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V. S. Viswanath

Gerhard Müller
University of Rhode Island, gmuller@uri.edu

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Recursion Method in Quantum Spin Dynamics: The Art of Terminating a Continued Fraction

Recursion method in quantum spin dynamics: The art of terminating a continued fraction

V. S. Viswanath and Gerhard Müller
Department of Physics, The University of Rhode Island, Kingston, Rhode Island 02881-0817

The results obtained from applications of the recursion method to quantum many-body dynamics can be greatly improved if an appropriate termination function is employed in the continued-fraction representation of the corresponding relaxation function. We present a general recipe for the construction and use of such termination functions along with two applications in spin dynamics. The method can be adapted to any other problem in quantum many-body dynamics.

The recursion method[1] as applied to problems in the dynamics of quantum and classical Hamiltonian model systems[2,3] is essentially a modern version of the projection operator formalism designed by Mori and Zwanzig, formulated in a language which makes it directly accessible to computational methods. However, the old problem of adequately terminating a continued fraction has resurfaced in recent dynamical studies which employ one or the other variant of the recursion method or the closely related moment method.[4] The present work was motivated in particular by a study of Gagliano and Balseiro,[2] in which they use the recursion method for the calculation of the dynamic structure factor $S_{zz}(q,\omega)$ of the one-dimensional (1D) $s=1/2$ XXZ model

$$H=-\sum_{l=1}^{N}(S_l^xS_{l+1}^x+S_l^yS_{l+1}^y+\Delta S_l^zS_{l+1}^z)$$

at zero temperature. The case $\Delta=0$ (XY model) can be taken as a convenient test case, since the function $S_{zz}(q,\omega)$ is exactly known[5]:

$$\begin{aligned}S_{zz}(q,\omega)&\equiv\int_{-\infty}^{+\infty}dte^{i\omega t}\langle S_q^z(t)S_{-q}^z\rangle\\&=2[4\sin^2(q/2)-\omega^2]^{-1/2}\Theta(\omega-\sin q)\\&\quad\times\Theta[2\sin(q/2)-\omega].\end{aligned}\tag{1}$$

For the implementation of the recursion method at $T=0$, it is convenient to use the fermion representation of the XXZ model; it has the advantage that the ground state has a simple structure in the limit $\Delta=0$ (noninteracting fermions). $S_{zz}(q,\omega)$ is then related to a fermion density correlation function.

The formulation of the recursion method used in Ref. 2 is based on an orthogonal expansion of the wave function

$$|\psi(t)\rangle\equiv G(t)|0\rangle=\sum_{k=0}^{\infty}D_k(t)|f_k\rangle,\tag{2}$$

where $|0\rangle$ is the ground-state wave function of a given quantum model Hamiltonian H and G is the dynamical variable whose time-dependent correlation function

$$\tilde{S}(t)\equiv\langle 0|G(t)G^\dagger|0\rangle=\langle 0|GG^\dagger|0\rangle D_0^*(-t)$$

we wish to determine. The orthogonal vectors $|f_k\rangle$ are generated recursively via the Gram-Schmidt orthogonalization procedure with initial condition $|f_0\rangle=G|0\rangle$, $|f_{-1}\rangle\equiv 0$:

$$|f_{k+1}\rangle=(H-E_0)|f_k\rangle-\sigma_k|f_k\rangle-\delta_k|f_{k-1}\rangle,$$

$$\sigma_k=\frac{\langle f_k|H-E_0|f_k\rangle}{\langle f_k|f_k\rangle},\quad \delta_k=\frac{\langle f_k|f_k\rangle}{\langle f_{k-1}|f_{k-1}\rangle}.$$

It is assumed that the ground-state energy E_0 and wave function $|0\rangle$ have been determined as accurately as possible. The sequences of recurrents σ_k, δ_k then contain all information necessary to reconstruct the function $D_0(t)$ as follows. Insert the orthogonal expansion (2) into the Schrödinger equation, $i(\partial/\partial t)|\psi(t)\rangle=(H-E_0)|\psi(t)\rangle$, to obtain an infinite set of difference-differential equations for the functions $D_k(t)$, which, upon Fourier–Laplace transform,

$$d_k(\zeta)\equiv\int_0^\infty dte^{i\zeta t}D_k(t),$$

can be solved for $d_0(\zeta)$ in the continued-fraction representation

$$d_0(\zeta)=\cfrac{i}{\zeta-\sigma_0-\cfrac{\delta_1}{\zeta-\sigma_1-\cdots}},\tag{3}$$

and from which the frequency-dependent correlation function can be directly recovered:

$$S(\omega)\equiv\int_{-\infty}^{+\infty}dte^{i\omega t}\tilde{S}(t)=2\langle 0|GG^\dagger|0\rangle\operatorname{Re}\lim_{\epsilon\to 0}d_0(\omega+i\epsilon).$$

Now consider the symmetrized correlation function

$$\tilde{\Phi}(t)=[\tilde{S}(t)+\tilde{S}(-t)]/2=\langle 0|GG^\dagger|0\rangle A_0(t)$$

and its Fourier transform, the fluctuation function $\Phi(\omega)$. $\tilde{\Phi}(t)$ is equal to the real part of $\tilde{S}(t)$. In Fourier space we have (at $T=0$) $S(\omega)=2\Phi(\omega)\Theta(\omega)$. The relaxation function $a_0(z)$, which is the Laplace transform of $A_0(t)$, can be expressed in a more concise continued-fraction representation than that of $d_0(\zeta)$:

$$a_0(z)=\int_0^\infty dte^{-zt}A_0(t)=\cfrac{1}{z+\cfrac{\Delta_1}{z+\cfrac{\Delta_2}{z+\cdots}}}.\tag{4}$$

The associated spectral density is recovered as

$$\Phi_0(\omega)=2\operatorname{Re}\lim_{\epsilon\to 0}a_0(\epsilon-i\omega)$$

and the fluctuation function as $\Phi(\omega)=\langle 0|GG^\dagger|0\rangle\Phi_0(\omega)$.

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The first n members of the sequence Δ_k are expressible in terms of the first n pairs of the sequences σ_k, δ_k and vice versa by elementary transformation formulas.[6] In a different formulation of the recursion method,[3] the sequence Δ_k is obtained directly. In most practical applications of the recursion method, only a limited number of recurrents σ_k, δ_k or recurrents Δ_k can be calculated, which makes it necessary to terminate the continued fractions (3) or (4) artificially. The main goal of this report is to demonstrate a way to terminate (3) in such a way that the information content of the known Δ_k is exploited to the fullest extent without introducing artificial features.

For the dynamical structure factor $S_{zz}(q,\omega)$ at fixed wave numbers $q = 3\pi/4$ and π for the XY model at $T = 0$, the first 13 recurrents Δ_k are displayed in the inset to Fig. 1. They can be obtained directly from Lee's[3] formulation of the recursion method or indirectly from the σ_k, δ_k in the approach taken by Gagliano and Balseiro.[2] The relatively simple patterns revealed by the two Δ_k sequences can be interpreted as follows: The almost uniform sequence for $q = \pi$, which is $\Delta_1 = 2$, $\Delta_2 = \Delta_3 = \ldots = 1$, is readily recognized as that of the Bessel function $A_0(t) = J_0(2t)$ or its Fourier transform, the spectral density $\Phi_0(\omega) = 2/\sqrt{4-\omega^2}$; it is consistent (for $q = \pi$) with the exact result (1).[7] For $q = 3\pi/4$, the Δ_{2k-1} and the Δ_{2k} converge (fairly rapidly) to different values, $\Delta_\infty^{(o)}$ and $\Delta_\infty^{(e)}$, respectively, which is the unmistakable signature of a spectral density whose spectral weight is confined to a finite interval with a gap in the center, $\omega_{\min} \leqslant |\omega| \leqslant \omega_{\max}$, and with the two cut-off frequencies determined by

$$\omega_{\max} = \sqrt{\Delta_\infty^{(e)}} + \sqrt{\Delta_\infty^{(o)}}, \quad \omega_{\min} = \sqrt{\Delta_\infty^{(e)}} - \sqrt{\Delta_\infty^{(o)}}.$$

The next step in the procedure proposed here is to choose the simplest model spectral density which is consistent with these conditions,

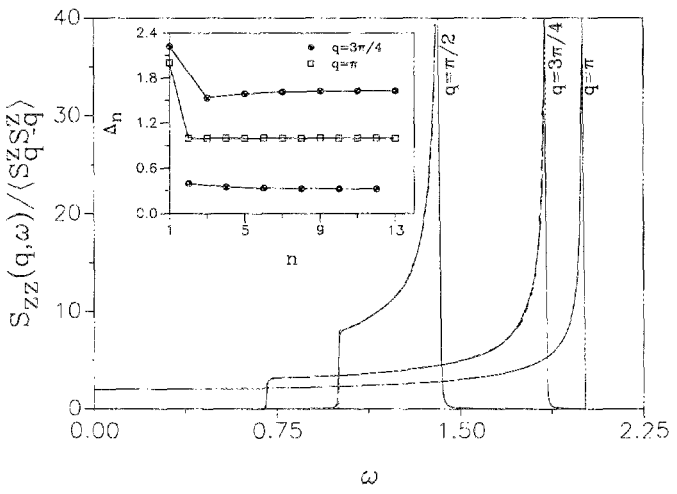

FIG. 1. Dynamic structure factor $S_{zz}(q,\omega)$ (normalized by $\langle S^z_q S^z_{-q}\rangle = q/2\pi$) for fixed $q = n\pi/4$, $n = 2,3,4$, of the 1D $s = 1/2$ XY model at $T = 0$. The full lines represent the result derived from the continued-fraction representation for $a_0(\epsilon - i\omega)$ (with $\epsilon = 0.001$) terminated at level $n = 5$ as explained in the text. The dashed lines represent the exact result (1). The inset shows the recurrents Δ_k, $k = 1,\ldots,13$, for $q = 3\pi/4$ and $q = \pi$.

$$\bar{\Phi}_0(\omega) = \frac{\pi}{\omega_{\max} - \omega_{\min}}\,\Theta(\omega - \omega_{\min})\Theta(\omega_{\max} - \omega),$$

and determine, via Hilbert transform, the associated model relaxation function

$$\bar{a}_0(z) = \frac{1}{2i(\omega_{\max} - \omega_{\min})}\left(\ln\frac{z + i\omega_{\max}}{z - i\omega_{\max}} - \ln\frac{z + i\omega_{\min}}{z - i\omega_{\min}}\right).$$

A good approximation of the relaxation function $a_0(z)$, of which we only know a continued fraction (4) down to level n, is then constructed as follows: First expand the known model relaxation function $\bar{a}_0(z)$ into a continued fraction down to the nth level,

$$\bar{a}_0(z) = \cfrac{1}{z + \cfrac{\bar{\Delta}_1}{z + \ldots \cfrac{}{\cdots + \cfrac{\bar{\Delta}_{n-1}}{z + \bar{\Delta}_n \Gamma_n(z)}}}} \tag{5}$$

which defines the nth-level termination function $\Gamma_n(z)$ along with the model recurrents $\bar{\Delta}_k$, $k = 1,\ldots,n$. Then insert this termination function into the continued-fraction representation of the actual relaxation function $a_0(z)$, again at the nth level. In other words, approximate $a_0(z)$ by taking $\bar{a}_0(z)$ in the representation (5) and replacing the model recurrents $\bar{\Delta}_k$, $k = 1,\ldots,n$, with the known recurrents Δ_k of the dynamical quantity under investigation. The termination can be performed at any level for which the true recurrents are known, and it can be expected that the degree of approximation improves systematically as more model recurrents are replaced by exact ones.

In the case of the dynamic structure factor $S_{zz}(q,\omega)$ for the XY model, only few exact recurrents are needed to recover a good representation of the exact result (1). Our results shown in Fig. 1 for $S_{zz}(q,\omega)$ at $q = n\pi/4$, $n = 2,3,4$, are based on a continued fraction terminated by $\Gamma_n(z)$ at the level $n = 5$. Comparison of these results with those of Fig. 1 in Ref. 2 demonstrates that there is much more information contained in the first few recurrents than can be retrieved from a finite continued fraction alone. The additional information is retrievable through the construction of a matching termination function.

For one more application of the method proposed here, consider the spin autocorrelation function $\langle S^x_l(t)S^x_l\rangle$ of the same model (the XY model at $T = 0$), which can be rigorously expressed in terms of the solution of a nonlinear ODE as described in Refs. 8 and 9. The associated spectral density $\Phi_0^{xx}(\omega)$ was determined in Ref. 9 on the basis of an exact long-time asymptotic expansion of $\langle S^x_l(t)S^x_l\rangle$ in conjunction with a precision numerical solution for short times. That spectral density, which is replotted in Fig. 2 (dashed line), has three singularities on the frequency range shown: an $\omega^{-1/2}$ divergence at $\omega = 0$, a logarithmic divergence at $\omega = 1$, and an $\omega^{1/2}$ cusp at $\omega = 2$.

The same nonlinear ODE from which these exact results were derived with much effort can be used to determine with relative ease a number of recurrents Δ_k, from which the spectral density can be reconstructed approximately according to our scheme. These recurrents up to Δ_{13} are shown in the inset to Fig. 2. They have a linear average growth rate,

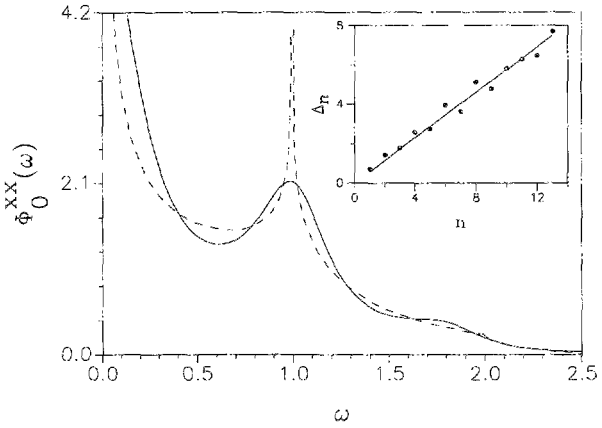

FIG. 2. Spectral density $\Phi_0^{xx}(\omega)$ for the spin autocorrelation function $\langle S_j^x(t)S_j^x\rangle$ of the 1D $s=1/2$ XY model at $T=0$. The full line represents the result derived from the continued-fraction representation for $a_0(\epsilon - i\omega)$ (with $\epsilon = 0.001$) terminated at level $n = 13$ as described in the text. The recurrents Δ_k, $k = 1,\ldots,13$, are shown in the inset along with the regression line $\Delta_k = 0.574k$. The dashed line represents the exact result from Ref. 9.

$\Delta_k \simeq 0.574k$, with considerable scattering about that line. In this case we select the model spectral density $\bar{\Phi}_0^{xx}(\omega)$ by the requirement that its $\bar{\Delta}_k$ sequence reproduces the average behavior of the actual Δ_k sequence. This condition is satisfied by a pure Gaussian[3]:

$$\bar{\Phi}_0^{xx}(\omega) = (2\sqrt{\pi}/\omega_0)\exp(-\omega^2/\omega_0^2), \quad \bar{\Delta}_k = k\omega_0^2/2.$$

The associated model relaxation function,

$$\bar{a}_0(z) = (\sqrt{\pi}/\omega_0)\exp(z^2/\omega_0^2)\mathrm{erfc}(z/\omega_0),$$

with the parameter ω_0 chosen to match the average growth rate of the Δ_k is then used to determine the nth-level termination function $\Gamma_n(z)$.[10] Inserted (at level $n = 13$) into the continued-fraction representation of the relaxation function $a_0(z)$ yields the spectral density shown as solid line in Fig. 2. The approximate result reproduces all the major features of the exact spectral density at least qualitatively. Note in particular that our scheme of approximation has not produced any artificial features which may invite misinterpretation, a problem with which less sophisticated termination methods have been plagued almost inevitably.

In summary, we have outlined a practical method to terminate a continued fraction as it arises from the recursion method for two particular test cases. That procedure can be adapted to virtually any situation which one is likely to encounter in quantum many-body dynamics.

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[10] Note that our procedure is quite distinct from phenomenological approximations (reviewed in Ref. 7) which employ one- or two-parameter Gaussians for the termination function itself. Such approximations almost always result in a mismatch between the average slope of the Δ_k and the slope of the $\bar{\Delta}_k$ even if the average growth rate of Δ_k is, in fact, linear in k. This is, however, not generally the case. We have positive evidence for the occurrence of quadratic and cubic growth rates, which require entirely different types of termination functions.