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The recursion method applied to the $T=0$ dynamics of the 1D $s=1/2$ Heisenberg and XY models

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The frequency-dependent spin autocorrelation functions for the 1D $s = 1/2$ Heisenberg and XY models at zero temperature are determined by the recursion method. These applications further demonstrate the efficacy of a new calculational scheme developed for the termination of continued fractions. A special feature of the recursion method highlighted here is its capability to predict the exponent of the infrared singularities in spectral densities.

The key to obtaining useful and reliable results from applications of the recursion method[1-4] to quantum many-body dynamics is the use of an appropriate termination function in the continued-fraction representation of the corresponding relaxation function. In a recent study,[4] we have presented a general recipe for the construction and use of such termination functions along with two applications in quantum spin dynamics. Meanwhile we have further refined this calculational technique, which will be demonstrated and illustrated with more applications in quantum spin dynamics. The focus here is on spectral densities

$$\Phi_0^{\mu\mu}(\omega) = \int_{-\infty}^{+\infty} dt e^{i\omega t} A_0^{\mu\mu}(t), \tag{1}$$

of symmetrized spin autocorrelation functions

$$A_0^{\mu\mu}(t) = [\langle S_l^\mu(t) S_l^\mu \rangle + \langle S_l^\mu(-t) S_l^\mu \rangle]/2 \langle S_l^\mu S_l^\mu \rangle, \tag{2}$$

of the 1D $s = 1/2$ Heisenberg and XY models at $T = 0$. These models are specified by the cases $\Delta = 0$ (XY model), $\Delta = 1$ (Heisenberg ferromagnet) and $\Delta = -1$ (Heisenberg antiferromagnet), respectively, of the Hamiltonian

$$H = -\sum_{l=1}^{N} [S_l^x S_{l+1}^x + S_l^y S_{l+1}^y + \Delta S_l^z S_{l+1}^z]. \tag{3}$$

The recursion method as formulated in Ref. 4 is based on an orthogonal expansion of the wave function $|\psi(t)\rangle = S_l^\mu(t)|0\rangle$, where $|0\rangle$ represents the ground-state of (3), and its most immediate result is a sequence of recurrents, Δ_k, $k = 1,2,...$ These numbers determine the relaxation function $a_0^{\mu\mu}(z)$, the Laplace transform of Eq. (2), in the continued-fraction representation

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

The spectral density [Eq. (1)] can be recovered directly from Eq. (4):

$$\Phi_0^{\mu\mu}(\omega) = \lim_{\epsilon \to 0} 2 \operatorname{Re}[a_0(\epsilon - i\omega)]. \tag{5}$$

In most applications of interest, only a limited number of recurrents Δ_k can be evaluated. The continued fraction in Eq. (4) must therefore be completed artificially if we

wish to recover a meaningful expression for the relaxation function. For this purpose we construct a termination function according to the general scheme that was introduced in Ref. 4.

Our first application is a test run on the spectral density $\Phi_0^{zz}(\omega)$ for the case $\Delta = 0$, a quantity which is exactly known[5] [see Eq. (3.9) of Ref. 6 for a closed-form expression]. In Fig. 1(a) we have plotted the recurrents Δ_k, $k = 1,...,15$, as determined by the recursion method. For the reconstruction of the spectral density, we first extract two important pieces of information directly from that Δ_k-sequence.

(i) The Δ_k tend to converge toward the value $\Delta_\infty = 1$. The implication is that $\Phi_0^{zz}(\omega)$ has compact support: the spectral weight is confined to the frequency interval $|\omega| < \omega_0 = 2\sqrt{\Delta_\infty} = 2$. (ii) The convergence toward the asymptotic value Δ_∞ is alternating in character. This indicates that the spectral density is singular at $\omega = 0$: $\Phi_0^{zz}(\omega) \sim |\omega|^\alpha$. The exponent α of that singularity determines the leading-order term of the large-k asymptotic expansion of the Δ_k-sequence:[7]

$$\sqrt{\Delta_k} = \sqrt{\Delta_\infty}[1 - (-1)^k(\alpha/2k) + ...]. \tag{6}$$

In Fig. 1(b) we have plotted the quantity

$$\alpha_k = (-1)^k 2k[1 - \sqrt{\Delta_k/\Delta_\infty}] \tag{7}$$

versus k. The sequence α_k tends to converge to the value $\alpha = 1$ (the exact result), albeit slowly and irregularly.

For the reconstruction of the spectral density $\Phi_0^{zz}(\omega)$ from the first 15 recurrents Δ_k according to the method outlined in Ref. 4, we need to select a model spectral density $\bar{\Phi}_0(\omega)$ which satisfies two conditions: (i) its spectral weight is confined to frequencies $|\omega| < \omega_0 = 2$; (ii) it has a singularity at $\omega = 0$, preferably with $\alpha = 1$. Our choice is the function

$$\bar{\Phi}_0(\omega) = \frac{\pi}{\omega_0^2} |\omega| (\omega_0^2 - \omega^2) \Theta(\omega_0 - |\omega|). \tag{8}$$

The associated model relaxation function is obtained from Eq. (8) by Hilbert transform:

$$\bar{a}_0(z) = \frac{2z}{\omega_0^2} \left(1 + \frac{z^2}{\omega_0^2}\right) \ln\left(1 + \frac{\omega_0^2}{z^2}\right) - \frac{2z}{\omega_0^2}. \tag{9}$$

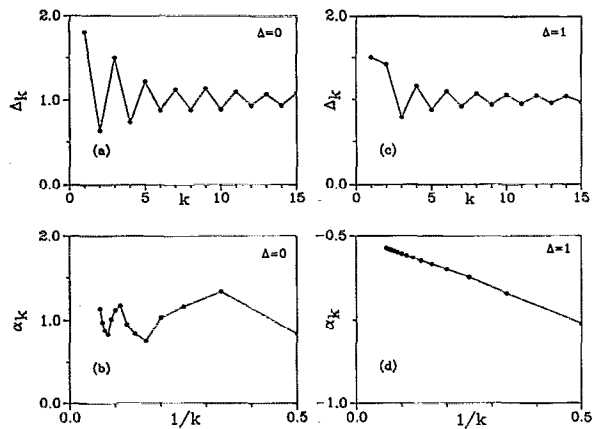Next we expand this function into a continued fraction down to the nth level:

FIG. 1. The two upper panels display the recurrents Δ_k, $k = 1,...,15$, vs k for the $T = 0$ spectral density $\Phi_0^{zz}(\omega)$ of (a) the 1D $s = 1/2$ XY model ($\Delta = 0$) and (c) the 1D $s = 1/2$ Heisenberg ferromagnet ($\Delta = 1$). The two lower panels show the sequences α_k, $k = 1,...,15$, plotted vs $1/k$ for these recurrents.

FIG. 3. Spectral density $\Phi_0^{zz}(\omega)$ for the 1D $s = 1/2$ Heisenberg antiferromagnet ($\Delta = -1$) at $T = 0$. The result shown is derived from the continued-fraction representation of $a_0^{zz}(\epsilon - i\omega)$ (with $\epsilon = 0.001$) terminated at level $n = 11$ as described in the text. The recurrents Δ_k, $k = 1,...,11$, are shown in the inset along with the regression line $\Delta_k = 0.807 k$.

$$\bar{a}_0(z) = \cfrac{1}{z + \cfrac{\Delta_1}{z + ... \cfrac{}{... + \cfrac{\Delta_{n-1}}{z + \Delta_n \Gamma_n(z)}}}} \quad (10)$$

This defines the nth-level termination function $\Gamma_n(z)$. The model recurrents $\bar{\Delta}_k$ are the following in this case:

$$\bar{\Delta}_{2k-1} = \frac{1}{4} \omega_0^2 \left(1 + \frac{1}{2k+1}\right), \quad \bar{\Delta}_{2k} = \frac{1}{4} \omega_0^2 \left(1 - \frac{1}{2k+1}\right). \quad (11)$$

The termination function $\Gamma_n(z)$ is then used in the continued-fraction representation of the actual relaxation function $a_0^{zz}(z)$, also expanded down to the nth level. In other words, we start with $\bar{a}_0(z)$ in the representation of Eq. (10), replace the model recurrents $\bar{\Delta}_k$, $k = 1,...,n$, by the
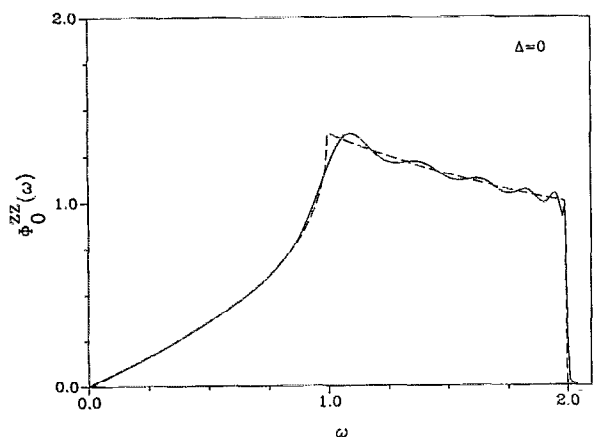

FIG. 2. Spectral density $\Phi_0^{zz}(\omega)$ for the 1D $s = 1/2$ XY model ($\Delta = 0$) at $T = 0$. The full line represents the result derived from the continued-fraction representation of $a_0^{zz}(\epsilon - i\omega)$ (with $\epsilon = 0.001$) terminated at level $n = 15$ as described in the text. The dashed line represents the exact result.
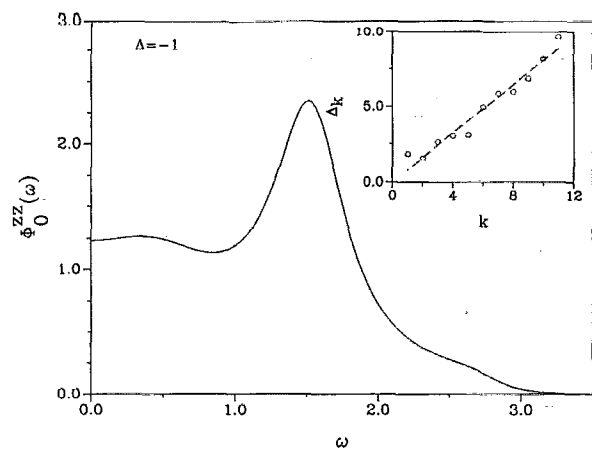
actual ones [those from Fig. 1(a)] and use Eq. (5) to arrive at the spectral density we set out to determine.

The result is shown in Fig. 2 along with the exact result. The agreement is not perfect, but very satisfactory if one takes into account that the reconstruction is based on a mere 15 numbers. The agreement is best at small ω, where both the exact result and our model spectral density have the same singularity exponent, $\alpha = 1$, previously inferred from the Δ_k-sequence directly. The agreement between the two curves is somewhat less than perfect near $\omega = 2$, where the exact spectral density has a discontinuity, whereas the model spectral density goes to zero linearly. Despite this mismatch in singularity exponent, the reconstructed spectral density reproduces the discontinuity fairly well. The agreement between the two curves is worst near $\omega = 1$, where the exact result has one more singularity, but the model spectral density has none.

The same spectral density $\Phi_0^{zz}(\omega)$ evaluated for the case $\Delta = 1$ of Hamiltonian (3) and for the ground state with all spins aligned parallel to the x-axis is the familiar spin-wave result,

$$\Phi_0^{zz}(\omega) = \int_{-\pi}^{+\pi} dq 1/2 [\delta(\omega - 1 + \cos q)$$
$$+ \delta(\omega + 1 - \cos q)]$$
$$= \Theta(2 - |\omega|)/\sqrt{|\omega|(2 - |\omega|)}. \quad (12)$$

We only want to use it here for the purpose of demonstrating one more time how the singularity exponent at $\omega = 0$ can be extracted from the first few recurrents. Figure 1(c) shows the Δ_k-sequence for that function up to $n = 15$ as obtained by the recursion method. The sequence again tends to converge toward the value $\Delta_\infty = 1$ in an alternating approach. The associated sequence α_k, plotted versus $1/k$ in Fig. 1(d), converges rather uniformly toward the value $\alpha = -1/2$, in agreement with the exact result.

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Now we turn to the case $\Delta = -1$ of Hamiltonian Eq. (3), for which the spectral density $\Phi_0^{zz}(\omega)$ is not known exactly. We have employed the recursion method to determine the Δ_k-sequence up to $n = 11$. These recurrents, which are plotted in the inset to Fig. 3, have the tendency to increase roughly linearly in k, albeit with considerable scattering. In Ref. 4 we have already analyzed a similar Δ_k-sequence, namely that for the spectral density $\Phi_0^{xx}(\omega)$ of the case $\Delta = 0$. Here we use the same criterion for the selection of the model spectral density: the model recurrents $\overline{\Delta}_k$ must follow the average linear growth of the actual Δ_k, indicated by the regression line $\overline{\Delta}_k = 0.807\,k$ in the inset to Fig. 3. This condition is satisfied by the functions

$$\overline{\Phi}_0(\omega) = (2\sqrt{\pi}/\omega_0)\exp(-\omega^2/\omega_0^2), \quad \overline{\Delta}_k = k\omega_0^2/2,$$
(13)

$$\overline{a}_0(z) = (\sqrt{\pi}/\omega_0)\exp(z^2/\omega_0^2)erfc(z/\omega_0),$$
(14)

with the parameter ω_0 chosen to match the average growth rate of the Δ_k. The model relaxation function (14) is then used to determine the nth-level termination function $\Gamma_n(z)$. Inserted (at level $n = 11$) into the continued fraction representation of the relaxation function $a_0^{zz}(z)$ produces the spectral density shown in the main plot of Fig. 3. This result is in qualitative agreement with all properties of the function $\Phi_0^{zz}(\omega)$ that can be inferred from exact information on the Heisenberg model: (i) the first three singularities in the spectral density occur at frequencies $\omega = 0, \pi/2, \pi$; (ii) the leading singularity exponent at $\omega = 0$ is $\alpha = 0$. In a previous study,[8] an approximate expression for the function $\Phi_0^{zz}(\omega)$ was proposed. That result is finite and nonzero at $\omega = 0$, has a logarithmic divergence at $\omega = \pi/2$ and a square-root cusp at $\omega = \pi$ (see Fig. 5 of Ref. 8). Its shape is qualitatively very similar to that of the result obtained by the recursion method.

How can we extract the exponent value α of the infrared singularity directly from the Δ_k-sequence if that sequence grows linearly in k on average? Consider the model spectral density

$$\overline{\Phi}_0(\omega) = \frac{2\pi}{\omega_0\Gamma[(\alpha/2) - \frac{1}{2}]}|\omega/\omega_0|^\alpha \exp(-\omega^2/\omega_0^2).$$
(15)

The associated $\overline{\Delta}_k$-sequence reads

$$\overline{\Delta}_{2k-1} = \tfrac{1}{2}\omega_0^2(2k - 1 + \alpha), \quad \overline{\Delta}_{2k} = \tfrac{1}{2}\omega_0^2(2k).$$
(16)

The singularity exponent α determines the displacement of the $\overline{\Delta}_{2k-1}$ from the line $\overline{\Delta}_{2k} = \omega_0^2 k$. In most applications, this easy-to-read signature of infrared singularities is obscured by the effects of further singularities at $\omega \ne 0$ in the spectral density (see inset to Fig. 3 of this paper and inset to Fig. 2 of Ref. 4). Under these circumstances, we could, for example, determine the value of α from the average difference in vertical displacement of the recurrents Δ_{2k} and the recurrents Δ_{2k-1} from the linear regression line, which was derived from the entire sequence. For the two cases mentioned we thus obtain the exponent values $\alpha = 0.3 \pm 0.7$ $(\Delta = -1)$ and $\alpha = -0.5 \pm 0.4$ $(\Delta = 0)$. Both values are consistent with the exact results $\alpha = 0$ and $\alpha = -1/2$, respectively, but have little predictive power. We are currently exploring more sophisticated techniques for the analysis of these exponents.

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