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

Robert E. Shrock

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

Gerhard Müller\(^1\) and Robert E. Shrock\(^2\)

\(^1\) Department of Physics, University of Rhode Island, Kingston RI 02881, USA
\(^2\) Institute for Theoretical Physics, State University of New York at Stony Brook, Stony Brook, NY 11974, USA

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

\[
H = -\sum_{l=1}^{N} \left[ J_x S^x_l S^x_{l+1} + J_y S^y_l S^y_{l+1} + J_z S^z_l S^z_{l+1} + h S^z_l \right],
\]

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 \(J_x \geq J_y\)):

\[
|G\rangle = \bigotimes_{l=1}^{N} |\Theta, l\rangle,
|\Theta, l\rangle = U_l(\Theta) |s, l\rangle
= \sum_{m=-s}^{s} |m, l\rangle D^{(s)}_{ms}(\cos \Theta/2, \sin \Theta/2)
= \sum_{m=-s}^{s} \sqrt{\frac{(2s)!}{(s+m)!(s-m)!}} (\cos \Theta/2)^{s+m} (\sin \Theta/2)^{s-m} |m, l\rangle.
\]

(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 \(D^{(s)}_{ms}\) as given above. For \(\Theta \neq 0\) such a GS is characterized by the presence of spontaneous long-range order. The order parameter is

\[
M = \langle \Theta, l | S^z | \Theta, l \rangle = (s \sin \Theta, 0, s \cos \Theta).
\]

(3)

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

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

\[
\tilde{H} = U^{-1} H U, \quad U = \bigotimes_{l=1}^{N} U_l(\Theta),
\]

(4)

has a GS wave function of the form

\[
|\tilde{G}\rangle = U^{-1} |G\rangle = \bigotimes_{l=1}^{N} |s, l\rangle,
\]

(5)
with all spins aligned parallel to the $z$-axis. The GS energy is invariant under this transformation:

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

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

$$\tilde{H} = \sum_{l=1}^{N} \left\{ J_y (S_l^x S_{l+1}^x + S_l^y S_{l+1}^y) + (J_x - J_y + J_z) S_l^x S_{l+1}^x + 2s(J_y - J_z) S_l^z \right. \right.$$  

$$\left. + \sqrt{(J_x - J_y)(J_y - J_z)} \left[ S_l^x S_{l+1}^x + S_l^y S_{l+1}^y - s (S_l^x + S_{l+1}^x) \right] \right\}. \tag{11}$$

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

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

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

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

where

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

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

$$S_{\mu\nu}(q, \omega) \equiv \sum_{R} e^{-iqR} \int_{-\infty}^{\infty} dt e^{i\omega t} \langle S_{\mu}^{R}(t) S_{\nu}^{R}(t) \rangle, \tag{15}$$

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 $\tilde{H}$ at $T = 0$:

$$S_{xx}(q, \omega)_{\tilde{R}} = S_{yy}(q, \omega)_{\tilde{R}} = \frac{1}{4} S_{+-}(q, \omega)_{\tilde{R}},$$

$$S_{zz}(q, \omega)_{\tilde{R}} = 4\pi^2 s^2 \delta(q) \delta(\omega),$$

$$S_{\mu\nu}(q, \omega)_{\tilde{R}} = 0 \quad \text{for} \quad \mu \neq \nu, \tag{16}$$
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where $S_{+-}(q, \omega)$ is the Fourier transform of $\langle S^+_{i}(t) S^{-}_{i+R} \rangle$ 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, $S_{+-}(q, \omega)_{\mathcal{H}}$, as follows:

$$S_{xx}(q, \omega)_{\mathcal{H}} = \frac{1}{4} S_{+-}(q, \omega)_{\mathcal{H}} \cos^2 \Theta + 4\pi^2 s^2 \sin^2 \Theta \delta(\omega) \delta(q),$$

$$S_{yy}(q, \omega)_{\mathcal{H}} = \frac{1}{4} S_{+-}(q, \omega)_{\mathcal{H}},$$

$$S_{zz}(q, \omega)_{\mathcal{H}} = \frac{1}{4} S_{+-}(q, \omega)_{\mathcal{H}} \sin^2 \Theta + 4\pi^2 s^2 \cos^2 \Theta \delta(\omega) \delta(q).$$

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

$$\mathcal{H}_s = -J \sum_{l=1}^{N} \left[ (1 + \gamma) S^z_{l} S^z_{l+1} + (1 - \gamma) S^x_{l} S^x_{l+1} \right] - h \sum_{l=1}^{N} S^y_{l}. \tag{18}$$

For this model, which maps onto a system of noninteracting fermions via the Jordan-Wigner transformation [3], the dynamic correlation function $\langle S^z_{l}(t) S^z_{l+R} \rangle$ 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]:

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

In contrast, the functions $\langle S^x_{l}(t) S^x_{l+R} \rangle$ and $\langle S^y_{l}(t) S^y_{l+R} \rangle$ 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.
7. This result was already suspected in ref. [5] on the basis of sum rule considerations.