11-1-1985

Implications of Direct-Product Ground States in the One-Dimensional Quantum XYZ and XY Spin Chains

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

Robert E. Shrock

Citation/Publisher Attribution

G. Müller and R.E. Shrock. *Implications of direct-product ground states in the one-dimensional quantum XYZ and XY spin chains.* Phys. Rev. B 32 (1985), 5845-5850.
Available at: http://dx.doi.org/10.1103/PhysRevB.32.5845.

Implications of direct-product ground states in the one-dimensional quantum XYZ and XY spin chains

Gerhard Müller
Department of Physics, University of Rhode Island, Kingston, Rhode Island 02881

Robert E. Shrock
Institute for Theoretical Physics, State University of New York, Stony Brook, New York 11794
(Received 21 May 1985)

We state the conditions under which the general spin-s quantum XYZ ferromagnet (H_-) and antiferromagnet (H_+) with an external magnetic field along one axis, specified by the Hamiltonian $H_\pm=\pm\sum_{l=1}^{N}(J_xS_l^xS_{l+1}^x+J_yS_l^yS_{l+1}^y+J_zS_l^zS_{l+1}^z)-h\sum_{l=1}^{N}S_l^z$ exhibits a fully ordered ground state described by a wave function which is a direct product of single-site wave functions. We present a detailed analysis of the implications for the zero-temperature dynamical properties of this model. In particular, we derive a rigorous relation between the three dynamic structure factors $S_{\mu\mu}(q,\omega)$, $\mu=x,y,z$ at $T=0$. For the special case of the $s=\frac{1}{2}$ anisotropic XY model ($J_z=0$), these relations are used to determine the dynamic structure factors $S_{xx}(q,\omega)$ and $S_{yy}(q,\omega)$ at $T=0$ and $h=(J_xJ_y)^{1/2}$ in terms of the known dynamic structure factor $S_{zz}(q,\omega)$.

I. INTRODUCTION

Quantum spin chains with short-range interactions belong to the category of strongly fluctuating statistical systems at all temperatures. Thermal fluctuations prevent the existence of spontaneous magnetic long-range order (LRO) at any $T>0$. At $T=0$, in general, quantum fluctuations still cause a considerable reduction of the LRO, indeed, sometimes a complete removal of it. The presence of strong zero-point fluctuations is commonly used as an argument for explaining the fact that the standard spin-wave-type approximation techniques routinely employed in the analysis of the collective excitations of magnetic insulators in two and three spatial dimensions (2D and 3D) frequently fail to reproduce the known properties of 1D quantum spin models amenable to rigorous analysis. Of considerable interest in this context are the results of a recent work.[1] in which it was found that there exist special circumstances where a spontaneously ordered ground state of the 1D spin-s XYZ antiferromagnet with no residual correlated quantum fluctuations can be stabilized by an external magnetic field. In a subsequent critical analysis of the validity of spin-wave theory for $T=0$ spin dynamics,[2] it was demonstrated, for the example of an exactly solvable case, that the presence of a fully ordered ground state is an insufficient criterion for the existence of linear spin-wave eigenstates, except in the classical limit $s\rightarrow\infty$. For $s=\frac{1}{2}$, the $T=0$ dynamic structure factors were shown to exhibit complicated behavior incompatible with the predictions of spin-wave theory, despite the fact that the ground state is characterized by zero spin reduction.

In this paper we present a comprehensive study of the circumstances under which the general spin-s XYZ model with an external magnetic field along one axis exhibits a fully ordered ground state and its implications for the $T=0$ dynamical properties of this model. We derive a rigorous relation between the three dynamic structure factors $S_{\mu\mu}(q,\omega)$, $\mu=x,y,z$, at $T=0$, which holds only for these special circumstances. For the $s=\frac{1}{2}$ anisotropic XY model, these relations are used to determine the dynamic structure factors $S_{xx}(q,\omega)$ and $S_{yy}(q,\omega)$ in terms of the known function $S_{zz}(q,\omega)$. In the light of our new work, we discuss a previous calculation by McCoy, Barouch, and Abraham[3] based on the analysis of infinite Toeplitz determinants. Finally, we use our new results to calculate exact expressions for the $T=0$ wave-number-dependent susceptibilities of the $s=\frac{1}{2}$ anisotropic XY model.

II. HAMILTONIAN AND GROUND STATE

In this section we analyze the conditions under which the ground state of the quantum 1D spin-s XYZ model in an external field, specified by the Hamiltonian

$$H_\pm=\pm\sum_{l-1}^{N}(J_xS_l^xS_{l+1}^x+J_yS_l^yS_{l+1}^y+J_zS_l^zS_{l+1}^z)-h\sum_{l=1}^{N}S_l^z \tag{2.1}$$

exhibits a ground state whose wave function is a direct product of single-site states.[4] In (2.1) we assume that $J_\mu\geq 0$ for $\mu=x,y,z$ and, without loss of generality, $J_x\geq J_y$. H_+ then characterizes the XYZ antiferromagnet (AFM) and H_- the XYZ ferromagnet (FM). For technical convenience, only even N and periodic boundary conditions are considered.

We search for realizations of a ground-state wave function with the following structure:

$$|G\rangle=\bigotimes_{l=1}^{N}|\theta_l,l\rangle ,$$

where

$$\begin{aligned}|\theta_l,l\rangle&=U_l(\theta_l)|s,l\rangle\\&=\sum_{m=-s}^{s}|m,l\rangle D_{ms}^{(s)}(\theta_l)\\&=\sum_{m=-s}^{s}\left[\frac{(2s)!}{(s+m)!(s-m)!}\right]^{1/2}[\cos(\theta_l/2)]^{s+m}\\&\qquad\times[\sin(\theta_l/2)]^{s-m}|m,l\rangle .\end{aligned}\tag{2.2}$$

Here $U_l(\theta_l)$ describes a unitary transformation representing a rotation of the spin direction at site l by an angle θ_l away from the z axis in the xz plane.[5] This rotation is generated by the $(2s+1)$-dimensional irreducible representation of the group SU(2) with matrix elements $D_{ms}^{(s)}$ as given above. The states $|m,l\rangle$ are the $2s+1$ eigenfunctions of S_l^2 and S_l^z with eigenvalues $s(s+1)$ and m, respectively.

For $\theta_l\neq 0$, such a ground state is characterized by the presence of spontaneous LRO. The order parameter is

$$\mathbf{M}=\langle\theta_l,l\,|\,\mathbf{S}_l\,|\,\theta_l,l\rangle=[s\sin(\theta_l),0,s\cos(\theta_l)] .\tag{2.3}$$

Note that there are no correlated fluctuations in this state. Its ordering is thus as complete as it can be for quantum spins. Obviously, we can assume that the ground state is uniform in the FM case and has a two-sublattice structure in the AFM case. This is incorporated in our ansatz

$$\theta_l^{\pm}=(\mp 1)^l\theta^{\pm}(J_x,J_y,J_z,h)\tag{2.4}$$

for $H_\pm$, respectively. In both cases, the state (2.2) with θ_l from (2.4) is degenerate with a state specified by $\bar{\theta}_l^{\pm}=-\theta_l^{\pm}$, obtained by rotating all spins by 180° about the axis of the magnetic field.

Applying the unitary transformation $U_l(\theta_l)$ to the spin operators S_l^μ defines a set of new spin operators $\widetilde{S}_l^\mu$, through the relation

$$\begin{aligned}\widetilde{S}_l^x&=U_l^{-1}S_l^xU_l=S_l^x\cos(\theta_l)+S_l^z\sin(\theta_l) ,\\ \widetilde{S}_l^y&=U_l^{-1}S_l^yU_l=S_l^y ,\\ \widetilde{S}_l^z&=U_l^{-1}S_l^zU_l=S_l^z\cos(\theta_l)-S_l^x\sin(\theta_l) .\end{aligned}\tag{2.5}$$

The problem of finding special cases of the Hamiltonian H for which the ground-state wave function $|G\rangle$ has the form (2.2), is then equivalent to finding special cases of the Hamiltonian

$$\widetilde{H}=U^{-1}HU,\quad U=\bigotimes_{l=1}^{N}U_l(\theta_l)\tag{2.6}$$

for which the ground-state wave function is

$$|\widetilde{G}\rangle=U^{-1}|G\rangle=\bigotimes_{l=1}^{N}|s,l\rangle ,\tag{2.7}$$

with all spins aligned parallel to the z axis. The ground-state energy is invariant under this transformation by virtue of the relation

$$\langle G|H|G\rangle=\langle\widetilde{G}|\widetilde{H}|\widetilde{G}\rangle=E_G .\tag{2.8}$$

The transformed Hamiltonian $\widetilde{H}$, if expressed in terms of the original spin operators, has the form

$$\begin{aligned}\widetilde{H}_\pm=\pm\sum_{l=1}^{N}\{&[J_x\cos^2(\theta^\pm)\mp J_z\sin^2(\theta^\pm)]S_l^xS_{l+1}^x+J_yS_l^yS_{l+1}^y\\&+[J_z\cos^2(\theta^\pm)\mp J_x\sin^2(\theta^\pm)]S_l^zS_{l+1}^z\mp h\cos(\theta^\pm)S_l^z\\&+(\mp1)^l(J_x\pm J_z)\sin(\theta^\pm)\cos(\theta^\pm)(S_l^zS_{l+1}^x\mp S_l^xS_{l+1}^z)\pm(\mp1)^l(h/2)\sin(\theta^\pm)(S_l^x\mp S_{l+1}^x)\}\end{aligned}\tag{2.9}$$

for the AFM (upper sign) and FM (lower sign), respectively. The condition for (2.7) to be an eigenstate of (2.9) implies that the first two terms in $\widetilde{H}$ have the same coefficient, and that the last two terms cancel each other for $S_l^z=S_{l+1}^z=s$:

$$J_x\cos^2(\theta^\pm)\mp J_z\sin^2(\theta^\pm)=J_y ,\tag{2.10a}$$

$$s(J_x\pm J_z)\cos(\theta^\pm)=h/2 .\tag{2.10b}$$

These conditions determine the magnitude of the magnetic field h and the angle θ of (2.4) entering in the wave function (2.2) as follows:

$$h=h_N^\pm=2s[(J_x\pm J_y)(J_y\pm J_z)]^{1/2} ,\tag{2.11}$$

$$\cos(\theta^\pm)=[(J_y\pm J_z)/(J_x\pm J_z)]^{1/2} ,\tag{2.12}$$

where the subscript N denotes Néel. For these special parameter values, (2.9) becomes

$$\begin{aligned}\widetilde{H}_\pm=\pm\sum_{l=1}^{N}\{&J_y(S_l^xS_{l+1}^x+S_l^yS_{l+1}^y)\mp(J_x-J_y\mp J_z)S_l^zS_{l+1}^z\mp 2s(J_y\pm J_z)S_l^z\\&+(\mp1)^l[(J_x-J_y)(J_y\pm J_z)]^{1/2}[S_l^zS_{l+1}^x\mp S_l^xS_{l+1}^z-s(S_{l+1}^x\mp S_l^x)]\} ,\end{aligned}\tag{2.13}$$

and the energy of the eigenstate $|\tilde{G}\rangle$, as obtained from (2.8), is

$$E_G=-Ns^2(J_x+J_y\pm J_z)\ , \tag{2.14}$$

whereas the exchange constants J_x, J_y, and J_z can have arbitrary (positive) values in the AFM case, they must satisfy the condition $J_z \le J_y$ or $J_z \ge J_x$ in the FM case.

For the proof[4] that $|\tilde{G}\rangle$ is the ground state of $\tilde{H}$ or, equivalently, that $|G\rangle$ is the ground state of H, it is useful to express the Hamiltonian (2.1) in terms of spin operators S_l^ξ, S_l^η, and S_l^ζ, which are obtained from the operators $\tilde{S}_l^x$, $\tilde{S}_l^y$, and $\tilde{S}_l^z$ of (2.5) by

$$S_l^\xi=(\mp 1)^l\tilde{S}_l^x,\ \ S_l^\eta=(\mp 1)^l\tilde{S}_l^y,\ \ S_l^\zeta=(\mp 1)^l\tilde{S}_l^z\ , \tag{2.15}$$

and in terms of the operators $S_l^{\bar{\xi}}$, $S_l^{\bar{\eta}}$, and $S_l^{\bar{\zeta}}$, which are obtained from S_l^ξ, S_l^η, and S_l^ζ via substitution of the angle θ_l by $\bar{\theta}_l=-\theta_l$ in the definition (2.5). The *XYZ* Hamiltonian (2.1) at $h=h_N^{\pm}$ can then be expressed in the following form:

$$\begin{aligned}H_\pm-E_G=\sum_{l=1}^{N}\{&\tfrac{1}{2}(J_x\pm J_z)[(s-S_l^\xi)(s-S_{l+1}^{\bar{\xi}})\\&+(s-S_l^{\bar{\xi}})(s-S_{l+1}^{\xi})]\\&+J_y[s^2-(S_l^\xi S_{l+1}^\xi+S_l^\eta S_{l+1}^\eta+S_l^\zeta S_{l+1}^\zeta)]\}\ .\end{aligned} \tag{2.16}$$

For the AFM (H_+), the right-hand side of (2.15) is a sum of positive operators for arbitrary (nonnegative) values of J_x, J_y, and J_z, which proves that $|G\rangle$ is the ground state. For the FM (H_-), on the other hand, the argument holds only for $J_x \ge J_z$. In conjunction with the condition stated after Eq. (2.14), this proves that $|G\rangle$ is the ground state of H_- if

$$J_x \ge J_y \ge J_z \ge 0\ \ (\text{for } H_-)\ . \tag{2.17}$$

Having established these special circumstances under which the ground state of the XYZ Hamiltonian (2.1) is characterized by a very simple wave function—a wave function of maximum spin ordering—we will next address the important question of the consequences of this simplifying feature on the structure of the zero-temperature dynamic correlation functions.

III. DYNAMIC STRUCTURE FACTORS

We consider the time-dependent two-spin correlation functions,

$$\langle S_l^\mu(t)S_{l+r}^\nu\rangle_H=\mathrm{Tr}[e^{iHt}S_l^\mu e^{-iHt}S_{l+r}^\nu e^{-\beta H}]/\mathrm{Tr}[e^{-\beta h}]\ , \tag{3.1}$$

of a given quantum spin Hamiltonian H at temperature T, with $\beta=(k_BT)^{-1}$. The unitary transformation (2.5), which relates the *XYZ* Hamiltonian H, Eq. (2.1), to the Hamiltonian $\tilde{H}$, Eq. (2.13), also provides a set of relations between the two-spin correlation functions of the two models:

$$\langle S_l^\mu(t)S_{l+r}^\nu\rangle_H=\langle \tilde{S}_l^\mu(t)\tilde{S}_{l+r}^\nu\rangle_{\tilde{H}};\ \ \mu,\nu=x,y,z\ . \tag{3.2}$$

Expressed in terms of the spin operators S_l^x, S_l^y, and S_l^z, this becomes

$$\begin{aligned}\langle S_l^x(t)S_{l+r}^x\rangle_{H_\pm}=&\langle S_l^x(t)S_{l+r}^x\rangle_{\tilde{H}_\pm}\cos^2(\theta^\pm)+\langle S_l^z(t)S_{l+r}^z\rangle_{\tilde{H}_\pm}(\mp 1)^r\sin^2(\theta^\pm)\\&+[\langle S_l^z(t)S_{l+r}^x\rangle_{\tilde{H}_\pm}(\mp 1)^l+\langle S_l^x(t)S_{l+r}^z\rangle_{\tilde{H}_\pm}(\mp 1)^{l+r}]\sin(\theta^\pm)\cos(\theta^\pm)\ ,\end{aligned} \tag{3.3a}$$

$$\langle S_l^y(t)S_{l+r}^y\rangle_{H_\pm}=\langle S_l^y(t)S_{l+r}^y\rangle_{\tilde{H}_\pm}\ , \tag{3.3b}$$

$$\begin{aligned}\langle S_l^z(t)S_{l+r}^z\rangle_{H_\pm}=&\langle S_l^z(t)S_{l+r}^z\rangle_{\tilde{H}_\pm}\cos^2(\theta^\pm)+\langle S_l^x(t)S_{l+r}^x\rangle_{\tilde{H}_\pm}(\mp 1)^r\sin^2(\theta^\pm)\\&-[\langle S_l^x(t)S_{l+r}^z\rangle_{\tilde{H}_\pm}(\mp 1)^l+\langle S_l^z(t)S_{l+r}^x\rangle_{\tilde{H}_\pm}(\mp 1)^{l+r}]\sin(\theta^\pm)\cos(\theta^\pm)\ .\end{aligned} \tag{3.3c}$$

Analogous relations hold between the dynamic structure factors

$$S_{\mu\nu}(q,\omega)=\sum_r e^{-iqr}\int_{-\infty}^{\infty}dt\,e^{i\omega t}\langle S_l^\mu(t)S_{l+r}^\nu\rangle \tag{3.4}$$

of the two Hamiltonians H and $\tilde{H}$, respectively. For our purposes it is useful to express $S_{\mu\nu}(q,\omega)$ in its spectral representation. For the model described by H at $T=0$ and $h=h_N$ this is[6]

$$\begin{aligned}S_{\mu\nu}(q,\omega)_{\tilde{H}}=2\pi\sum_\lambda\langle\tilde{G}\,|\,S_q^\mu\,|\,\lambda\rangle\langle\lambda\,|\,S_{-q}^\nu\,|\,\tilde{G}\rangle\\ \times\delta(\omega+E_G-E_\lambda)\ ,\end{aligned} \tag{3.5}$$

where

$$S_q^\mu=N^{-1/2}\sum_{l=1}^{N}e^{-iql}S_l^\mu,\ \ \mu=x,y,z\ ; \tag{3.6}$$

$|\tilde{G}\rangle$ is the ground-state wave function (2.7); and the sum in (3.5) runs over all excited states $|\lambda\rangle$ of $\tilde{H}$ with energy E_λ. Owing to the fact that $|\tilde{G}\rangle$ describes a state with all spins aligned in the z direction, we have

$$S_{xx}(q,\omega)_{\tilde{H}}=S_{yy}(q,\omega)_{\tilde{H}}=\tfrac{1}{4}S_{+-}(q,\omega)_{\tilde{H}}\ \ (T=0)\ , \tag{3.7a}$$

$$S_{zz}(q,\omega)_{\tilde{H}}=4\pi^2s^2\delta(q)\delta(\omega)\ \ (T=0)\ , \tag{3.7b}$$

$$S_{\mu\nu}(q,\omega)_{\tilde{H}}=0\ \ \text{for } \mu\neq\nu\ \ (T=0)\ , \tag{3.7c}$$

where $S_{+-}(q,\omega)$ is the Fourier transform of $\langle S_l^+(t)S_{l+r}^-\rangle$ with $S_l^\pm\equiv S_l^x\pm iS_l^y$.

Using the unitary transformation (2.5), we can now express the dynamic structure factors $S_{\mu\nu}(q,\omega)_H$ of the XYZ model at $T=0$ and $h=h_N$ in terms of the function $S_{+-}(q,\omega)_{\tilde{H}}$. From (3.7) with (3.3) and (3.4) we obtain

$$S_{xx}(q,\omega)_{H_\pm}=\tfrac{1}{4}S_{+-}(q,\omega)_{\tilde{H}_\pm}\cos^2(\theta^\pm)+4\pi^2s^2\sin^2(\theta^\pm)\delta(\omega)\delta(q+Q_\pm)\ , \quad (3.8a)$$

$$S_{yy}(q,\omega)_{H_\pm}=\tfrac{1}{4}S_{+-}(q,\omega)_{\tilde{H}_\pm}\ , \quad (3.8b)$$

$$S_{zz}(q,\omega)_{H_\pm}=\tfrac{1}{4}S_{+-}(q+Q_\pm,\omega)_{\tilde{H}_\pm}\sin^2(\theta^\pm)+4\pi^2s^2\cos^2(\theta^\pm)\delta(\omega)\delta(q)\ , \quad (3.8c)$$

where $Q_+=\pi$ and $Q_-=0$ for $H_\pm$, respectively. Thus, the special structure of the ground-state wave function of the XYZ model at $h=h_N$ has the consequence that the three diagonal dynamic structure factors $S_{\mu\mu}(q,\omega)_H$, $\mu=x,y,z$ at $T=0$ are expressible in terms of a single function, $S_{+-}(q,\omega)_{\tilde{H}}$, which, in general, is nontrivial.

One category of circumstances under which the function $S_{+-}(q,\omega)_{\tilde{H}}$ can be determined explicitly is the following. If for any given wave number q, the ferromagnetic linear spin-wave excitation whose wave function is defined by

$$|\,q\,\rangle=S_q^-\,|\,\tilde{G}\,\rangle \quad (3.9)$$

is an exact eigenstate of H, then it is the only state which can contribute to $S_{+-}(q,\omega)$ at $T=0$. If this is the case, then the general expression (3.5) for $S_{+-}(q,\omega)_{\tilde{H}}$ reduces to the simple result

$$S_{+-}(q,\omega)_{\tilde{H}}=2\pi\delta[\omega-\omega_{\rm SW}(q)] \quad (3.10)$$

where $\omega_{\rm SW}(q)$ is the spin-wave excitation energy. The condition for (3.9) to be an exact eigenstate of $\tilde{H}$ can be stated by the equation

$$[\,\tilde{H}_\pm,S_q^-\,]\,|\,\tilde{G}\,\rangle=\omega_{\rm SW}(q)S_q^-\,|\,\tilde{G}\,\rangle\ . \quad (3.11)$$

With $\tilde{H}$ from (2.9), the left-hand side of (3.11) becomes

$$[\,\tilde{H}_\pm,S_q^-\,]\,|\,\tilde{G}\,\rangle=\omega_{\rm SW}(q)S_q^-\,|\,\tilde{G}\,\rangle\mp\tfrac{1}{2}[(J_x-J_y)(J_y\pm J_z)]^{1/2}\times(1\mp e^{-iq})N^{-1/2}\times\sum_l(\mp1)^le^{-iql}S_l^-S_{l+1}^-\,|\,\tilde{G}\,\rangle\ , \quad (3.12)$$

where

$$\omega_{\rm SW}(q)=2s[J_x\pm J_y\cos(q)] \quad (3.13)$$

is the dispersion relation predicted by linear-spin-wave theory.

From (3.12) we thus conclude that linear spin waves are exact eigenstates of $\tilde{H}$ (i) for arbitrary q if $J_x=J_y$ or (for $\tilde{H}_-$ only) $J_y=J_z$ and (ii) for arbitrary J_x, J_y, and J_z (subject to our conventions) if $q=0$ (for $\tilde{H}_+$) or $q=\pi$ (for $\tilde{H}_-$). The second term on the right-hand side of (3.12) reflects the anharmonic terms which cause the dynamic structure factor to become nontrivial in all other cases, even though they have no effect on the ground state. From (3.12) with (3.13) we also conclude that in the classical limit $s\to\infty$, these anharmonic terms are always negligible for the $T=0$ dynamic structure factor.

In the following, we focus on a case for which the relations (3.8) lead directly to new nontrivial exact results. This is the $s=\frac{1}{2}$ anisotropic XY model, specified by the Hamiltonian (2.1) with $J_x=J(1+\gamma)$, $J_y=J(1-\gamma)$, and $J_z=0$, i.e.,

$$H_\pm^{(\gamma)}=\pm J\sum_{l=1}^{N}\{(1+\gamma)S_l^xS_{l+1}^x+(1-\gamma)S_l^yS_{l+1}^y\}-h\sum_{l=1}^{N}S_l^z\ . \quad (3.14)$$

This model, which can be expressed as a system of noninteracting fermions, has been the object of numerous studies which have yielded exact results for its thermodynamic properties[7–9] and its static[7,10–13] and dynamic[2,3,14–30] correlation functions. The structure of the Jordan-Wigner transformation between spin operators and fermion operators implies that the correlation function $\langle S_l^z(t)S_{l+r}^z\rangle$ can be expressed as a fermion density-density correlation function, i.e., a function involving a product of four fermion operators.[14] In contrast, the functions $\langle S_l^x(t)S_{l+r}^x\rangle$ and $\langle S_l^y(t)S_{l+r}^y\rangle$ are represented by infinite block Toeplitz determinants in terms of fermion operators, i.e., quantities involving infinite products of these operators.[3] The spectrum of the corresponding $T=0$ dynamic structure factors $S_{xx}(q,\omega)$ and $S_{yy}(q,\omega)$ thus represents not just two-fermion excitations as is the case for $S_{zz}(q,\omega)$, but rather the excitation of m-fermion states with m arbitrarily large. It is thus understandable that whereas the evaluation of $\langle S_l^z(t)S_{l+r}^z\rangle$ is straightforward (although quite tedious if pursued to the stage of explicit analytic expressions), explicit results for $\langle S_l^x(t)S_{l+r}^x\rangle$ and $\langle S_l^y(t)S_{l+r}^y\rangle$ have been rather limited. A detailed analysis of the latter correlation functions at $T=0$ was carried out recently for two special cases: the transverse Ising model at the critical field ($\gamma=0$, $h=J$); and the isotropic XY model in zero field ($\gamma=0$, $h=0$).[27,28] This study revealed, among many other interesting features, that the dynamic structure factors $S_{xx}(q,\omega)$ and $S_{yy}(q,\omega)$ have contributions from excitations at arbitrarily high energies ω, whereas $S_{zz}(q,\omega)$ is of compact support as a function of ω and is governed by the two-particle excitations alone.

Here we are interested in the special case of the Hamiltonian (3.14) with

$$h=h_N^\pm=J(1-\gamma^2)^{1/2}\ , \quad (3.15)$$

for which we have established the relations (3.8) between the dynamic structure factors at $T=0$. These exact relations lead to the important conclusion that for $h=h_N$, the $T=0$ dynamic structure factors $S_{xx}(q,\omega)$ and $S_{yy}(q,\omega)$ do not have a more complicated structure than $S_{zz}(q,\omega)$, in sharp contrast to what was found for the cases studied previously. We can then obtain the former two functions from the latter one, which was recently calculated in closed form,[2] via the relations (3.8):

$$S_{xx}(q,\omega)=\frac{1-\gamma}{1+\gamma}\sigma(q+Q_\pm,\omega)+\frac{2\gamma}{1+\gamma}\pi^2\delta(\omega)\delta(q+Q_\pm)\ , \quad (3.16a)$$

$$S_{yy}(q,\omega)=\sigma(q+Q_\pm,\omega)\ , \tag{3.16b}$$

$$S_{zz}(q,\omega)=\frac{2\gamma}{1+\gamma}\sigma(q,\omega)+\frac{1-\gamma}{1+\gamma}\pi^2\delta(\omega)\delta(q)\ , \tag{3.16c}$$

$$\sigma(q,\omega)=\frac{\gamma}{2(1-\gamma)}\frac{[4J^2(1-\gamma^2)\cos^2(q/2)-(\omega-2J)^2]^{1/2}}{[\omega-2J\sin^2(q/2)]^2+J^2\gamma^2\sin^2(q/2)}$$
$$\times\Theta[4J^2(1-\gamma^2)\cos^2(q/2)-(\omega-2J)^2]\ , \tag{3.16d}$$

for $H_\pm^{(\gamma)}$ at $h=h_N$ and $T=0$. Note that all three of these components of the dynamics structure factor are nonzero only for (q,ω) in the range of the two-particle spectrum, i.e., for $|\omega-2|\geq\cos(q/2)$. Apart from the $\delta(\omega)$ terms, they differ only by γ-dependent factors, a property which was previously found to hold for the frequency integrals.[2]

In a previous study of the correlation functions $\langle S_l^x(t)S_{l+r}^x\rangle$ and $\langle S_l^y(t)S_{l+r}^y\rangle$ based on an analysis of infinite Toeplitz determinants, McCoy, Barouch, and Abraham[3] presented a result for $S_{xx}(q,\omega)$ and $S_{yy}(q,\omega)$ [Eqs. (5.10) and (5.11) of Ref. 3] originating from the two-particle contribution and thus constituting the first term in an expansion indexed by the contributions of m-particle excitations with $m=2,4,6,\ldots$. Since it is the two-particle contribution, their result is kinematically restricted to be nonzero over the same range as our exact answer, but it differs from (3.16) in its functional dependence on q and ω. The only way to render their result compatible with our exact answer (3.16) is to invoke the contributions of the higher-lying excitations with $m=4,6,\ldots$; however, if one tries to do this, one must explain how these additional terms can contribute only in the (q,ω) range of the two-particle spectrum while miraculously cancelling to zero for all (q,ω) outside this range. If, in particular, the terms with $m>2$ vanish at $h=h_N$, which would provide a natural explanation of why our exact result is nonzero only in the range of the two-particle excitations, then our result is clearly incompatible with the one given in Ref. 3.

As an immediate consequence of our exact result (3.16) for the $T=0$ dynamic structure factors, we can infer new exact results for the q-dependent susceptibilities of the 1D $s=\frac{1}{2}$ anisotropic XY model (3.14). These susceptibilities are defined as follows:

$$\chi_{\mu\mu'}(q)=\partial M_\mu(q)/\partial h_{\mu'}(q),\ \ \mu,\mu'=x,y,z\ , \tag{3.17a}$$

where

$$M_\mu(q)\equiv N^{-1}\sum_l e^{-iql}\langle S_l^\mu\rangle\ , \tag{3.17b}$$

and

$$h_\mu(q)\equiv N^{-1}\sum_l e^{-iql}h_l^\mu\ , \tag{3.17c}$$

and h_l^μ denotes an inhomogeneous magnetic field. For given dynamic structure factors $S_{\mu\mu}(q,\omega)$, the q-dependent susceptibilities are determined, as discussed, e.g., in Refs. 29 and 30, through the relation

$$\chi_{\mu\mu}(q)=\frac{1}{\pi}\int\frac{d\omega}{\omega}S_{\mu\mu}(q,\omega)\ . \tag{3.18}$$

Using the exact results (3.16), we thus obtain

$$\chi_{xx}(q)=\frac{1-\gamma}{1+\gamma}f(q+Q_\pm) \tag{3.19a}$$

$$\chi_{yy}(q)=f(q+Q_\pm)\ , \tag{3.19b}$$

and

$$\chi_{zz}(q)=\frac{2\gamma}{1+\gamma}f(q)\ , \tag{3.19c}$$

where

$$f(q)=\frac{1}{J(1-\gamma)\sin^2(q/2)}\times\left[1-\frac{\gamma}{[\sin^2(q/2)+\gamma\cos^2(q/2)]^{1/2}}\right]\ , \tag{3.19d}$$

for $H_\pm^{(\gamma)}$ at $T=0$. These expressions thus extend the list of exact results for $T=0$ susceptibilities of the 1D $s=\frac{1}{2}$ anisotropic XY model which have been reported in a recent comprehensive study.[29,30]

ACKNOWLEDGMENTS

The research of R.E.S. was supported in part by the National Science Foundation under Grant No. PHY-81-9110-A01. The research of G. M. was supported by a Grant-in-Aid from the Research Council of the University of Rhode Island.

[1]J. Kurmann, H. Thomas, and G. Müller, Physica **112**, 235 (1982).
[2]J. H. Taylor and G. Müller, Phys. Rev. B **28**, 1529 (1983).
[3]B. M. McCoy, E. Barouch, and D. B. Abraham, Phys. Rev. A **4**, 2331 (1971).
[4]For ground-state properties, this analysis complements that reported in Ref. 1, which focused on the XYZ antiferromagnet (H_+), but with a field in an arbitrary direction.
[5]Our convention $J_x\geq J_y$ implies that the spins are parallel to the xz plane, provided that a product ground state exists.
[6]In Eq. (3.5) we have ignored the fact that the ground state is six-fold degenerate, as explained earlier; taking into account the degeneracy does not affect the functions $S_{\mu\nu}(q,\omega)$ for the cases considered here.
[7]E. Lieb, T. Schultz, and D. Mattis, Ann. Phys. (N.Y.) **16**, 407 (1961).
[8]S. Katsura, Phys. Rev. **127**, 1508 (1962).
[9]M. Suzuki, Prog. Theor. Phys. **46**, 1337 (1971).
[10]B. M. McCoy, Phys. Rev. **173**, 531 (1968).
[11]E. Barouch and B. M. McCoy, Phys. Rev. A **3**, 786 (1971).
[12]T. Tonegawa, Solid State Commun. **40**, 938 (1981).
[13]P. Pfeuty, Ann. Phys. (N.Y.) **57**, 79 (1970).
[14]T. Niemeiger, Physica **36**, 377 (1967).
[15]S. Katsura, T. Horiguchi, and M. Suzuki, Physica **46**, 67 (1976).
[16]T. N. Tommet and D. L. Huber, Phys. Rev. B **11**, 450 (1975).
[17]M. W. Puga and H. Beck, J. Phys. C **15**, 2441 (1982).
[18]M. Mohan and G. Müller, Phys. Rev. B **27**, 1776 (1983); J. H.

Taylor and G. Müller, Physica **130A**, 1 (1985).
[19]J. H. H. Perk, H. W. Capel, and T. J. Siskens, Physica **89A**, 304 (1977).
[20]H. W. Capel and J. H. H. Perk, Physica **87A**, 211 (1977); J. H. H. Perk and H. W. Capel, *ibid.* **89A**, 265 (1977); **100A**, 1 (1980).
[21]U. Brandt and K. Jacoby, Z. Phys. B **25**, 181 (1976).
[22]A. Sur, B. Jasnow, and I. J. Lowe, Phys. Rev. B **12**, 3845 (1975).
[23]W. Pesch and H. J. Mikeska, Z. Phys. B **30**, 177 (1978).
[24]J. Lajzerowicz and P. Pfeuty, Phys. Rev. B **11**, 4560 (1975).
[25]H. G. Vaidya and C. A. Tracy, Physica **92A**, 1 (1978).
[26]J. H. H. Perk, Phys. Lett. **79A**, 1 (1980).
[27]B. M. McCoy, J. H. H. Perk, and R. E. Shrock, Nucl. Phys. B **220** [FS8], 35 (1983); *ibid.,* **220** [FS8], 269 (1983).
[28]G. Müller and R. E. Shrock, Phys. Rev. Lett. **51**, 219 (1983); Phys. Rev. B **29**, 288 (1984).
[29]G. Müller and R. E. Shrock, Phys. Rev. B **30**, 5254 (1984).
[30]G. Müller and R. E. Shrock, Phys. Rev. B **31**, 637 (1985).