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Dynamics of quantum spin chains and multi-fermion excitation continua

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Abstract

We use the Jordan-Wigner representation to study dynamic quantities for the spin-$\frac{1}{2}$ XX chain in a transverse magnetic field. We discuss in some detail the properties of the four-fermion excitation continuum which is probed by the dynamic trimer structure factor.

Key words: spin-$\frac{1}{2}$ XX chain, dynamic quantities, multi-fermion excitations
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Recently the subject of multi-magnon excitations of quasi-one-dimensional quantum spin systems has attracted considerable interest. With high-resolution inelastic neutron scattering experiments one may expect to examine not only the bound two-magnon states but also the continua of multi-magnon states. Some properties of multi-magnon continua were examined in [1]. More recently, we have noted that the spin-$\frac{1}{2}$ transverse XX chain, which can be mapped via the Jordan-Wigner transformation onto noninteracting spinless fermions, is a model whose dynamics is governed by continua of multi-fermion excitations. In particular, the dynamic trimer structure factor involves two-fermion and four-fermion excitations [2]. In the present report we compare and contrast the general and specific properties of the four-fermion excitation continuum, which contributes to the dynamics of trimer fluctuations.

To be specific, we consider the spin-$\frac{1}{2}$ transverse XX chain with the Hamiltonian

$$H = \sum_n J\left(s_n^x s_{n+1}^x + s_n^y s_{n+1}^y\right) + \sum_n \Omega s_n^z. \tag{1}$$

We will set further $J = -1$. The trimer operator is defined as $T_n = s_n^x s_{n+2}^x + s_n^y s_{n+2}^y$ and the corresponding dynamic structure factor

$$S_{TT}(\kappa,\omega) = \sum_l \mathrm{e}^{-\mathrm{i}\kappa l} \int_{-\infty}^{\infty} \mathrm{d}t \mathrm{e}^{\mathrm{i}\omega t} \langle \Delta T_n(t) \Delta T_{n+l}(0)\rangle, \tag{2}$$

$\Delta T_n(t) = T_n(t) - \langle T\rangle$ can be written as a sum of the two-fermion contribution $S_{TT}^{(2)}(\kappa,\omega)$ and the four-fermion contribution $S_{TT}^{(4)}(\kappa,\omega)$ with

$$S_{TT}^{(2)}(\kappa,\omega) = \int \mathrm{d}\kappa_1 \mathrm{d}\kappa_2 C^{(2)}(\kappa_1,\kappa_2) n_{\kappa_1}(1-n_{\kappa_2}) \cdot\delta(\omega + \Lambda_{\kappa_1} - \Lambda_{\kappa_2})\delta_{\kappa+\kappa_1-\kappa_2,0}, \tag{3}$$

$$S_{TT}^{(4)}(\kappa,\omega) = \frac{1}{4\pi^2}\int \mathrm{d}\kappa_1 \ldots \mathrm{d}\kappa_4 C^{(4)}(\kappa_1,\ldots,\kappa_4) \cdot n_{\kappa_1} n_{\kappa_2}(1-n_{\kappa_3})(1-n_{\kappa_4}) \cdot\delta(\omega + \Lambda_{\kappa_1} + \Lambda_{\kappa_2} - \Lambda_{\kappa_3} - \Lambda_{\kappa_4})\delta_{\kappa+\kappa_1+\kappa_2-\kappa_3-\kappa_4,0}. \tag{4}$$

Here $C^{(2)}(\kappa_1,\kappa_2)$, $C^{(4)}(\kappa_1,\ldots,\kappa_4) \geq 0$ are certain functions the explicit expressions for which are given in [2], $n_\kappa = (1+\exp(\beta\Lambda_\kappa))^{-1}$ is the Fermi function, $\Lambda_\kappa =$

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$\Omega + J\cos\kappa$, and $-\pi \leq \kappa < \pi$ is the quasi-momentum which parameterizes the Jordan-Wigner fermions. It is easy to note that Eq. (3) coincides with the dynamic zz structure factor if $C^{(2)}(\kappa_1,\kappa_2) = 1$ or with the dynamic dimer structure factor if $C^{(2)}(\kappa_1,\kappa_2) = \cos^2\frac{\kappa_1+\kappa_2}{2}$ (see [2]). These dynamic quantities are governed exclusively by the two-fermion (one particle and one hole) excitations. The properties of the two-fermion excitation continuum were examined in [3,4].

In contrast, Eq. (4) is governed exclusively by the four-fermion (two particles and two holes) excitation continuum the properties of which are described concisely below. The specific features of the four-fermion contribution to $S_{TT}(\kappa,\omega)$ (2) are controlled by the function $C^{(4)}(\kappa_1,\ldots,\kappa_4)$. To display the generic behavior of a four-fermion dynamic quantity we also consider Eq. (4) with $C^{(4)}(\kappa_1,\ldots,\kappa_4) = 1$ (compare Figs. 1 and 2).

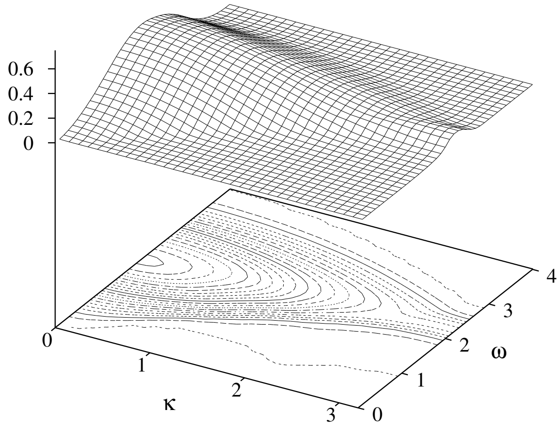

Fig. 1. $S^{(4)}_{TT}(\kappa,\omega)$ (4) for the chain (1) with $J = -1$, $\Omega = 0.25$ at zero temperature ($\beta \to \infty$).

The four-fermion dynamic quantity can have nonzero values only in a restricted region of the κ–ω plane. At nonzero temperatures one immediately finds the upper boundary of the four-fermion excitation continuum, $4|J|\cos\frac{\kappa}{4}$. At zero temperature the Fermi functions in (4) come into play and both the upper and the lower boundaries of the four-fermion excitation continuum become complicated Ω-dependent functions of κ. For $\Omega = 0.25$ the upper boundary remains $4|J|\cos\frac{\kappa}{4}$, whereas the lower boundary assumes the following values as κ increases from 0 to π: $\omega_l^{(1)} = 2|J|\sin\frac{\kappa}{2}\sin(\alpha - \frac{\kappa}{2})$, $\omega_l^{(2)} = 4|J|\cos\frac{\kappa}{4}\cos(\alpha + \frac{\kappa}{4})$, $\omega_l^{(3)} = -2|J|\sin(\alpha + \frac{\kappa}{2})\sin(2\alpha + \frac{\kappa}{2})$, $\omega_l^{(1)}$, $\omega_l^{(4)} = -2|J|\sin(\alpha - \frac{\kappa}{2})\sin(2\alpha - \frac{\kappa}{2})$ with $\cos\alpha = \frac{\Omega}{|J|}$. To find these boundaries we (numerically) seek for the extrema of $\cos\kappa_1 + \cos\kappa_2 - \cos\kappa_3 - \cos\kappa_4$ with the restrictions imposed by the Fermi functions (see (4))

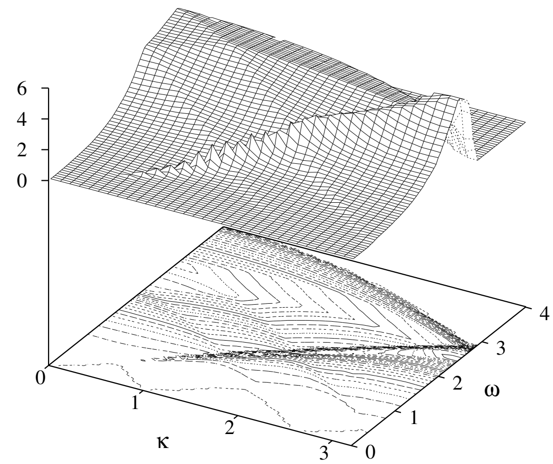

Fig. 2. The same as in Fig. 1 but with $C^{(4)}(\kappa_1,\ldots,\kappa_4) = 1$.

for $0 \leq \kappa \leq \pi$ and determine the values of $\kappa_1,\ldots,\kappa_4$ at which such extrema occur. We find simple relations between the quantities $\kappa_1,\ldots,\kappa_4$ and κ, α obtaining as a result the upper and the lower boundaries of the four-fermion excitation continuum.

The four-fermion dynamic quantities may exhibit Van Hove cusp singularities akin to the three dimensional density of states. These singularities occur along the lines $2|J|\sin\frac{\kappa}{2}$, $4|J|\sin\frac{\kappa}{4}$, and $4|J|\cos\frac{\kappa}{4}$.

Comparing Figs. 1 and 2 we see how some characteristic features of the four-fermion excitation continuum are smeared out owing to $C^{(4)}(\kappa_1,\ldots,\kappa_4) \neq 1$.

Finally, we note that spin-$\frac{1}{2}$ XX chains are realized in some quasi-one-dimensional magnetic insulators (e.g. such as Cs_2CoCl_4 [5]). The dynamic dimer structure factor is relevant to phonon-assisted optical adsorption [6,7]; the direct experimental relevance of the dynamic trimer structure factor is less evident. However, our results may be important from the theoretical point of view since the four-fermion dynamic trimer structure factor is a quantity of intermediate complexity between the two-fermion dynamic zz structure factor and the multi-fermion dynamic xx (yy) structure factor.

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