Dynamics of quantum spin chains and multi-fermion excitation continua

Oleg Derzhko

Taras Krokhmalskii

Joachim Stolze

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

Terms of Use

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O. Derzhko [a,*], T. Krokhmalskii [a], J. Stolze [b], G. Müller [c]

[a] *Institute for Condensed Matter Physics NASU, 1 Svientsitskii Str., L'viv-11, 79011, Ukraine*
[b] *Institut für Physik, Universität Dortmund, 44221 Dortmund, Germany*
[c] *Department of Physics, University of Rhode Island, Kingston, Rhode Island 02881-0817, USA*

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.

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

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

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

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

$\Delta T_n(t) = T_n(t) - \langle T \rangle$ 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

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

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

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, $\Lambda_\kappa =$

$\Omega + J\cos\kappa$, and $-\pi \le \kappa < \pi$ 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).
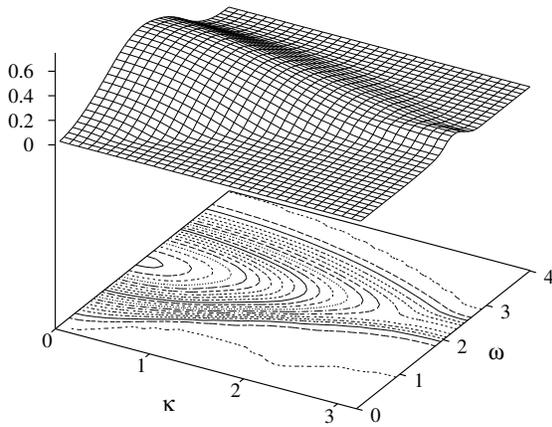
Fig. 1. $S_{TT}^{(4)}(\kappa, \omega)$ (4) for the chain (1) with $J = -1$, $\Omega = 0.25$ at zero temperature ($\beta \to \infty$).

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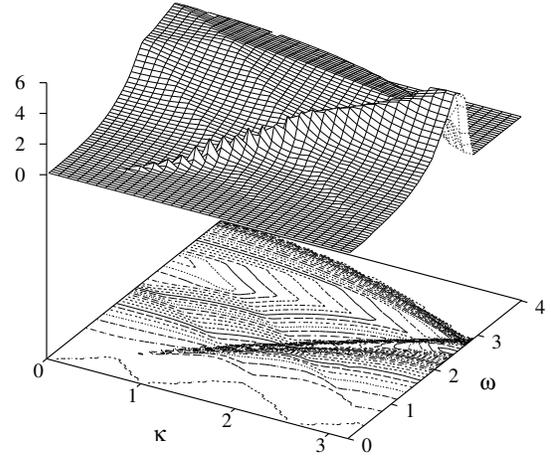
Fig. 2. The same as in Fig. 1 but with $C^{(4)}(\kappa_1, \ldots, \kappa_4) = 1$.

for $0 \le \kappa \le \pi$ 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 $C^{(4)}(\kappa_1, \ldots, \kappa_4) \ne 1$.

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.

References

[1] T. Barnes, Phys. Rev. B **67** (2003) 024412.

[2] O. Derzhko et al., Phys. Rev. B **71** (2005) 104432.

[3] G. Müller et al., Phys. Rev. B **24** (1981) 1429.

[4] J. H. Taylor and G. Müller, Physica A **130** (1985) 1.

[5] M. Kenzelmann et al., Phys. Rev. B **65** (2002) 144432.

[6]   H. Suzuura et al., Phys. Rev. Lett. **76** (1996) 2579.

[7]   J. Lorenzana and R. Eder, Phys. Rev. B **55** (1997) R3358.