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Dynamic Correlation Functions for the One-Dimensional XYZ Model: New Exact Results

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It is found that there exist special circumstances for which a rigorous relation between the three dynamic structure factors $S_{\mu\mu}(q,\omega)$, $\mu = x,y,z$, at $T=0$ of the one-dimensional spin-s XYZ model in a uniform magnetic field can be derived. This relation is used to infer new exact results for $S_{xx}(q,\omega)$ and $S_{yy}(q,\omega)$ of the $s=\frac{1}{2}$ anisotropic XY model.

We study the circumstances under which the general spin-s XYZ ferromagnet in a uniform magnetic field, specified by the Hamiltonian

$$\mathcal{H} = -\sum_{l=1}^{N}\Big[J_x S_l^x S_{l+1}^x + J_y S_l^y S_{l+1}^y + J_z S_l^z S_{l+1}^z + hS_l^z\Big], \tag{1}$$

for $J_x, J_y, J_z \geq 0$, even N and periodic boundary conditions exhibits a ground state (GS) wavefunction of the simple product type (without loss of generality we also assume $J_x \geq J_y$):

$$\begin{aligned} |G\rangle &= \bigotimes_{l=1}^{N} |\Theta, l\rangle, \\ |\Theta, l\rangle &= U_l(\Theta)|s,l\rangle \\ &= \sum_{m=-s}^{s} |m,l\rangle D_{ms}^{(s)}(\cos\Theta/2, \sin\Theta/2) \\ &= \sum_{m=-s}^{s} \sqrt{\frac{(2s)!}{(s+m)!(s-m)!}}(\cos\Theta/2)^{s+m}(\sin\Theta/2)^{s-m}|m,l\rangle. \end{aligned} \tag{2}$$

Here $U_l(\Theta)$ describes a unitary transformation representing a rotation of the spin direction at the site l by an angle Θ away from the z-axis in the xz-plane, generated by the $(2s+1)$-dimensional irreducible representation of the group SU(2) with matrix elements $D_{ms}^{(s)}$ as given above. For $\Theta \neq 0$ such a GS is characterized by the presence of spontaneous long-range order. The order parameter is

$$\mathbf{M} = \langle \Theta, l|\mathbf{S}_l|\Theta, l\rangle = (s\sin\Theta, 0, s\cos\Theta). \tag{3}$$

There are evidently no correlated fluctuations in this state of maximum spin ordering.

The problem of finding special cases of the Hamiltonian $\mathcal{H}$ for which the GS wave function $|G\rangle$ has the form (2) is equivalent to finding the circumstances under which the Hamiltonian

$$\tilde{\mathcal{H}} = U^{-1}\mathcal{H}U, \quad U = \bigotimes_{l=1}^{N} U_l(\Theta), \tag{4}$$

has a GS wave function of the form

$$|\tilde{G}\rangle = U^{-1}|G\rangle = \bigotimes_{l=1}^{N} |s,l\rangle, \tag{5}$$

with all spins aligned parallel to the z-axis. The GS energy is invariant under this transformation:

$$\langle G|\mathcal{H}|G\rangle = \langle\tilde{G}|\tilde{\mathcal{H}}|\tilde{G}\rangle = E_G. \tag{6}$$

The solution of this well-defined problem is that the XYZ model (1) does indeed have a GS wavefunction of the form (2) with [1]

$$\cos\Theta = \sqrt{(J_y - J_z)/(J_x - J_z)}, \tag{7}$$

and energy

$$E_G = -s^2(J_x + J_y - J_z), \tag{8}$$

provided the exchange constants satisfy the constraints [2]

$$J_x \geq J_y \geq J_z, \tag{9}$$

and the strength of the magnetic field is

$$h = h_N = 2s\sqrt{(J_x - J_z)(J_y - J_z)}. \tag{10}$$

The transformed Hamiltonian $\tilde{\mathcal{H}}$ whose GS wave function is $|\tilde{G}\rangle$ reads:

$$\begin{aligned}\tilde{\mathcal{H}} = \sum_{l=1}^{N} \Big\{ & J_y(S_l^x S_{l+1}^x + S_l^y S_{l+1}^y) + (J_x - J_y + J_z)S_l^z S_{l+1}^z + 2s(J_y - J_z)S_l^z \\ & + \sqrt{(J_x - J_y)(J_y - J_z)}\big[S_l^z S_{l+1}^x + S_l^x S_{l+1}^z - s(S_l^x + S_{l+1}^x)\big]\Big\}.\end{aligned} \tag{11}$$

Note that the presence of a ferromagnetic GS does not guarantee that the ferromagnetic spin-wave states are also eigenstates of $\mathcal{H}$ or $\tilde{\mathcal{H}}$. The spin-wave excitations with respect to the ferromagnetic state $|\tilde{G}\rangle$, for example, are characterized by the wave functions

$$|\tilde{q}\rangle = S_q^-|\tilde{G}\rangle, \quad S_q^- = N^{-1/2}\sum_{l=1}^{N} \mathrm{e}^{-\mathrm{i}ql} S_l^-. \tag{12}$$

The condition for these states to be eigenstates of $\tilde{\mathcal{H}}$ is that the second term on the right-hand side of the following equation vanishes:

$$\big[\tilde{\mathcal{H}}, S_q^-\big]|\tilde{G}\rangle = \omega_{sw}(q)|\tilde{G}\rangle + \frac{1}{2}\sqrt{(J_x - J_y)(J_y - J_z)}(1 + \mathrm{e}^{-\mathrm{i}q})N^{-1/2}\sum_l \mathrm{e}^{-\mathrm{i}ql} S_l^- S_{l+1}^-|\tilde{G}\rangle, \tag{13}$$

where

$$\omega_{sw}(q) = 2s(J_x - J_y\cos q) \tag{14}$$

is the dispersion predicted by the linear spin-wave analysis. For general values of J_x, J_y, J_z and h satisfying the constraints (9) and (10), this condition is only met for $q = \pi$, for general q only in the classical limit $s \to \infty$.

Thus the second term in (13) or, equivalently, the last term in (11) is responsible for nontrivial features in the $T = 0$ dynamic structure factors defined as

$$S_{\mu\nu}(q,\omega) \equiv \sum_R \mathrm{e}^{-\mathrm{i}qR}\int_{-\infty}^{+\infty} \mathrm{d}t\, \mathrm{e}^{\mathrm{i}\omega t}\langle S_l^\mu(t) S_{l+R}^\nu\rangle, \tag{15}$$

in spite of the very special structure of the GS wave function. However, the fact that $|\tilde{G}\rangle$ describes a state with all spins aligned in the z-direction implies the following general structure for the $S_{\mu\nu}(q,\omega)$ of $\tilde{\mathcal{H}}$ at $T = 0$:

$$\begin{aligned} & S_{xx}(q,\omega)_{\tilde{\mathcal{H}}} = S_{yy}(q,\omega)_{\tilde{\mathcal{H}}} = \frac{1}{4}S_{+-}(q,\omega)_{\tilde{\mathcal{H}}}, \\ & S_{zz}(q,\omega)_{\tilde{\mathcal{H}}} = 4\pi^2 s^2\delta(q)\delta(\omega), \\ & S_{\mu\nu}(q,\omega)_{\tilde{\mathcal{H}}} = 0 \quad \text{for} \quad \mu \neq \nu, \end{aligned} \tag{16}$$

where $S_{+-}(q,\omega)$ is the Fourier transform of $\langle S_l^+(t) S_{l+R}^-\rangle$ and is, in general, nontrivial. This special structure is translated by the unitary transformation (4) into a relation between the three diagonal structure factors $S_{\mu\nu}(q,\omega)_{\mathcal{H}}$ of the XYZ model at $T=0$ and $h=h_N$. They are all expressible in terms of a single function, $S_{+-}(q,\omega)_{\tilde{\mathcal{H}}}$, as follows:

$$\begin{aligned} S_{xx}(q,\omega)_{\mathcal{H}} &= \frac{1}{4} S_{+-}(q,\omega)_{\tilde{\mathcal{H}}} \cos^2\Theta + 4\pi^2 s^2 \sin^2\Theta\,\delta(\omega)\,\delta(q), \\ S_y(q,\omega)_{\mathcal{H}} &= \frac{1}{4} S_{+-}(q,\omega)_{\tilde{\mathcal{H}}}, \\ S_{zz}(q,\omega)_{\mathcal{H}} &= \frac{1}{4} S_{+-}(q,\omega)_{\tilde{\mathcal{H}}} \sin^2\Theta + 4\pi^2 s^2 \cos^2\Theta\,\delta(\omega)\,\delta(q). \end{aligned} \tag{17}$$

There exists a particular case of the XYZ model (1) for which these relations directly lead to new nontrivial exact results: the $s=1/2$ anisotropic XY model

$$\mathcal{H}_\gamma = -J\sum_{l=1}^{N}\left[(1+\gamma)S_l^x S_{l+1}^x + (1-\gamma)S_l^y S_{l+1}^y\right] - h\sum_{l=1}^{N} S_l^z. \tag{18}$$

For this model, which maps onto a system of noninteracting fermions via the Jordan-Wigner transformation [3], the dynamic correlation function $\langle S_l^z(t) S_{l+R}^z\rangle$ can be expressed as a fermion density-density correlation function [4]. The corresponding $T=0$ dynamic structure factor at $h=h_N=J\sqrt{1-\gamma^2}$ was recently determined in closed form [5]:

$$\begin{aligned} S_{zz}(q,\omega) = \pi^2 \frac{1-\gamma}{1+\gamma}\,\delta(q)\delta(\omega) \\ + \frac{\gamma^2}{1-\gamma^2} \frac{\left[4J^2(1-\gamma^2)\cos^2(q/2) - (\omega-2J)^2\right]^{1/2}}{\left[\omega - 2J\sin^2(q/2)\right]^2 + J^2\gamma^2\sin^2 q} \\ \times\Theta\Big[4J^2(1-\gamma^2)\cos^2(q/2) - (\omega-2J)^2\Big]. \end{aligned} \tag{19}$$

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 the fermion language, i.e. quantities involving infinite products of fermion operators [6]. The spectrum of the corresponding $T=0$ dynamic structure factors $S_{xx}(q,\omega)$ and $S_{yy}(q,\omega)$ thus represent 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. On the other hand, the newly found relations (17) imply that for $h=h_N$ all three dynamic structure factors are zero for values of (q,ω) outside the range of the two-particle spectrum, i.e. for $|\omega-2J| > 2Jh_N\cos(q/2)$. They differ from one another (apart from the δ-function at $q=\omega=0$) only by an overall γ-dependent factor [7].

These peculiar properties are far from evident in the formal expressions for $S_{xx}(q,\omega)$ and $S_{yy}(q,\omega)$ in the fermion representation. In fact, expressions (5.10) of ref. [6] which are stated to represent the two-particle contributions to $S_{xx}(q,\omega)$ are incompatible with our exact result unless one assumes that there are also contributions to these functions at $h=h_N$ from m-particle excitations with $m>2$. This would imply, however, that such contributions miraculously cancel one another for all (q,ω) outside the range of the two-particle spectrum.

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1. As far as the ground-state properties are concerned, this analysis complements that reported by J. Kurmann, H. Thomas and G. Müller, Physica **112A** (1982) 235, which focused on the XYZ antiferromagnet, but with a field in an arbitrary direction.
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