).

Therefore, one can now use the following form in our calculations and exploit the existing direct summation method of evaluating FCF's recently introduced by Sen and co-workers [3,5],

$$a_0^L(z)=\cfrac{1}{z+\cfrac{\Delta_1}{z+\cfrac{\Delta_2}{z+\cfrac{\vdots}{z+\cfrac{\Delta_{L-1}}{z+\cfrac{\Delta_L}{z+\cfrac{-\Delta_L^0}{z+\cfrac{\Delta_{L-1}^0}{z+\cfrac{\vdots}{z+\cfrac{\Delta_2^0}{z+\cfrac{\Delta_1^0}{z-\cfrac{1}{a_0^0(z)}}}}}}}}}}}} \tag{16}$$

Often one finds that $\Delta_0 \to \gamma^2 \Delta_n^0$ for some problem. In these cases, one can simply substitute $a_0^0(z/\gamma)/\gamma$ for $a_0^0(z)$ and $\gamma^2\Delta_n^0$ for Δ_n^0 in the above formula.

The error in $a_0^L(z)$ can be estimated as $|a_0^L(z)-a_0^{L+1}(z)|/|a_0^L(z)|$. In order to test the accuracy and correctness of our algorithm, however we let $\Delta_n=\Delta_n^0=n^2$ for all n and set $L=5000$. A quadratic growth law for Δ_n^0 provides an exactly soluble ICF [7]. Therefore, in this special case, $a_0^L(z)=a_0^0(z)=\int_0^\infty du \exp(-zu)\operatorname{sech} u$ in Eq. (16). We then evaluate $a_0^L(z)$ using Eq. (16) by putting $a_0^0(z)$ at the $L=5000$th level. Since in this test case $\Delta_n=\Delta_n^0$, the $a_0^L(z)$ thus obtained was equal to $a_0^0(z)$. It is worth noting here that the construction of the inversion lemma allows us to perturbatively evaluate an ICF with a quadratic or faster growth rate without costing excessive computer time.

The same $a_0^L(z)$ can then be used to recalculate $a_0^0(z)$ by substituting the ICF in Eq. (16) by $a_0^L(z)$ at the 5000th level. The inverse Laplace transform of $a_0^L(z)$, i.e., $a_0^L(t)=\operatorname{sech} t$ can then be calculated numerically by integrating $a_0^L(z)$ along the line $\mathcal{R}(z)=0$ using the method of Krump [3,5,15]. This calculation yields an $a_0^L(t)$ for $L=5000$. As shown in Fig. 1, the error incurred in our GDCM calculation tends to 0 as t increases. It is important to note that the relatively large error in Fig. 1 as $t \to 0$ enters while performing the inverse Laplace transform and does not reflect any limitations of the GDCM. In fact, the $t \to 0$ calculation can always be accurately performed via short-time expansion of $a_0^0(t)$. The above calculation was also repeated for other L values and equally good results were obtained. Tests were also made with $\Delta_n=\gamma^2\Delta_n^0=\gamma^2 n^2$ by varying L and no change in $a_0^L(t)$ (for constant γ) was detected.

Two important advantages of the GDCM, which by definition permits studies of long-time dynamics, are as follows: (i) provided enough Δ_n's are known for the insoluble ICF to be evaluated and provided this ICF converges sufficiently rapidly to a soluble ICF, it may be possible to extract a significant amount of information on the asymptotic behavior of $a_0(t)$ using this method. This is precisely what we are able to obtain for the case of a two-spin XX cluster, a problem that has been recently studied by Liu and Müller [8]. (ii) It is well known [7] that ICF's with $\phi \to 2$ approach the limit of convergence, implying that they can no longer be approximated by FCF's for studying long-time dynamics. The GDCM does not rely on approximating an ICF via a FCF although it treats an insoluble ICF as an effectively FCF with the inversion lemma. Hence the computation of the insoluble ICF can be carried out efficiently in this approach.

IV. APPLICATION TO THE TWO-SPIN *XX* CLUSTER

Consider a Hamiltonian of a classical *XX* model with only two classical spins, i.e., with angular-momentum vector S_i. The Hamiltonian for this system is given by

$$H=(S_1^x\cdot S_2^x+S_1^y\cdot S_2^y)=\cos(\phi_1-\phi_2)\ , \tag{17}$$

where the angles ϕ_1 and ϕ_2 describe the orientations of the two classical vectors in the x-y plane with respect to the x axis. The Liouville equation of motion for $S_{1,2}^x(t)$ has been studied recently by Liu and Müller [8] for this problem. They find that the dynamical correlation $\langle S_{1,2}^x(t)S_{1,2}^x\rangle$ for this problem at $T=\infty$ can be described by the following sequence of Δ_n's for $1\le n\le 18$ (see Table I). The sequence appears to increase very nearly quadratically.

In what follows we present results from a calculation in which we used the first 18 Δ_n's as obtained from the actual calculations in the Liu-Müller [8] work and replaced the rest of the Δ_n's by a quadratic formula for Δ_n. It turns out that for corrections up to level n equal to 7 and 8, we obtained correlation functions that were very stable with respect to further corrections (see Fig. 2). The corresponding frequency spectrum is given in Fig. 3 and shows a well-defined shallow peak that would not enter without the corrections we have performed. There was a slight shift of the shallow peak toward a higher frequency when the highest-level, i.e., $L=18$, corrections were made with a marginal difference in the peak positions between the $L=17$ and $L=18$ cases. The time-domain results also show very little difference between $L=17$ and $L=18$ order corrections. Interestingly, a plot of $\log a_0(t)$ vs $\log t$ (not shown here) reveals that the oscillatory envelope for the relaxation function decays as an exponential with the following law: $a_0(t)\rightarrow\exp(-0.1t)$, which has a prefactor to time in the exponential function that is half of the prefactor if the entire set of Δ_n's were approximated by $\Delta_n=n^2$. Therefore, the GDCM reveals that the asymptotic behavior of the dynamical-spin pair correlation is actually altered in this problem and is distinctly slower than what has been previously found in the approximate calculations of Liu and Müller [8]. The numerical estimates of the long-time decay characteristics of the dynamical correlation can, in principle, be made exact via an extensive analysis of the perturbed ICF with the perturbation running through all the infinite number of levels.

TABLE I. Δ_n vs n for the two-spin *XX* model.

n	Δ_n
1	0.33333
2	0.66667
3	2.28000
4	3.39669
5	5.38884
6	8.81650
7	10.22152
8	15.88268
9	17.80241
10	23.91886
11	28.21480
12	33.47531
13	40.64990
14	45.43127
15	54.41163
16	60.11017
17	69.53225
18	77.19229

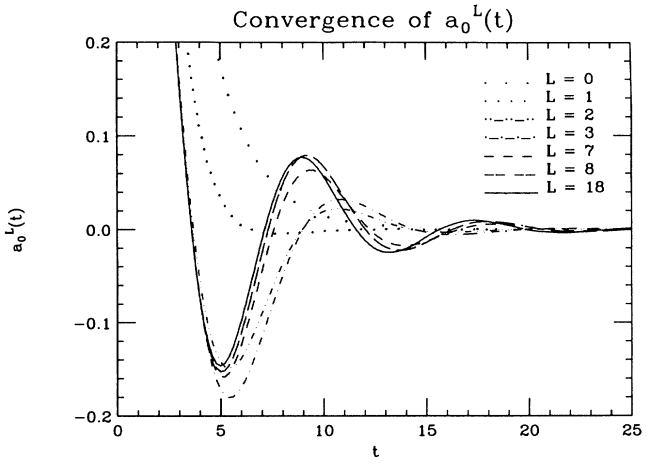

FIG. 2. Plot of $a_0^L(t)$ for various L values for the two-spin classical *XX* model of Liu and Müller [8].

V. CONCLUSION

In conclusion, we have shown that the dynamical correlations of systems with insoluble ICF's may be estimable via the GDCM if a closely related ICF is exactly soluble. The method relies upon expressing the insoluble ICF via an "effectively" FCF using the newly introduced inversion lemma. There is no truncation of the ICF in-

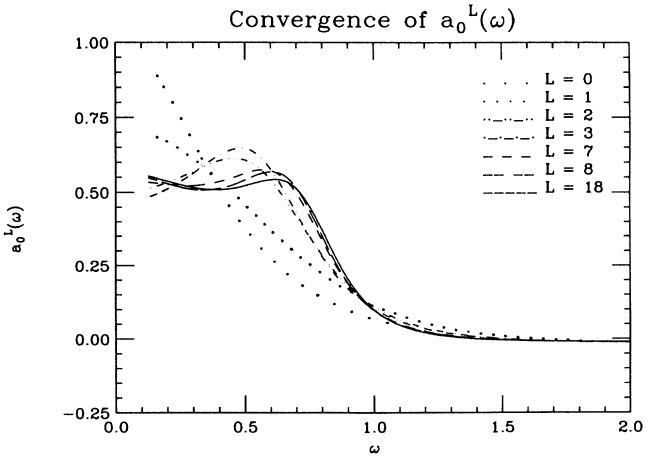

FIG. 3. Plot of frequency spectrum of the dynamical-spin pair correlation $a_0^L(\omega)$ vs ω for system in Fig. 2.

volved here. Thus, asymptotic behavior of dynamical correlation is, in principle, estimable via a GDCM calculation. The method, when feasible, is also independent of the convergence properties of the ICF under study. Finally, we have applied this method to estimate the dynamical-spin pair correlations in a two-spin classical XX cluster. The ICF corresponding to the dynamical-spin pair correlations in this problem is insoluble. We use the GDCM to estimate the solution to the insoluble ICF by replacing the actual ICF with the soluble ICF for level $L > 18$. The results reveal that the relaxation function exhibits damped oscillations which are stable against corrections to the ICF. The corresponding frequency spectrum reveals a well-defined side peak at a higher frequency that was not found in a previous calculation [8]. Furthermore, we estimate that the damped oscillatory dynamical-spin pair correlation decays approximately exponentially as $\exp(-0.1t)$, which is significantly slower than the behavior $\exp(-0.2t)$ previously estimated [8].

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