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# Spin dynamics for the one-dimensional $XY$ model at infinite temperature*†

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The infinite-temperature space- and time-dependent spin-correlation functions $g_r^x(t)$ are studied for the one-dimensional $XY$ model. Numerical calculations are performed to obtain the exact autocorrelation function $g_0^x(t)$ for chains containing 5, 7, and 9 spins ($S = 1/2$). This yields exact results for the first 16 moments of the frequency autocorrelation function of the infinite chain, and estimates for a few of the higher moments as well. The analysis suggests that $g_0^x(t)$ for the infinite chain is identical to $\exp(-J^2t^2)/4$. We show that $g_r^x(t)$ for $r\neq 0$ vanishes identically for all values of time, implying a wave-vector-independent relaxation shape function. Our result for $g_0^x(t)$ is compared with that obtained by Huber for the classical ($S = \infty$) chain.

## I. INTRODUCTION

The one-dimensional $XY$ model has attracted considerable attention as a nontrivial many-body problem having interesting physical properties.[1] The Hamiltonian is described by

$$\mathcal{H}_\gamma = 2J\sum_i [(1+\gamma)S_i^xS_{i+1}^x + (1-\gamma)S_i^yS_{i+1}^y], \qquad (1)$$

where $J$ is the strength of the interaction, $\vec{S}_i$ is the spin vector of the $i$th particle ($S=\frac{1}{2}$), and $\gamma$ is the anisotropy parameter. Lieb, Schultz, and Mattis[2] showed that $\mathcal{H}_\gamma$ can be transformed into one describing a set of noninteracting fermions and made a detailed study of its ground-state ($T=0$) properties. Katsura[3] introduced a magnetic field in the $z$ direction and obtained exact results for the temperature and magnetic field dependence of the various thermodynamic properties. McCoy[4] and later Barouch and McCoy[5] made a detailed investigation of the various space-dependent spin-correlation functions at different temperatures. Suzuki[6] studied the effect of introducing a staggered magnetic field along the $z$ direction. He later introduced a generalized $XY$ model and examined its relationship to other exactly soluble magnetic models.[7]

Recently, the dynamic behavior of this system has also received a great deal of attention. Barouch, McCoy, and Dresden[8] introduced a time-dependent external magnetic field in the $z$ direction and solved the Liouville equation exactly. They demonstrated that for $\gamma\neq 0$ the magnetization shows nonergodic behavior. This rather peculiar behavior was also observed by Mazur,[9] Suzuki,[10] and Girardeau.[11] The space- and time-dependent spin pair-correlation functions $\tilde{g}_r^\nu(t)$, defined by

$$\tilde{g}_r^\nu(t) = \langle S_0^\nu(t)S_r^\nu\rangle, \qquad (2)$$

are of considerable interest also. Niemeijer[12] and also Katsura, Horiguchi, and Suzuki[13] obtained exactly the longitudinal correlation functions $\tilde{g}_r^z(t)$. Because of mathematical complexity, however, the knowledge of transverse correlation functions $\tilde{g}_r^x(t)$ is rather limited. Barouch and McCoy[14] examined the asymptotic behavior of $\tilde{g}_r^x(t)$ at $T=0$ as $r\to\infty$ and $t\to\infty$. They found it to be an oscillatory factor times $t^{-p}$, where $p$ is a fraction depending on the values of the parameters of the Hamiltonian. Very recently, Capel, Van Dongen, and Siskens[15] obtained analytically a few of the high-temperature and short-time series expansion coefficients of $\tilde{g}_r^x(t)$ for $r\leq 5$.

Here we focus our attention on the isotropic $XY$ model where the Hamiltonian $\mathcal{H}_0$ is given by Eq. (1) with $\gamma=0$. We also confine ourselves to the infinite-temperature correlation functions

$$g_r^\nu(t) = \mathrm{Tr}(e^{i\mathcal{H}_0t}S_0^\nu e^{-i\mathcal{H}_0t}S_r^\nu)/\mathrm{Tr}(1) = \tilde{g}_r^\nu(t)\big|_{T=\infty}, \qquad (3)$$

and also its frequency Fourier transform $f_r^\nu(\omega)$, defined by

$$f_r^\nu(\omega) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} e^{-i\omega t}g_r^\nu(t)\,dt, \quad \nu=x,y,z. \qquad (4)$$

The trace in Eq. (3) can be taken over any complete set of states.

We present here a study of the autocorrelation functions $g_0^z(t)$ and $g_0^x(t)$ for the short-time region ($Jt\sim 3$) for the infinite linear chain on the basis of *ab initio* calculation for finite linear chains containing $N$ spins for $N=5, 7$, and 9. Our result for $g_0^z(t)$ is in excellent agreement with the exact result and confirms the accuracy of our method. The first 16 moments of $f_0^x(\omega)$ for the infinite chain are found to be identical to those of a Gaussian. The transverse crosscorrelation functions $g_r^x(t)$ for $r\neq 0$ are shown to vanish identically for all values of $t$. This, however, is not true for the general anisotropic Heisenberg model.

The results are presented in Sec. II and some concluding remarks are added in Sec. III.

## II. RESULTS

The method of obtaining $g_0^\nu(t)$ ($\nu=x$ or $z$) for a finite chain containing $N$ spins is identical to that of a recent study of linear Heisenberg chains.[16] We first introduce the periodic boundary condition,

$$\vec{S}_{i+N}=\vec{S}_i \tag{5}$$

for each $i$. This enables one to diagonalize $\mathcal{H}_0$ numerically in a representation in which the translation operator $T$ and the $z$ component of the total spin $S^z$ are diagonal. The trace in Eq. (3) is then evaluated over the eigenfunctions of $\mathcal{H}_0$. The moments $(\mu_r^x)_{2k}$ of $f_r^x(\omega)$, which are given by the Taylor series expansion of $g_r^x(t)$ around $t=0$, namely,

$$g_r^x(t)=(\mu_r^x)_0+\sum_{k=1}^{\infty}(-1)^k(\mu_r^x)_{2k}\frac{t^{2k}}{(2k)!}\,,$$
$$(\mu_r^x)_0=\tfrac{1}{4}\delta_{0,r}\,, \tag{6}$$

can also be evaluated in this representation. We shall on occasion use the normalized correlation functions $G_0^\nu(t)$, defined by

$$G_0^\nu(t)=g_0^\nu(t)/g_0^\nu(0)=4g_0^\nu(t)\,. \tag{7}$$

To illustrate the accuracy of our method, we have plotted in Fig. 1 our numerical results for $G_0^z(t)$ for $N=5, 7$, and 9, and also the analytic result for the infinite chain obtained by Niemeijer,[12] namely,

$$G_0^z(t)=[J_0(2Jt)]^2, \tag{8}$$

where $J_0$ is the Bessel function of order 0. As has been observed previously,[16] addition of spins to a chain modifies $G_0^z(t)$ at successively longer times, keeping the short-time behavior relatively unchanged (see Fig. 1). We define $\tau_N$ to be the time domain up to which the $N$-spin result for $G_0^z(t)$ reproduces that of the infinite chain accurately. Figure 1 indicates that $J\tau_5\sim 1$, $J\tau_7\sim 2$, and $J\tau_9\sim 3$. The result for $G_0^z(t)$ for each value of $N$ investigated is

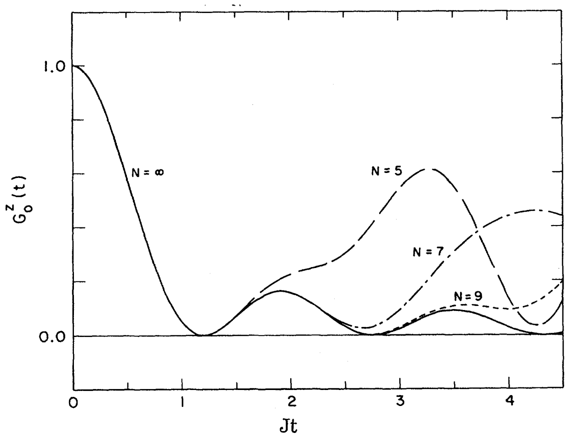


FIG. 1. Exact normalized infinite-temperature longitudinal autocorrelation function $G_0^z(t)$ for the nearest-neighbor one-dimensional $XY$ model for different values of $N$. The solid curve is the analytical result of Niemeijer (Ref. 12) for the infinite chain.

in excellent agreement (within the accuracy of our computations[17]) with the exact result for $N=\infty$, if $t<\tau_N$.

The moments of $f_0^x(\omega)$ are shown in Table I. The $N$-spin result is expected to reproduce the moments of the infinite chain up through $(\mu_0^x)_{2N-2}$ exactly.[16] Empirically (see Table I), it also seems to provide lower bounds for a few of the higher moments as well. A comparison of our results for $N=5$ and $N=7$ shows that the moments $(\mu_0^x)_2$ through $(\mu_0^x)_8$ are identical in these two cases. One also notes that $(\mu_0^x)_{10}$ and $(\mu_0^x)_{12}$ for $N=5$ are within 1.2% and 5%, respectively, of those obtained for $N=7$. Similarly, $(\mu_0^x)_{14}$ and $(\mu_0^x)_{16}$ for $N=7$ are within 0.03% and 0.2%, respectively, of those obtained for $N=9$. We believe that this trend continues for higher values of $N$ as well and probably arises because of the

TABLE I. Moments of the infinite-temperature transverse autocorrelation function $f_0^x(\omega)$ for the nearest-neighbor one-dimensional $XY$ model. Entries up through those marked (a) are identical to those of the infinite chain for each finite value of $N$ investigated. In the fifth column ($N=\infty$) entries up through $(\mu_0^x)_{16}$ are identical to those for $N=9$. The $(\mu_0^x)_{18}$, marked (b) in the table, and the higher entries in the same column should be considered as lower bounds of the exact results only.

| | | | $\mu_0^x 2k/J^{2k}$ | | |
|---|---|---|---|---|---|
| $2k$ | $N=5$ | $N=7$ | $N=9$ | $N=\infty$ | $\frac{1}{4}(e-J^2t^2)$ |
| 0 | 0.25 | 0.25 | 0.25 | 0.25 | 0.25 |
| 2 | 0.500000 | 0.500000 | 0.500000 | 0.500000 | 0.50 |
| 4 | 3.00000 | 3.00000 | 3.00000 | 3.00000 | 3.00 |
| 6 | 30.0000 | 30.0000 | 30.0000 | 30.0000 | 30.00 |
| 8 | 420.000[a] | 420.000 | 420.000 | 420.000 | 420.00 |
| 10 | 7469.00 | 7560.00 | 7560.00 | 7560.00 | 7560.00 |
| 12 | $0.157878\times10^6$ | $0.166320\times10^6$ [a] | $0.166320\times10^6$ | 166320.0 | 166320.00 |
| 14 | $0.378744\times10^7$ | $0.432307\times10^7$ | $0.432432\times10^7$ | $0.432432\times10^7$ | 4324320.00 |
| 16 | $0.998628\times10^8$ | $0.129498\times10^9$ | $0.129730\times10^9$ [a] | $0.129730\times10^9$ | $0.12972960\times10^9$ |
| 18 | $0.282815\times10^{10}$ | $0.438355\times10^{10}$ | $0.441079\times10^{10}$ | $0.44108\times10^{10}$ [b] | $0.44108064\times10^{10}$ |
| 20 | $0.845415\times10^{11}$ | $0.164966\times10^{12}$ | $0.167605\times10^{12}$ | $0.1676\times10^{12}$ | $0.16761064\times10^{12}$ |
| 22 | | | $0.703861\times10^{13}$ | $0.704\times10^{13}$ | $0.70396470\times10^{13}$ |
| 24 | | | $0.323669\times10^{15}$ | $0.32\times10^{15}$ | $0.32382376\times10^{15}$ |

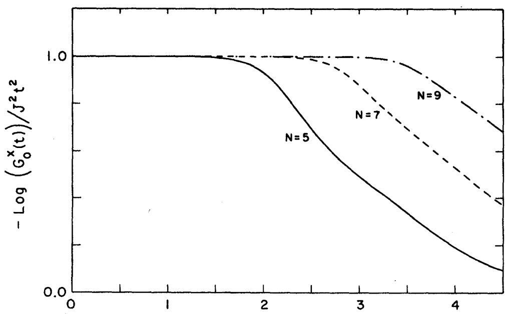


FIG. 2. Test for Gaussian hypothesis for the normalized infinite-temperature transverse autocorrelation function $G_0^x(t)$ for the nearest-neighbor one-dimensional $XY$ model.

lower dimensionality of our system. In column 5 of Table I, we provide exact results for the first 16 moments and also estimate lower bounds for $(\mu_0^x)_{18}$ through $(\mu_0^x)_{24}$ for the infinite chain. Our results for $(\mu_0^x)_2$ and $(\mu_0^x)_4$ are in excellent agreement with those obtained by McFadden and Tahir-Kheli.[18] The $(\mu_0^x)_6$ and higher moments have not been calculated previously. The last column in Table I contains the moments of a Gaussian $f(t)$, defined by

$$f(t)=\tfrac{1}{4}e^{-J^2t^2}\ . \tag{9}$$

A comparison of the last two columns in Table I shows that each of the known moments for $N=\infty$ is identical to that of $f(t)$. This suggests that $g_0^x(t)$ for the infinite chain may be identical to $f(t)$. We know of no rigorous proof of this result.

To investigate how $g_0^x(t)$ for finite chains approaches the Gaussian behavior, we have plotted $h(t)$, defined by

$$h(t)=-[\log G_0^x(t)]/J^2t^2, \tag{10}$$

against $Jt$ for $N=5, 7$, and 9, as shown in Fig. 2, which indicates $J\tau_5\sim 1$, and $J\tau_7\sim 2$. Assuming the same trend to continue for $N=9$, one obtains $J\tau_9\sim 3$. We note that for $t$ within $\tau_N$ $h(t)$ is identical to 1 (within the accuracy of our calculations). Our numerical result on $G_0^x(t)$ for $N=9$ shows that it has already decayed to $10^{-4}$ when $Jt\sim 3$. We therefore hypothesize that $G_0^x(t)$ for the infinite chain is given by

$$G_0^x(t)=e^{-J^2t^2}. \tag{11}$$

Recently, Huber[19] has obtained numerical results on $g_0^x(t)$ for a classical ($S=\infty$) chain by Monte Carlo methods. To compare our result with his, we scale his result according to the transformation

$$J=J_H/\sqrt{3}\ , \tag{12}$$

where $J_H$ is the exchange constant, as defined in Ref. 19. This ensures that the two models have the same second moment. We also properly normalize his result. A comparison of the two cases is illustrated in Fig. 3. The asymptotic behavior for large values of $t$ is quite different for the two cases, in contrast to the Heisenberg chain, where it was found to be rather insensitive to the $S$ value.[16]

At infinite temperatures, the transverse off-site (or crosscorrelation) functions $g_r^x(t)$ for $r\neq 0$ vanish identically. This can be seen term by term in, say, the diagram expansion discussed by Wortis,[20] where classes of diagrams vanish either because $J_{\parallel}=J_z=0$ or because $\beta=1/k_BT=0$. The correlations for $r$ an odd integer can be seen to vanish by the usual symmetry arguments.[21] These results are of course reproduced explicitly in the calculations on the finite chains.

## III. CONCLUDING REMARKS

Since $g_r^x(t)$ vanishes for $r\neq 0$, the wave-vector-dependent transverse relaxation shape function[22] $F_q^x(t)$ for our model is given by

$$F_q^x(t)=e^{-J^2t^2}, \tag{13}$$

independent of $q$. In the theory of magnetic resonance, the $q=0$ mode of $F_q^x(t)$ is referred to as the free-induction decay function.[23] Its frequency Fourier transform is identical to the NMR line shape.[24] We therefore conclude that the NMR line shape for the one-dimensional $XY$ model is a Gaussian, provided that the magnetic field is applied along the $z$ direction. The usual phenomenological arguments[25] which predict a Gaussian line shape, however, cannot be valid for this system. A simple physical interpretation and a rigorous proof of our result is still lacking.

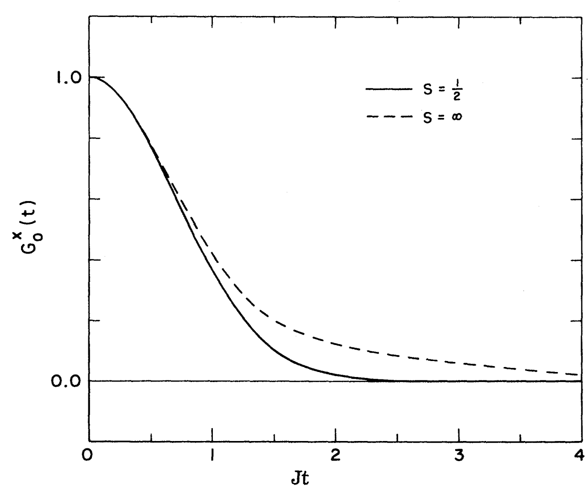


FIG. 3. Comparison of normalized infinite-temperature transverse autocorrelation function for the nearest-neighbor one-dimensional $XY$ model for different values of $S$. The solid curve is our present result for $S=\frac{1}{2}$. The dashed curve is the numerical result obtained by Huber (Ref. 19) for $S=\infty$.

Our arguments that the cross-correlation functions vanish can be generalized to other loose-packed lattices. In particular, this shows that $F_q^x(t)$ for the square and simple-cubic lattices[26] are also independent of $q$. Results for the second $(m_2)$ and fourth $(m_4)$ moments of the frequency Fourier transform of $G_0^x(t)$ for hypercubic lattices[18] show that

$$m_4/(m_2)^2 = (\mu_0^x)_4/4[(\mu_0^x)_2]^2 = 5 - 2/d\,, \qquad (14)$$

where $d$ is the dimensionality of the lattice. Since the ratio in Eq. (14) must be exactly three for a Gaussian function, $F_q^x(t)$ cannot be Gaussian for all times when $d > 1$.


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*Note added in proof*. The question as to what happens when $\gamma \neq 0$ in Eq. (1) has been raised (B. M. McCoy, private communication). One can show (see Ref. 15) that for this case $m_4/(m_2)^2$ $3[1+\gamma(\gamma - \frac{2}{3})]$. This shows that for a general nonzero value of $\gamma$, other than $\gamma = \frac{2}{3}$, $G_0^x$ cannot be a Gaussian. It remains to be seen if the higher moments for $\gamma = \frac{2}{3}$ are also equal to those of a Gaussian.

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