Proceedings of the CSMAG'07 Conference, Košice, July 9–12, 2007

Spin-1/2 XX Chains with Three-Spin Interactions

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We consider a spin-1/2 XX chain with three-spin interactions which is equivalent to a system of noninteracting spinless fermions.We examine some dynamic quantities of the spin model.In particular,we calculate analytically the dynamic transverse (zz) structure factor which is governed by a two-fermion excitation continuum.Moreover,we compute numerically the dynamic xx structure factor which is a many-fermion dynamic quantity.We illustrate how the three-spin interactions manifest themselves in the dynamic probes.

PACS numbers: 75.10.Jm, 75.40.Gb

1. Introduction

Spin-1/2 XY chains are well-known exactly solvable models: by applying the Jordan-Wigner transformation they can be mapped onto a model of noninteracting spinless fermions. Within such an approach some additional many-spin interactions may be also included into the spin Hamiltonian leaving the model exactly solvable. Recently there has been renewed interest in the spin-1/2 XY chains with many-spin interactions [1–4]. Such models provide rigorous statements which may be important for understanding of more complicate quantum spin chains with many-spin interactions.

2. Model

In what follows we consider N spins 1/2 in a row with the Hamiltonian

$$H=\sum_n \big[\Omega s_n^z + J\left(s_n^x s_{n+1}^x + s_n^y s_{n+1}^y\right) + D\left(s_n^x s_{n+1}^y - s_n^y s_{n+1}^x\right) + K\left(s_n^x s_{n+1}^z s_{n+2}^x + s_n^y s_{n+1}^z s_{n+2}^y\right) + E\left(s_n^x s_{n+1}^z s_{n+2}^y - s_n^y s_{n+1}^z s_{n+2}^x\right)\big]. \quad (1)$$

Here Ω is the transverse (z) external magnetic field, J and D are the isotropic XY (or XX) exchange interaction and the z-component of the Dzyaloshinskii–Moriya interaction between the neighboring sites. K and E are two types of three-site exchange interaction introduced in [2, 3] and [1], respectively.After applying the Jordan–Wigner transformation the Hamiltonian (1) becomes

$$H = \sum_n \left[\Omega \left(c_n^\dagger c_n - \frac{1}{2} \right) + \frac{J + \mathrm{i}D}{2} c_n^\dagger c_{n+1} - \frac{J - \mathrm{i}D}{2} c_n c_{n+1}^\dagger \right.$$
$$\left. - \frac{K + \mathrm{i}E}{4} c_n^\dagger c_{n+2} + \frac{K - \mathrm{i}E}{4} c_n c_{n+2}^\dagger \right], \tag{2}$$

that is the Hamiltonian of spinless fermions with complex nearest-neighbor and next-nearest-neighbor hoppings. The fermionic Hamiltonian (2) can be diagonalized by the Fourier transformation, $c_n^\dagger = \left(1/\sqrt{N}\right) \sum_\kappa \exp\left(\mathrm{i}\kappa n\right) c_\kappa^\dagger$, with the result

$$H = \sum_\kappa \Lambda_\kappa \left(c_\kappa^\dagger c_\kappa - \frac{1}{2} \right),$$
$$\Lambda_\kappa = \Omega + J\cos\kappa + D\sin\kappa - \frac{K}{2}\cos(2\kappa) - \frac{E}{2}\sin(2\kappa). \tag{3}$$

The three-spin interactions lead to the terms proportional to $\cos(2\kappa)$ and $\sin(2\kappa)$ in the formula for the elementary excitation energy Λ_κ (3).

3. Dynamic structure factors

In this study we focus on the dynamic structure factors defined by

$$S_{\alpha\alpha}(\kappa,\omega) = \frac{1}{N} \sum_{j=1}^{N} \sum_{m=1}^{N} \exp\left(-\mathrm{i}\kappa m\right) \int_{-\infty}^{\infty} \mathrm{d}t \exp\left(\mathrm{i}\omega t\right) \langle \Delta s_j^\alpha(t) \Delta s_{j+m}^\alpha \rangle, \tag{4}$$

where $\alpha = x, y, z$, $\langle (\ldots) \rangle = \mathrm{Tr}\left(\exp\left(-\beta H\right)(\ldots)\right) / \mathrm{Tr}\exp\left(-\beta H\right)$, $\Delta s_j^\alpha(t) = s_j^\alpha(t) - \langle s_j^\alpha \rangle$, $s_j^\alpha(t) = \exp\left(\mathrm{i}Ht\right) s_j^\alpha \exp\left(-\mathrm{i}Ht\right)$.

The dynamic transverse structure factor $S_{zz}(\kappa,\omega)$ can be calculated after using the Wick–Bloch–de Dominicis theorem ([5] and references therein). We obtain

$$S_{zz}(\kappa,\omega) = \int_{-\pi}^{\pi} \mathrm{d}\kappa_1 n_{\kappa_1} \left(1 - n_{\kappa+\kappa_1}\right) \delta\left(\omega + \Lambda_{\kappa_1} - \Lambda_{\kappa+\kappa_1}\right), \tag{5}$$

where n_κ is the Fermi function.

We display gray-scale plots for $S_{zz}(\kappa,\omega)$ at low temperature in the left parts in Fig. 1 taking as an example the case of chain (1) with $\Omega = D = E = 0$. The dynamic zz structure factor (5) is governed exclusively by a two-fermion (particle–hole) excitation continuum.The existing theory of the two-fermion excitation continuum [5] has to be extended to the case of the more complicated elementary excitation energy spectrum Λ_κ [6]. From Fig. 1 one immediately notes that the two-fermion excitation continuum probed by the ground-state $S_{zz}(\kappa,\omega)$ is characterized by a number of characteristic lines in the κ–ω plane (bound-

aries, lines of potential van Hove singularities etc.).The dynamic zz structure factor is almost structureless within the permitted region of the κ–ω plane apart from peculiarities along the boundaries. We also note that a nonzero value of the three-site interaction $K \neq 0$ leads to a shift of the soft mode $|\kappa_c| = \pi$ to $|\kappa_c| = \pi - 2\arcsin\left(\sqrt{\frac{J^2}{4K^2} + \frac{1}{2}} - \frac{J}{2K}\right)$ and opens a gap at $|\kappa| = \pi$ (compare the lower and the upper parts in the left column in Fig. 1).

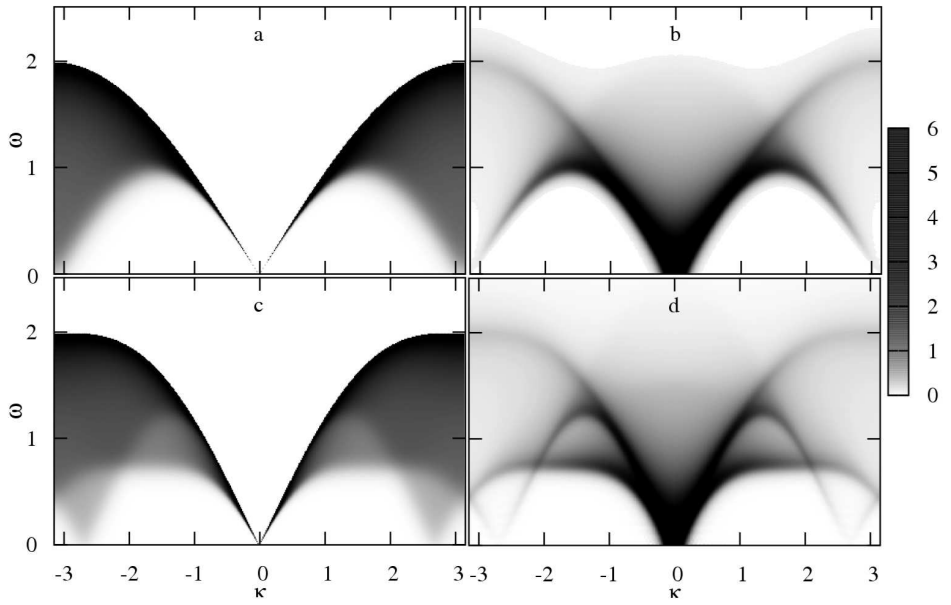

Fig. 1. $S_{zz}(\kappa,\omega)$ (left parts) and $S_{xx}(\kappa,\omega)$ (right parts) for the spin-1/2 chain (1) with $\Omega = 0$, $J = -1$, $D = 0$, $K = 0$ (upper parts) or $K = -0.5$ (lower parts), $E = 0$ at low temperature $\beta = 20$.

We compute $S_{xx}(\kappa,\omega)$ numerically following the scheme elaborated earlier ([7] and references therein).We express the relevant time-dependent correlation functions $\langle s_j^x(t)s_{j+m}^x\rangle$ as Pfaffians constructed from the known elementary contractions (which contain the elementary excitation energy Λ_κ (3)) and compute the Pfaffians for chains of $N = 400$ sites assuming $j = 41$ and taking m up to 100 and $t|J|$ up to ± 100 (see (4)).Our findings for the set of parameters fixed above are shown in the right parts in Fig. 1. In contrast to the dynamic zz structure factor, the dynamic xx structure factor is a many-particle quantity which is not restricted to some region in the κ–ω plane. However, as can be seen from Fig. 1 $S_{xx}(\kappa,\omega)$ at low temperatures is concentrated mainly along several washed-out excitation branches which roughly correspond to the characteristic lines of the two-fermion excitation continuumin the κ–ω plane.Again by comparing the lower and the upper parts in the right column in Fig. 1 we see a number of prominent

features (e.g. around $|\kappa| = \pi$) which unambiguously indicate the presence of the three-site interaction.

4. Conclusions

To summarize, we have examined some dynamic quantities for the spin-1/2 XX chain with three-site interactions. Within the Jordan–Wigner description the three-site interactions complicate the elementary excitation energy that influences not only the static quantities but also the dynamic quantities of the spin model. The three-site interactions clearly manifest themselves in the frequency or wave-vector scans of the dynamic structure factors.

Acknowledgments

NATO support is acknowledged (CBP.NUKR.CLG 982540).

References

[1] D. Gottlieb, J. Rössler, *Phys. Rev. B* **60**, 9232 (1999).

[2] O. Derzhko, J. Richter, V. Derzhko, *Ann. Phys. (Leipzig)* **8**, SI-49 (1999).

[3] I. Titvinidze, G.I. Japaridze, *Eur. Phys. J. B* **32**, 383 (2003).

[4] A.A. Zvyagin, *Phys. Rev. B* **73**, 104414 (2006).

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

[6] T. Krokhmalskii, O. Derzhko, J. Stolze, T. Verkholyak, in preparation.

[7] O. Derzhko, T. Krokhmalskii, J. Stolze, *J. Phys. A* **33**, 3063 (2000); O. Derzhko, T. Krokhmalskii, J. Stolze, *J. Phys. A* **35**, 3573 (2002).