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Dynamical correlation functions for one-dimensional quantum spin systems: New results based on a rigorous approach

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We present new results on the time-dependent correlation functions $\Xi_n(t) = 4\langle S_0^\xi(t) S_n^\xi\rangle, \xi = x,y$ at zero temperature of the one-dimensional $S = 1/2$ isotropic XY model $(h = \gamma = 0)$ and of the transverse Ising model (TI) at the critical magnetic field $(h = \gamma = 1)$. Both models are characterized by special cases of the Hamiltonian $H = -J\sum_l[(1+\gamma)S_l^x S_{l+1}^x + (1-\gamma)S_l^y S_{l+1}^y + hS_l^z]$. We have derived exact results on the long-time asymptotic expansions of the autocorrelation functions (ACF's) $\Xi_0(t)$ and on the singularities of their frequency-dependent Fourier transforms $\Phi_0^{\xi\xi}(\omega)$. We have also determined the latter functions by high-precision numerical calculations. The functions $\Phi_0^{\xi\xi}(\omega)$, $\xi = x,y$ have singularities at the infinite sequence of frequencies $\omega = m\omega_0$, $m = 0, 1, 2, 3, \ldots$ where $\omega_0 = J$ for the XY model and $\omega_0 = 2J$ for the TI model. In both models the singularities in $\Phi_0^{xx}(\omega)$ for $m = 0, 1$ are divergent, whereas the nonanalyticities at higher frequencies become increasingly weaker. We point out that the nonanalyticities at $\omega \neq 0$ are intrinsic features of the discrete quantum chain and have therefore not been found in the context of a continuum analysis.

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Exact results are available for the thermodynamic properties of many one-dimensional (1D) classical and quantum spin systems. But for most of these "exactly solvable" model systems, no rigorous results are known for dynamic correlation functions. However, the knowledge of dynamic correlation functions is crucial for understanding the excitation spectrum of the underlying model and its observability in dynamical experiments.

In this paper, we study the dynamics at temperature $T = 0$ of the 1D, $S = 1/2$ transverse Ising (TI) model at the critical external magnetic field and the 1D, $S = 1/2$ isotropic XY model in zero field, specified, respectively, by the Hamiltonians

$$H_{\mathrm{TI}} = -\sum_{l=1}^{N}[2JS_l^x S_{l+1}^x + h_c S_l^z], \quad h_c = J, \tag{1}$$

$$H_{XY} = -J\sum_{l=1}^{N}[S_l^x S_{l+1}^x + S_l^y S_{l+1}^y] \tag{2}$$

in the limit $N \to \infty$, with periodic boundary conditions imposed. We are interested in the time-dependent correlation functions

$$\Xi_n(t) = 4\langle S_0^\xi(t) S_n^\xi\rangle, \quad \xi = x,y,z, \tag{3}$$

and their frequency-dependent Fourier transforms

$$\Phi_n^{\xi\xi}(\omega) = \int_{-\infty}^{+\infty} dt e^{i\omega t}\langle S_0^\xi(t) S_n^\xi\rangle. \tag{4}$$

A brief report of some of our results was given in Ref. 1. Here we present the results of a newly extended long-time asymptotic expansion (LTAE) of the time-dependent autocorrelation functions (ACF's) $X_0(t)$ and $Y_0(t)$ for the TI and the XY models, together with an analysis of their general structural features, and an analytical determination of the singularities in their frequency-dependent Fourier transforms $\Phi_0^{\xi\xi}(\omega)$, $\xi = x,y$. Our results are of direct experimental interest, since there are several compounds which exhibit quasi-1D interactions described by Eq. (1) or (2). $\Phi_0^{\xi\xi}(\omega)$ is important since it is the integral over q of the dynamic structure factor $S_{\xi\xi}(q,\omega)$ measured by inelastic neutron scattering, and for small ω, is related to the spin-lattice relaxation rate measured by nuclear magnetic resonance experiments. Whereas the functions $Z_n(t)$ have been known analytically for many years for both models at arbitrary temperature,[2] there has never been any complete calculation of $X_n(t)$ for general T and, in particular, for the case $T = 0$ of interest here. Recently, however, substantial progress was made in this direction.[3]

In Ref. 3, it was shown that the time-dependent correlation function $X_n(t)_{\mathrm{TI}}$ at $T = 0$ can be expressed in terms of a related function $\sigma_n(z)$ as

$$X_n(t)_{\mathrm{TI}} = X_n(0)_{\mathrm{TI}} \exp\left\{-(1/2)t^2 + \int_0^{2t} dt'\sigma_n(it')/t'\right\}, \tag{5}$$

where the units are chosen such that $J = 1$, and where the static correlation function is given by $X_0(0)_{\mathrm{TI}} = 1$ and for the nontrivial case $n > 0$ by

$$X_n(0)_{\mathrm{TI}} = \left(\frac{2}{\pi}\right)^{|n|}\prod_{l=1}^{|n|}\left[1 - \frac{1}{4l^2}\right]^{l-|n|}, \tag{6}$$

and $\sigma_n(z)$ satisfies the nonlinear ordinary differential equation (ODE)

$$(z\sigma_n'')^2 + 4[z\sigma_n' - \sigma_n - n^2][z\sigma_n' - \sigma_n + (\sigma_n')^2] = 0, \tag{7}$$

with certain initial conditions. For the case $n = 0$ of interest here, the solution for $z \to 0$ can be represented by the series

$$\sigma_0(z) = \sum_{k=1}^{\infty} a_{0,k} z^{2k} + z\sum_{k=0}^{\infty} b_{0,k} z^{2k}, \tag{8}$$

where all coefficients $a_{0,k}$ and $b_{0,k}$ can be calculated recursively in terms of $b_{0,0} = 1/\pi$.

For Ref. 3, the ODE (7) was solved numerically for $n = 0$. From this numerical solution, an analytic ansatz for the LTAE of $\sigma_0(it)$ was inferred and then verified analytically. From this LTAE, the resultant LTAE of $X_0(t)_{\mathrm{TI}}$ was calculated to $0(t^{-11/4})$. For the present work, we have extended the LTAE of $X_0(t)_{\mathrm{TI}}$ to $0(t^{-33/4})$. We find that the

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LTAE's of $X_0(t)_{\rm TI}$ and $Y_0(t)_{\rm TI}$ have the following structure as far as we have determined it:

$$\Xi_0(t)_{\rm TI} \sim \overline{A}\,(it)^{-1/4} \sum_{m=0}^{\infty} T^{(\rm TI)}_{\xi,m}, \tag{9a}$$

$$T^{(\rm TI)}_{\xi,m} = (2\pi)^{-m/2} e^{-2imt}(-2it)^{-\alpha^{(\xi)}_m} \times \sum_{n=0}^{\infty} a_n^{(\xi,m)}(-2it)^{-n}, \tag{9b}$$

for $\xi = x,y$, where

$$\overline{A} = 2^{1/12}\exp[3\zeta'(-1)] = 0.64500248\ldots . \tag{10}$$

The coefficients $a_n^{(\xi,m)}$ are rational numbers with $a_{2n+1}^{(\xi,0)} = 0$ for $\xi = x,y$, and all n in Eq. (9). The exponents $\alpha_m^{(\xi)}$ are positive integers or half integers. The values of $a_n^{(x,m)}$ and $\alpha_m^{(x)}$ which have so far been calculated are listed in Table I. We have also calculated the corresponding $a_n^{(y,m)}$ and $\alpha_m^{(y)}$ from these results.

Some general features of the LTAE (9) are as follows: It consists of an infinite sum of terms $T^{(\rm TI)}_{\xi,m}$, $m = 0, 1, 2\ldots$, each with a specific oscillatory t dependence given by the phase factor e^{-2imt}. Each term $T^{(\rm TI)}_{\xi,m}$ is itself an infinite sum of terms with ascending powers of t^{-1}. We thus denote it as a "tower." Each successive tower enters first at a progressively higher level in the expansion. Our results in Table I strongly suggest that the exponent $\alpha_m^{(x)}$ is given by $\alpha_m^{(x)} = m^2/2$. It follows that $\alpha_m^{(y)} = m^2/2$ also, except for the nonoscillatory tower, which is suppressed by two units: $\alpha_0^{(y)} = 2$.

We have also calculated the LTAE of $X_0(t)_{XY} = Y_0(t)_{XY}$ and found the following result ($\perp$ denotes x or y)[4]:

$$X_0(t)_{XY} \sim (\overline{A})^2 2^{1/2}(it)^{-1/2} \sum_{m=0}^{\infty} T^{(XY)}_{\perp,m}, \tag{11a}$$

$$T^{(XY)}_{\perp,m} = (2\pi)^{-m/2} e^{-imt}(-it)^{-\beta^{(\perp)}_m} \sum_{n=0}^{\infty} b_n^{(\perp,m)}(-it)^{-n}. \tag{11b}$$

TABLE I. Values for the exponents $\alpha_m^{(x)}$ and the coefficients $a_n^{(x,m)}$ of the LTAE Eq. (9) of $X_0(t)_{\rm TI}$ which have been calculated. We have also calculated two values for the next column ($m = 4$): $\alpha_4^{(x)} = 8$, $a_0^{(x,4)} = 3/2^{10}$.

m	0	1	2	3
$\alpha_m^{(x)}$	0	$\frac{1}{2}$	2	$\frac{9}{2}$
$a_0^{(x,m)}$	1	1	$\frac{1}{2^2}$	$\frac{1}{2^5}$
$a_1^{(x,m)}$	0	$\frac{9}{2^3}$	$\frac{15}{2^4}$	$\frac{75}{2^8}$
$a_2^{(x,m)}$	$\frac{1}{2^3}$	$\frac{297}{2^7}$	$\frac{489}{2^7}$	$\frac{8881}{2^{12}}$
$a_3^{(x,m)}$	0	$\frac{7587}{2^{10}}$	$\frac{9387}{2^9}$	$\frac{516\,609}{2^{15}}$
$a_4^{(x,m)}$	$\frac{81}{2^7}$	$\frac{1\,027\,035}{2^{15}}$	$\frac{851\,427}{2^{13}}$	
$a_5^{(x,m)}$	0	$\frac{43\,594\,695}{2^{18}}$	$\frac{22\,520\,925}{2^{15}}$	
$a_6^{(x,m)}$	$\frac{11\,259}{2^{10}}$	$\frac{4\,418\,168\,445}{2^{22}}$	$\frac{1\,368\,815\,805}{2^{18}}$	
$a_7^{(x,m)}$	0	$\frac{260\,700\,970\,635}{2^{25}}$		
$a_8^{(x,m)}$	$\frac{13\,516\,875}{2^{15}}$			

Again, the coefficients $b_n^{(\perp,m)}$ are rational numbers, with $b_{2n+1}^{(\perp,0)} = 0$ for all n in Eq. (11), and the exponents $\beta_m^{(\perp)}$ are positive integers or half integers. Evidently, the structure of Eq. (11) is very similar to that of Eq. (9). In contrast to the TI case, however, all non-negative integral frequencies, not only the even ones, occur in the LTAE of $X_0(t)_{XY}$. In this case, our results suggest that the exponent in the prefactor for the mth tower is given by $\beta_m^{(\perp)} = (1/2)[(m^2+1)/2]$, where $[\nu]$ denotes the integer part of ν.

We have generated the function $\Phi_0^{xx}(\omega)_{\rm TI}$ numerically by a fast Fourier transform program using the precise numerical results for $X_0(t)_{\rm TI}$ for $t < 40$ and the LTAE (9) for $t > 40$. At $t = 40$, our numerical solution matches the known LTAE to within an error of 10^{-6}. The resulting $\Phi_0^{xx}(\omega)_{\rm TI}$ is plotted in Fig. 1. The accuracy of the curve is estimated to be better than 1 part in 10^3 over the range shown. Figure 1 also shows $\Phi_0^{yy}(\omega)_{\rm TI}$, which is given by[4] $\Phi_0^{yy}(\omega)_{\rm TI} = \omega^2\phi_0^{xx}(\omega)_{\rm TI}$. Our numerical results, shown in Fig. 1, exhibit singularities at $\omega = 0, 2$, and 4. It is a rigorous property that the singularities in the frequency-dependent correlation functions are determined by the long-time asymptotic behavior of the corresponding time-dependent correlation functions. Using our result Eq. (9) on the LTAE of $X_0(t)_{\rm TI}$, we find that $\Phi_0^{xx}(\omega)_{\rm TI}$ has further (finite) singularities at $\omega = 6, 8, \ldots$, dominated by the leading term in each successive tower of the LTAE. Specifically, the dominant singularity of $\Phi_0^{xx}(\omega)_{\rm TI}$ at frequency $\omega_m^{(\rm TI)} = 2m$, $m = 0, 1, 2, \ldots$ has the following form:

$$\Phi_0^{xx}(\omega)^{(m)}_{\rm TI} \sim \tfrac{1}{2}A_m^{(x)}\Gamma(\tfrac{3}{4} - \tfrac{1}{2}m^2)|\omega - 2m|^{\nu^{(\rm TI)}_{x,m}} \times \{(1/2)[1-(-1)^m]\theta(2m-\omega) + 2^{-1/2}\theta(\omega - 2m)\}, \tag{12}$$

where

$$A_m^{(x)} = \overline{A}\,(2\pi)^{-m/2}2^{-m^2/2}a_0^{(x,m)}, \tag{13}$$

and $\nu^{(\rm TI)}_{x,m} = m^2/2 - 3/4$. Note that the power-type singularities in $\Phi_0^{xx}(\omega)_{\rm TI}$ at $\omega = \omega_m^{(\rm TI)}$ are one sided for even m and two sided for odd m. Two of the singularities are divergent, viz. $\sim\omega^{-3/4}\theta(\omega)$ at $\omega = 0$ and $\sim|\omega - 2|^{-1/4} \times [\theta(2-\omega) + 2^{-1/2}\theta(\omega - 2)]$ at $\omega = 2$. Since $\nu^{(\rm TI)}_{x,m}$ is a monotonically increasing function of m, the singularities become progressively weaker for larger m. The dominant singulari-

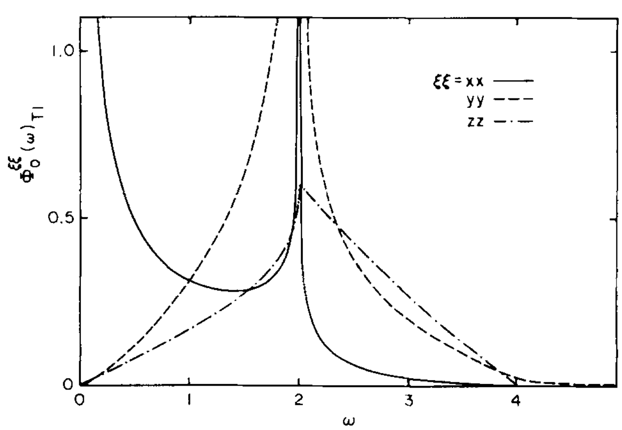

FIG. 1. Frequency-dependent autocorrelation functions $\Phi_0^{xx}(\omega)_{\rm TI}$ (solid line), $\Phi_0^{yy}(\omega)_{\rm TI}$ (dashed line), and $\Phi_0^{zz}(\omega)_{\rm TI}$ (dot-dashed line).

ties in $\Phi_0^{yy}(\omega)_{\rm TI}$ are of the same type as those in $\Phi_0^{xx}(\omega)_{\rm TI}$ except the one at $\omega = 0$. In fact, $\Phi_0^{yy}(\omega)_{\rm TI}$ vanishes like $\omega^{5/4}\theta(\omega)$ as $\omega \to 0$ whereas $\Phi_0^{xx}(\omega)_{\rm TI}$ is divergent there. Physically, the difference in the singularity at $\omega = 0$ can be attributed to the fact that x is the "easy" axis and y the "hard" axis for spin fluctuations.

By the same method as for the TI model and with equally high precision, we have numerically determined $\Phi_0^{xx}(\omega)_{XY} = \Phi_0^{yy}(\omega)_{XY} \equiv \Phi_0^{\perp\perp}(\omega)_{XY}$. Our result is plotted in Fig. 2. From the analysis of the LTAE (11), we find that the dominant singularities of $\Phi_0^{\perp\perp}(\omega)_{XY}$ at frequencies $\omega_m^{(XY)} = m$, $m = 0, 1, 2, \ldots$ have the following form:

$$\Phi_0^{\perp\perp}(\omega)_{XY}^{(m)} \sim \begin{cases} \frac{1}{2}B_m^{(\perp)}\Gamma\left(\frac{1}{2} - \frac{1}{4}m^2\right)(\omega - m)^{\nu_{\perp,m}^{(XY)}}\theta(\omega - m), & \text{even } m, \qquad (14a) \\ -\frac{1}{2}B_m^{(\perp)}\dfrac{1}{\left[\frac{1}{4}(m^2 - 1)\right]!}\,|\omega - m|^{\nu_{\perp,m}^{(XY)}}\ln|\omega - m|, & \text{odd } m, \qquad (14b) \end{cases}$$

where

$$B_m^{(\perp)} = (\bar{A})^2 2^{1/2}(2\pi)^{-m/2} b_0^{(\perp,m)}. \tag{15}$$

The singularity exponents $\nu_{\perp,m}^{(XY)}$ are determined to be $\nu_{\perp,m}^{(XY)} = m^2/4 - 1/2$ for even m and $\nu_{\perp,m}^{(XY)} = m^2/4 - 1/4$ for odd m. The $B_m^{(\perp)}$ can be determined explicitly up to $m = 4$ from the values of $b_0^{(\perp,m)}$ which we have calculated. The singularities in $\Phi_0^{xx}(\omega)_{XY}$ at $\omega_m^{(XY)}$ are alternatingly one sided power-type (m even) and two sided power-type with logarithmic corrections (m odd). In particular, the singularities shown in Fig. 2 are the two divergences $\sim \omega^{-1/2}\theta(\omega)$ at $\omega = 0$, $\sim \ln|\omega - 1|$ at $\omega = 1$ and the cusp $\sim (\omega - 2)^{1/2}\theta(\omega - 2)$ at $\omega = 2$.

For a physical interpretation of $\Phi_0^{xx}(\omega)_{\rm TI}$, $\Phi_0^{yy}(\omega)_{\rm TI}$, and $\Phi_0^{\perp\perp}(\omega)_{XY}$, it is instructive to compare these functions with $\Phi_0^{zz}(\omega)_{TI}$ and $\Phi_0^{zz}(\omega)_{XY}$, both of which can be evaluated exactly in terms of elliptic integrals. These functions, which are also plotted in Figs. 1 and 2, have only three singularities and vanish for $\omega > 4$ (TI case) and $\omega > 2$ (XY case), respectively. This difference in behavior can be understood in the framework of the fermion representation of the models (1) and (2): the ground state is characterized by a half-filled band of noninteracting, spinless fermions with one-particle energies

$$\epsilon_1(q)_{\rm TI} = 2\cos\frac{q}{2}, \quad \epsilon_1(q)_{XY} = \cos q. \tag{16}$$

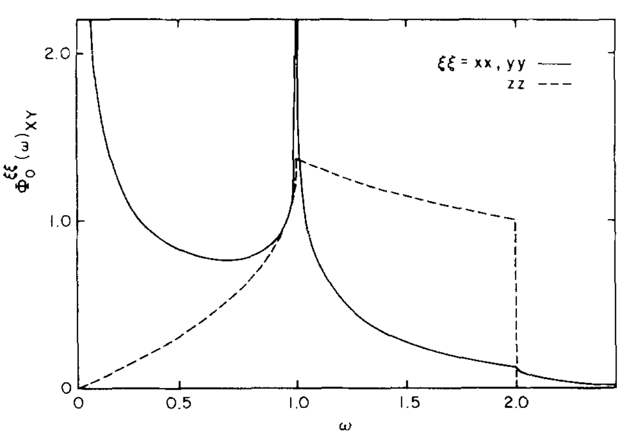

FIG. 2. Frequency-dependent autocorrelation functions $\Phi_0^{xx}(\omega)_{XY} = \Phi_0^{yy}(\omega)_{XY}$ (solid line) and $\Phi_0^{zz}(\omega)_{XY}$ (dashed line).

The spin operator S_l^z, if applied onto the ground state, couples to the two-particle excitations only, whereas the operators S_l^x, S_l^y couple to m-particle excitations with m arbitrarily large. Consequently, the two-particle spectrum exhausts all spectral weight in $\Phi_0^{zz}(\omega)$, whereas $\Phi_0^{xx}(\omega)$, and $\Phi_0^{yy}(\omega)$ include also contributions from m-particle excitations with $m > 2$.

In addition to our work reported above, we have gone on to carry out the analogous studies of the general correlation functions $X_n(t)_{\rm TI}$, $Y_n(t)_{\rm TI}$, and $X_n(t)_{XY} = Y_n(t)_{XY}$. We find, for example, that the LTAE of $X_n(t)_{\rm TI}$ has the same leading order asymptotic t dependence for each tower as that of $X_0(t)_{\rm TI}$, except with a factor $(-1)^{mn}$ adjoined, where m denotes the index of the mth tower of $X_n(t)_{\rm TI}$. This is actually a consequence of the finite-n, large-t asymptotic expansions calculated in Ref. 3. It follows that the singularity exponents of $\Phi_n^{xx}(\omega)_{\rm TI}$ are the same for all n. The same statements apply to $Y_n(t)_{\rm TI}$ and $\Phi_n^{yy}(\omega)_{\rm TI}$, respectively. In the case of XY model, the singularity exponents of $\Phi_n^{\perp\perp}(\omega)_{XY}$ are the same for all even n. These are given above. For odd n, however, we have the relations $\nu_{\perp,m}^{(XY)} = m^2/4 - 1/2$ if m is even, and $\nu_{\perp,m}^{(XY)} = m^2/4 + 3/4$ if m is odd. Further details will be published elsewhere.

Finally, our new results bear strong relevance for low-temperature dynamical experiments on quasi-1D compounds such as the XY-like substance Cs_2CoCl_4 and $PrCl_3$ and the $S = 1/2$ Ising-like substance $CsCoCl_3 \cdot 3H_2O$.

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[4]Once $X_0(t)_{\rm TI}$ is determined, we can determine $Y_0(t)_{\rm TI}$ and $X_0(t)_{XY} = Y_0(t)_{XY}$ by means of the relations $Y_0(t)_{\rm TI} = -(d^2/dt^2)X_0(t)_{\rm TI}$ and $X_0(t)_{XY} = [X_0(t/2)_{\rm TI}]^2$; see Refs. 1 and 3 for more details.