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Continued-fraction formalism applied to the spin-$\frac{1}{2}$ XYZ model

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In this paper, we evaluate the correlation functions of the spin-$\frac{1}{2}$ XYZ model for some particular cases by using the Mori continued-fraction formalism. The results are exactly the same as those well-known ones. This removes any doubt about the convergence of the continued fraction recently raised by some authors.

By introducing a projection-operator technique, it has been demonstrated by Mori[1] that the Laplace transform of the correlation function (the relaxation function) could be written as an infinite continued fraction. This continued fraction can be obtained by solving a set of coupled Volterra equations for a hierarchy of memory functions. In general, it cannot be evaluated exactly for most of the physical systems. Consequently, some approximation is required in order to obtain a closed-form expression for the relaxation function. A very often used one is the N-pole approximation in which the Nth-order memory function is taken as a constant. This formalism has been revealed itself as a powerful computational method of calculating the relaxation function, and it has been applied successfully in many problems of theory of relaxation (for instance, see Refs. 2 and 3).

Very recently, Oitmaa, Linbasky and Aydin[4] have evaluated numerically the relaxation function of the spin-$\frac{1}{2}$ XYZ model (spin-$\frac{1}{2}$ anisotropic Heisenberg chain). In contrast to previous works, their results show that the continued-fraction approach, together with the N-pole approximation, suffers from a serious lack of convergence. In this paper some analytical calculations will be presented which are in total disagreement with this conclusion. In other words, we will prove that the continued fraction converges and provide results which coincide with previous well-established ones. We then point out what might be the mistake in those numerical works.

The system to be investigated is the spin-$\frac{1}{2}$ anisotropic Heisenberg chain described by the Hamiltonian[5(a),6]

$$H=-\tfrac{1}{2}\sum_{l}(J_x\sigma_l^x\sigma_{l+1}^x+J_y\sigma_l^y\sigma_{l+1}^y+J_z\sigma_l^z\sigma_{l+1}^z)\ . \qquad (1)$$

where σ^α ($\alpha=x,y,z$) are the Pauli operators. The correlation functions for this system at infinite temperature are defined by

$$C^\alpha(n,t)=\langle\sigma_0^\alpha(t)\sigma_n^\alpha(0)\rangle_{T=\infty}=\lim_{N\to\infty}2^{-N}\mathrm{Tr}[\sigma_0^\alpha(t)\sigma_n^\alpha(0)]\ , \qquad (2)$$

where N is the number of spins. The spatial Fourier transform of $C^\alpha(n,t)$ is defined by

$$\tilde{C}^\alpha(k,t)=\sum_{n=-\infty}^{\infty}e^{-ikn}C^\alpha(n,t)\ . \qquad (3)$$

For the special case $J_z=0$, these correlation functions can be evaluated exactly.[5a] Let us analyze separately two branches of this particular case.

(a) Calculation of $C^z(n,t)$ for $J_x=J_y=J$. The expansions of the $\tilde{C}^\alpha(k,t)$ in powers of t is given by the moments according to

$$\tilde{C}^\alpha(k,t)=\sum_{l=0}^{\infty}\frac{(-1)^l}{(2l)!}\tilde{M}_{2l}^\alpha(k)t^{2l}\ , \qquad (4)$$

where

$$\tilde{M}_{2l}^\alpha(k)=M_{2l}^\alpha(0)+2\sum_{n=1}^{l}M_{2l}^\alpha(n)\cos(nk)\ , \qquad (5)$$

where $M_{2l}^\alpha(n)$ are the moments of the power-series expansion of $C^\alpha(n,t)$. In fact, the sum in Eq. (5) should go up to $n=\infty$. Nevertheless, $M_{2l}^\alpha(n)=0$ if $n\geq l+1$,[5a] so that we can stop at $n=l$. These moments were found in Ref. 5(a) up to tenth order. For our purpose, it will be sufficient to retain terms only up to sixth order. We have

$$\tilde{M}_0^z(k)=1\ , \qquad (6a)$$

$$\tilde{M}_2^z(k)=2(J_x^2+J_y^2)-4J_xJ_y\cos k\ , \qquad (6b)$$

$$\tilde{M}_4^z(k)=4[2(J_x^4+J_y^4)+5J_x^2J_y^2+(J_x^2+J_y^2)J_z^2]-8J_xJ_y[3(J_x^2+J_y^2)+J_z^2]\cos k+12J_x^2J_y^2\cos 2k\ , \qquad (6c)$$

$$\begin{aligned}\tilde{M}_6^z(k)=&4\{8(J_x^6+J_y^6)+42J_x^2J_y^2(J_x^2+J_y^2)+[18(J_x^4+J_y^4)+19J_x^2J_y^2]J_z^2+4(J_x^2+J_y^2)J_z^4\}\\&-4J_xJ_y[32(J_x^4+J_y^4)+86J_x^2J_y^2+35(J_x^2+J_y^2)J_z^2+8J_z^4]\cos k\\&+60J_x^2J_y^2[2(J_x^2+J_y^2)+J_z^2]\cos(2k)-40J_x^3J_y^3\cos(3k)\ .\end{aligned} \qquad (6d)$$

For the special case $J_z=0$, $J_x=J_y=J$, tedious but straightforward calculation leads us to

$$\widetilde{M}\,{}_0^z(k)=1,\quad \widetilde{M}\,{}_2^z(k)=8a^2=2^3a^2\ ,$$
$$\widetilde{M}\,{}_4^z(k)=96a^4=3\times 2^5a^4\ , \tag{7}$$
$$\widetilde{M}\,{}_6^z(k)=1280a^6=5\times 2^8a^6\ ,$$

where $a=J\sin(k/2)$.

Let $\Gamma^\alpha(k,s)$ denote the Laplace transform of $\widetilde{C}\,{}^\alpha(k,t)$. According to Mori,[1] the continued-fraction representation of this function is

$$\Gamma^\alpha(k,s)=\cfrac{1}{s+\cfrac{\delta_1^\alpha(k)}{s+\cfrac{\delta_2^\alpha(k)}{s+\ddots}}}\ , \tag{8}$$

where the Mori parameters are given by[7]

$$\delta_1^\alpha(k)=\frac{\widetilde{M}\,{}_2^\alpha(k)}{\widetilde{M}\,{}_0^\alpha(k)}\ ,$$
$$\delta_2^\alpha(k)=\frac{\widetilde{M}\,{}_4^\alpha(k)}{\widetilde{M}\,{}_2^\alpha(k)}-\frac{\widetilde{M}\,{}_2^\alpha(k)}{\widetilde{M}\,{}_0^\alpha(k)}\ , \tag{9}$$
$$\delta_3^\alpha(k)=\frac{\widetilde{M}\,{}_6^\alpha(k)-[\widetilde{M}\,{}_4^\alpha(k)]^2/\widetilde{M}\,{}_2^\alpha(k)}{\widetilde{M}\,{}_4^\alpha(k)-[\widetilde{M}\,{}_2^\alpha(k)]^2/\widetilde{M}\,{}_0^\alpha(k)}\ ,$$

which are particular cases of a more general expression $\delta_l^\alpha(k)=\Delta_l\Delta_{l-2}/(\Delta_{l-1})^2$, where $\Delta_{-1}=\Delta_0=1$, and for $l\geq 1$,

$$\Delta_l=\begin{vmatrix} C_0 & C_1 & \cdots & C_l \\ C_1 & C_2 & \cdots & C_{l+1} \\ \cdot & \cdot & \cdots & \cdot \\ \cdot & \cdot & \cdots & \cdot \\ \cdot & \cdot & \cdots & \cdot \\ C_l & C_{l+1} & \cdots & C_{2l}\end{vmatrix}\ , \tag{10}$$

with $C_{2l+1}=0$ and $C_{2l}=\widetilde{M}\,{}_{2l}^\alpha(k)$.

Now, it follows from Eqs. (7) and (9) that $\delta_1^z(k)=8a^2$, $\delta_2^z(k)=\delta_3^z(k)=\cdots=4a^2$.[8] Introducing these expressions into Eq. (8), we obtain $\Gamma(k^z,s)=1/[s+2f(k,s)]$, where $f(k,s)=4a^2/[s+f(s,k)]$. This immediately gives $f(s,k)=-s/2+(s^2/4+4a^2)^{1/2}$ and $\Gamma^z(k,s)=1/(s^2+16a^2)^{1/2}$. Hence $\widetilde{C}\,{}^z(k,t)$ is just the Laplace transform of the Bessel function of order zero, $J_0(4at)=J_0[4Jt\sin(k/2)]$. This is exactly the same result which was found in Ref. 5(a) by using a different approach. For completeness, we just quote the result $C^z(n,t)=[J_n(2Jt)]^2$, which may be easily obtained by taking inverse Fourier transform of $\widetilde{C}\,{}^z(k,t)$.

(b) Calculation of $C^x(0,t)$ and $C^y(0,t)$. The moments of the expansion of $\widetilde{C}\,{}^\alpha(k,t)$ $(\alpha=x,y)$ may be found from Eq. (6) by making the changes $J_x\to J_y$, $J_y\to J_z$, and $J_z\to J_x$. We then obtain, with $J_z=0$,

$$\widetilde{M}\,{}_0^x(k)=1\ , \tag{11a}$$
$$\widetilde{M}\,{}_2^x(k)=2J_y^2\ , \tag{11b}$$
$$\widetilde{M}\,{}_4^x(k)=4(2J_y^4+J_y^2J_x^2)\ , \tag{11c}$$
$$\widetilde{M}\,{}_6^x(k)=4(8J_y^6+18J_y^4J_x^2+4J_y^2J_x^4)\ , \tag{11d}$$
$$\widetilde{M}\,{}_0^y(k)=1\ , \tag{12a}$$
$$\widetilde{M}\,{}_2^y(k)=2J_x^2\ , \tag{12b}$$
$$\widetilde{M}\,{}_4^y(k)=4(2J_x^4+J_x^2J_y^2)\ , \tag{12c}$$
$$\widetilde{M}\,{}_6^y(k)=4(8J_x^6+18J_x^4J+4J_x^2J_y^4)\ . \tag{12d}$$

Note that as we make the change specified above, all the k-dependent terms in the moments are proportional to J_z. Because we are considering $J_z=0$, $\widetilde{M}\,{}_{2l}^\alpha(k)$ become k independent. It has been pointed out in Ref. 5(a) that, for $J_z=0$, $M_{2l}^\alpha(n)$ is nonzero only if $n=0$. Therefore, Eq. (3) implies that $\widetilde{C}\,{}^\alpha(k,t)=C^\alpha(0,t)$. Thus, substituting Eqs. (11) and (12) into Eq. (9), the Mori parameters take the form

$$\delta_1^x(k)=2J_y^2\ , \tag{13a}$$
$$\delta_2^x(k)=2(J_x^2+J_y^2)\ , \tag{13b}$$
$$\delta_3^x(k)=\frac{2J_x^2(5J_x^2+J_y^2)}{(J_x^2+J_y^2)}\ , \tag{13c}$$
$$\delta_1^y(k)=2J_x^2\ , \tag{14a}$$
$$\delta_2^y(k)=2(J_x^2+J_y^2)\ , \tag{14b}$$
$$\delta_3^x(k)=\frac{2J_y^2(5J_y^2+J_x^2)}{(J_x^2+J_y^2)}\ . \tag{14c}$$

For the Ising case $J_x\neq 0$ and $J_y=0$, Eqs. (13a) and (14) are reduced to $\delta_1^x(0)=0$, $\delta_1^y(0)=\delta_2^y(0)=2J_x^2$, and $\delta_3^y(0)=0$. Consequently, with the help of Eq. (8), the relaxation functions become $\Gamma^x(0,s)=1/s$ and $\Gamma^y(0,s)=(s^2+2J_x^2)/s(s^2+4J_x^2)$, which are the Laplace transform of $C^x(0,t)=1$ and $C^y(0,t)=\cos^2 J_xt$, respectively. This is again in agreement with the results of Ref. 5(b). As a final case, let us take the isotropic situation $J_x=J_y=J$ for which $C^x(0,t)=C^y(0,t)$. Then $\delta_1^\alpha(0)=2J^2$, $\delta_2^\alpha(0)=4J^2$, $\delta_3^\alpha(0)=6J^2$, etc., and

$$\Gamma^\alpha(0,s)=\cfrac{1}{s+\cfrac{2J^2}{s+\cfrac{4J^2}{s+\cfrac{6J^2}{s+\ddots}}}}\ , \tag{15}$$

with $\alpha=x,y$.

This expression can be rearranged in a more convenient form as follows:

$$\Gamma^\alpha(0,s)=\cfrac{1/\sqrt{2}J}{\cfrac{s}{\sqrt{2}J}+\cfrac{1}{\cfrac{s}{\sqrt{2}J}+\cfrac{2}{\cfrac{s}{\sqrt{2}J}+\cfrac{3}{\cfrac{s}{\sqrt{2}J}+\ddots}}}}\ . \tag{16}$$

According to Wall,[9] this continued fraction converges to

$$(1/\sqrt{2J})\exp(-s^2/4J^2)\int_{s/\sqrt{2J}}^{\infty} e^{-u^2/2}du ,$$

which in turn is precisely the Laplace transform of $e^{-J^2t^2}$. Once more, this is a merely confirmation of well-known results.[5]

To the best of my knowledge, I could not find any closed form of the relaxation function for which the continued fraction converges in the anisotropic case $J_x \neq J_y$. Even so, I consider that the previous calculation is sufficient to believe that the continued-fraction approach produces the correct answer for the correlation functions of the spin-$\frac{1}{2}$ XYZ model in any situation.

Let us now make some comments about the convergence of the continued fraction. The relaxation function of Eq. (8) can be generated from a hierarchy of relaxation functions coupled one each other by

$$\Gamma_l^\alpha(k,s)=\delta_l^\alpha(k)/[s+\Gamma_{l+1}^\alpha(k,s)] ,$$

with $\delta_0^\alpha(k)=1$ and $\Gamma_0^\alpha(k,z)=\Gamma^\alpha(k,z)$. We can also write this as $\Gamma_{l+1}^\alpha(k,s)=-s+\delta_l^\alpha(k)/\Gamma_l^\alpha(k,s)$. Having knowledge of the exact result for $\Gamma_0^\alpha(k,z)$, in Ref. 4 they evaluated (numerically) $\Gamma_l^\alpha(k,s)$ up to $l=5$. Surprisingly, they did not find any function $g(k,s)$ for which $\Gamma_l^\alpha(k,s)$ approaches with increasing values of l. For instance, in case (a) investigated above, $\Gamma_l^\alpha(k,s) = s/2 + (s^2/4+4a^2)^{1/2}$ for all $l \geq 2$. It must be emphasized that Eq. (8) converges for all $\mathrm{Re}(s)>0$ (the proof of this fact can be found in Ref. 7). It seems that in Ref. 4 they did not attempt to solve this problem. This might be the origin of all their difficulties in not finding the convergence of the continued fraction. It is hard to affirm whether this is in fact the problem; nevertheless, our analysis certainly indicates that those numerical works must be revised.

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[8]To convince ourselves that $\delta_l^z(k)=4a^2$ for all $l \geq 2$, one could say that we should go a few more stages beyond $l=3$. In fact, from Eqs. (2.19) and (2.20) of Ref. 5(a) with $J_z=0$ and $J_x=J_y=J$, we find $\tilde{M}_8^z(k)=35\times 2^9 a^8$, $\tilde{M}_{10}^z(k)=315\times 2^{10}a^{10}$. These moments and those of Eq. (7) as substituted into Eq. (10) produce $\Delta_1=2^3a^2$, $\Delta_2=2^8a^6$, $\Delta_3=2^{15}a^{12}$, $\Delta_4=2^{24}a^{20}$, and $\Delta_5=2^{35}a^{30}$. This sequence suggests to us that $\Delta_l=2^{l(l+2)}a^{l(l+1)}$ for all $l \geq 1$. Upon using $\delta_l^z(k)=\Delta_l\Delta_{l-2}/(\Delta_{l-1})^2$, one finally obtains $\delta_l^z(k)=4a^2$ for all $l \geq 2$.

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