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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) wave-function of the simple product type (without loss of generality we also assume $J_x \geq J_y$):

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

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

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

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:

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

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]:

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

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, 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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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.

3. E. Lieb, T. Schultz and D. Mattis, Ann. Phys. (N.Y.) **16** (1961) 407; S. Katsura, Phys. Rev. **127** (1962) 1508;
4. T. Niemeijer, Physica **36** (1967) 377.
5. J.H. Taylor and G. Müller, Phys. Rev. B **28** (1983) 1529.
6. B.M. McCoy, E. Barouch and D.B. Abraham, Phys. Rev. A **4** (1971) 2331.
7. This result was already suspected in ref. [5] on the basis of sum rule considerations.