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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

$$\mathcal{H} = - \sum_{l=1}^N \left[ J_x S_l^x S_{l+1}^x + J_y S_l^y S_{l+1}^y + J_z S_l^z S_{l+1}^z + h S_l^z \right], \quad (1)$$

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  $J_x \geq J_y$ ):

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

Here  $U_l(\Theta)$  describes a unitary transformation representing a rotation of the spin direction at the site  $l$  by an angle  $\Theta$  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  $D_{m,s}^{(s)}$  as given above. For  $\Theta \neq 0$  such a GS is characterized by the presence of spontaneous long-range order. The order parameter is

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

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

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

has a GS wave function of the form

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

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

$$\langle G|\mathcal{H}|G\rangle = \langle \tilde{G}|\tilde{\mathcal{H}}|\tilde{G}\rangle = E_G. \quad (6)$$

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]

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

and energy

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

provided the exchange constants satisfy the constraints [2]

$$J_x \geq J_y \geq J_z, \quad (9)$$

and the strength of the magnetic field is

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

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

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

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

$$|\tilde{q}\rangle = S_q^- |\tilde{G}\rangle, \quad S_q^- = N^{-1/2} \sum_{l=1}^N e^{-iql} S_l^-. \quad (12)$$

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:

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

where

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

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  $s \rightarrow \infty$ .

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

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

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  $T = 0$ :

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

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:

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

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

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

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]:

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

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  $(q, \omega)$  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  $\delta$ -function at  $q = \omega = 0$ ) only by an overall  $\gamma$ -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  $(q, \omega)$  outside the range of the two-particle spectrum.

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## References

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.
2. The constraint  $J_x \geq J_y$  is just a convention.

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7. This result was already suspected in ref. [5] on the basis of sum rule considerations.