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Динамічні властивості спін-1/2 XX ланцюжка з тривузловими взаємодіями $XZY - YZX$ типу

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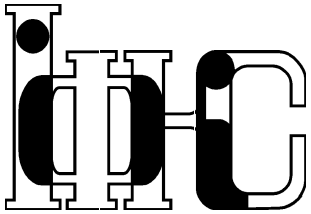

ІНСТИТУТ ФІЗИКИ КОНДЕНСОВАНИХ СИСТЕМ

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DYNAMIC PROPERTIES OF SPIN-1/2 XX CHAIN WITH THREE-SITE INTERACTIONS OF $(XZY - YZX)$-TYPE

ЛЬВІВ

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Динамічні властивості спін-1/2 XX ланцюжка з тривузловими взаємодіями $XZY-YZX$ типу

М.Топілко, О.Держко, Т.Крохмальський

Анотація. Розглядається спін-1/2 ізотропний XY ланцюжок у поперечному полі з тривузловими взаємодіями $XZY-YZX$ типу, який може бути перетворений у систему невзаємодіючих безспінових ферміонів. Досліджуються динамічні властивості спінової моделі. Зокрема, обчислено динамічні структурні фактори, які обумовлені континуумом двоферміонних збуджень. Показано, як тривузлові взаємодії проявляють себе у динамічних властивостях квантового спінового ланцюжка.
Ця робота була представлена на 14ій чеській і словацькій конференції з магнетизму CSMAG'10 (6–9 липня 2010, Кошіце, Словаччина).

Dynamic properties of spin-1/2 XX chain with three-site interactions of $(XZY-YZX)$-type

M.Topilko, O.Derzhko, T.Krokhmalskii

Abstract. We consider the spin-1/2 isotropic XY chain in a transverse field with three-site interactions of $(XZY-YZX)$-type, which can be transformed into a system of noninteracting spinless fermions. We study dynamic properties of the spin model. In particular, we calculate the dynamic structure factors which are governed by a two-fermion excitation continuum. We demonstrate how the three-site interactions manifest themselves in the dynamic properties of the quantum spin chain.
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Consider the spin-1/2 system with the Hamiltonian

$$H=\sum_n\left[J\left(s_n^xs_{n+1}^x+s_n^ys_{n+1}^y\right)\right.$$
$$\left.+E\left(s_n^xs_{n+1}^zs_{n+2}^y-s_n^ys_{n+1}^zs_{n+1}^x\right)+\Omega s_n^z\right], \qquad (1)$$

where J is the isotropic XY interaction between neighboring sites, E is the three-site interaction [1–4], Ω is the transverse field, and the sum runs over all N lattice sites of a simple chain. Spin system (1) admits accurate statistical-mechanics analysis and provides an excellent ground for studying quantum phase transitions [2,3]. We also notice that model (1) may emerge in a theory of the spin-1/2 XX chain with the energy current [5].

The reason why spin model (1) is amenable to exact calculations is generally known: After applying the Jordan-Wigner transformation the Hamiltonian (1) becomes a simple bilinear form in terms of spinless fermions and further can be put into a diagonal form after performing the Fourier transformation. The final result reads:

$$H=\sum_k\Lambda_k\left(c_k^\dagger c_k-\frac{1}{2}\right),$$
$$\Lambda_k=J\cos k-\frac{E}{2}\sin(2k)+\Omega. \qquad (2)$$

The term proportional to $\sin(2k)$ in the elementary excitation spectrum Λ_k emerges due to the three-site interactions and it drastically modifies various properties of the spin chain. The ground-state and thermodynamic properties as well as the static spin correlations of spin model (1) were examined in Refs. [2,3]. In the present paper we focus on the dynamic properties of the model which were not discussed so far.

To be specific, we consider the dynamic structure factor

$$S_A(k,\omega)=\sum_{l=1}^{N}e^{-ikl}\int_{-\infty}^{\infty}dte^{i\omega t}\langle\Delta A_n(t)\Delta A_{n+l}(0)\rangle, \qquad (3)$$

where $\langle(\ldots)\rangle=\mathrm{Tr}[e^{-\beta H}(\ldots)]/\mathrm{Tr}e^{-\beta H}$, $\Delta A_n(t)=A_n(t)-\langle A\rangle$, $A_n(t)=e^{iHt}A_ne^{-iHt}$, A_n is some local operator attached to the site n, $\langle A\rangle=(1/N)\sum_n\langle A_n\rangle$. Furthermore, we consider five local spin operators A_n, which in the Jordan-Wigner representations are products of two Fermi operators, namely, s_n^z, $d_n^{(1)}=s_n^xs_{n+1}^x+s_n^ys_{n+1}^y$, $d_n^{(2)}=s_n^xs_{n+1}^y-s_n^ys_{n+1}^x$, $t_n^{(1)}=s_n^xs_{n+1}^zs_{n+2}^x+s_n^ys_{n+1}^zs_{n+2}^y$, and $t_n^{(2)}=s_n^xs_{n+1}^zs_{n+2}^y-s_n^ys_{n+1}^zs_{n+2}^x$.

Following the usual procedure (see, e.g., Ref. [6]) we calculate the dynamic structure factors $S_{s^z}(k,\omega)$, $S_{d^{(1)}}(k,\omega)$, $S_{d^{(2)}}(k,\omega)$, $S_{t^{(1)}}(k,\omega)$, and $S_{t^{(2)}}(k,\omega)$. The final result can be written compactly as follows:

$$S_A(k,\omega) = \int_{-\pi}^{\pi} dk_1 B_A(k_1,k_2) C(k_1,k_2) D(k_1,k_2);$$

$$B_{s^z}(k_1,k_2) = 1,$$

$$B_{d^{(1)}}(k_1,k_2) = \cos^2\frac{k_1+k_2}{2},$$

$$B_{d^{(2)}}(k_1,k_2) = \sin^2\frac{k_1+k_2}{2},$$

$$B_{t^{(1)}}(k_1,k_2) = \frac{1}{4}\cos^2(k_1+k_2),$$

$$B_{t^{(2)}}(k_1,k_2) = \frac{1}{4}\sin^2(k_1+k_2);$$

$$C(k_1,k_2) = n_{k_1}\left(1-n_{k_2}\right), \quad n_k = \frac{1}{e^{\beta\Lambda_k}+1};$$

$$D(k_1,k_2) = \delta\left(\omega+\Lambda_{k_1}-\Lambda_{k_2}\right)\delta_{k_2,k_1+k}. \qquad (4)$$

From Eq. (4) it is clear that the obtained dynamic structure factors are governed by a two-fermion excitation continuum. They should have many common features conditioned by the factors $D(k_1,k_2)$ and $C(k_1,k_2)$ and some specific peculiarities due to the factor $B_A(k_1,k_2)$, see Eq. (4). *In the high-temperature limit* ($\beta = 0$) $C(k_1,k_2) \to 1/4$ and $S_A(k,\omega)$ does not depend on Ω. Furthermore, $S_A(k,\omega)$ may have nonzero values only within a restricted region in the wavevector–frequency plane since $-\Lambda_{k_1}+\Lambda_{k_2}$ is bounded above. Due to the presence of a two-particle density of states, $S_A(k,\omega)$ may exhibit a van Hove singularity. *In the zero-temperature limit* ($\beta \to \infty$) the Fermi functions, which enter the factor $C(k_1,k_2)$, impose extra demands to have nonzero values of $S_A(k,\omega)$ ($\Lambda_{k_1} \le 0$ and $\Lambda_{k_1+k} \ge 0$) leading, in general, to further restrictions on the region in the k–ω plane, where $S_A(k,\omega)$ may have nonzero values. Furthermore, considering the condition $S_A(k_0,\omega=0) \neq 0$ we may find soft modes k_0. In the zero-temperature limit $S_A(k,\omega) = 0$ if the value of Ω becomes sufficiently large, since in such a case the inequalities $\Lambda_{k_1} \le 0$ and $\Lambda_{k_1+k} \ge 0$ cannot be satisfied. The detailed distribution of different structure factors should be different, compare different factors $B_A(k_1,k_2)$ in Eq. (4). For example, the behavior of $S_A(k,\omega)$ along the line of (potential) van Hove singularities depends essentially on the specific factor $B_A(k_1,k_2)$. Further analysis of generic and specific properties of the two-fermion excitation continuum probed by dynamic structure factors (4) will be given in an extended publication.

In Fig. 1 we present the grayscale plots for two ground-state structure factors (4), $S_{s^z}(k,\omega)$ (panels a and b) and $S_{d^{(1)}}(k,\omega)$ (panels c and d), for $\Omega = 0$, $J = 1$ and two values of the three-site interaction, $E = 0.5$ (panels a and c) and $E = 1.5$ (panels b and d). $S_{s^z}(k,\omega)$ and $S_{d^{(1)}}(k,\omega)$ exhibit generic and specific features discussed above [nonzero values within a restricted region in the k–ω plane, singularities, soft modes, definite differences between $S_{s^z}(k,\omega)$ and $S_{d^{(1)}}(k,\omega)$]. We recall that for the case $E = 0$ the upper [lower] boundary of the two-fermion excitation continuum is given by $\omega_u(k) = 2|J|\sin(|k|/2)$ [$\omega_l(k) = |J|\sin|k|$], see Ref. [7]. Clearly, the three-site interactions drastically modify these boundaries even for small values of E leading, in particular, to a loss of symmetry with respect to the change $k \to -k$. Furthermore, the considered spin model exhibits two different spin-liquid ground states with phase transition points at $E = \pm|J|$ (for $\Omega = 0$). Comparing panels a and c ($E = 0.5$) with panels b and d ($E = 1.5$) in Fig. 1 we see that the calculated two-fermion dynamic quantities undoubtedly reflect the change of the ground state of spin model (1).

As a final remark, we wish to compare our findings for the case of three-site interactions of $(XZY - YZX)$-type with the corresponding results obtained earlier for the case of three-site interactions of $(XZX + YZY)$-type [4]. The main difference is connected with the symmetry $\Lambda_k = \Lambda_{-k}$ which exists in the latter case but does not hold for the model under consideration, see Eq. (2).

To summarize, we have reported the first results on dynamic properties of the spin-1/2 XX chain with three-site interactions of $(XZY - YZX)$-type. Our study concerns two-fermion dynamic structure factors and (together with paper [4]) generalizes earlier works on conventional XY chains [7]. Although we do not discuss many-fermion dynamic structure factors [like $S_{s^x}(k,\omega)$], from the previous works [4,6,7] we may expect that in the low-temperature limit these quantities are concentrated in the k–ω plane mostly along characteristic lines of the two-fermion excitation continuum.

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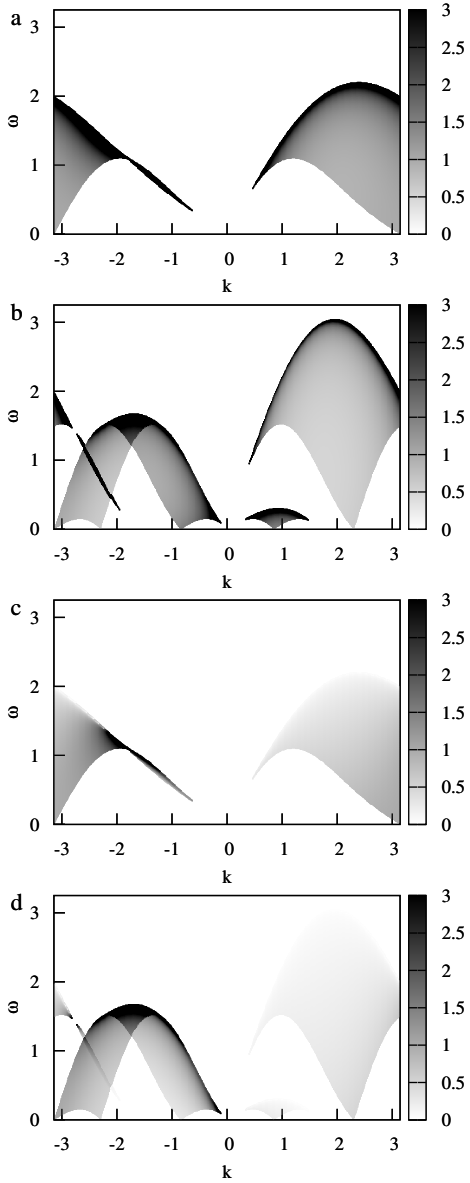

Figure 1. Ground-state two-fermion dynamic structure factors $S_{s^z}(k,\omega)$ (a, b) and $S_{d^{(1)}}(k,\omega)$ (c, d) of spin model (1) for $\Omega = 0$, $J = 1$, and $E = 0.5$ (a, c) or $E = 1.5$ (b, d).

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