Condensed Matter Physics, 2005, Vol. 8, No. 4(44), pp. 859–867

CONDENSED MATTER PHYSICS

Dynamics of dimer and z spin component fluctuations in spin-$1/2$ XY chain

O.Derzhko, T.Krokhmalskii, P.Hlushak

Institute for Condensed Matter Physics
of the National Academy of Sciences of Ukraine,
1 Svientsitskii Str., 79011 Lviv, Ukraine

Received August 15, 2005

One-dimensional quantum spin- $1/2$ XY models admit the rigorous analysis not only of their static properties (i.e. the thermodynamic quantities and the equal-time spin correlation functions) but also of their dynamic properties (i.e. the different-time spin correlation functions, the dynamic susceptibilities, the dynamic structure factors). This becomes possible after exploiting the Jordan-Wigner transformation which reduces the spin model to a model of spinless noninteracting fermions. A number of dynamic quantities (e.g. related to transverse spin operator or dimer operator fluctuations) are entirely determined by two-fermion excitations and can be examined in much detail. We consider the spin- $1/2$ XY chain in a transverse ($\|$ z) magnetic field with the Hamiltonian

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

and calculate the dynamic structure factors

$$S_{AB}(\kappa,\omega)=\sum_n \exp\left(-\mathrm{i}\kappa n\right)\int_{-\infty}^{\infty}\mathrm{d}t\exp\left(\mathrm{i}\omega t\right)\langle A_j(t)B_{j+n}(0)\rangle$$

for the local spin operators $\{A_m,B_m\}=\left\{s_m^z,D_m\right\}$ where $D_m=s_m^x s_{m+1}^x+s_m^y s_{m+1}^y$ is the dimer operator. The results for the dynamic transverse structure factor $S_{zz}(\kappa,\omega)$ and for the dynamic dimer structure factor $S_{\mathrm{DD}}(\kappa,\omega)$ are known, whereas the analysis of the dynamic structure factor $S_{z\mathrm{D}}(\kappa,\omega)=(S_{\mathrm{D}z}(\kappa,\omega))^{\star}$ has not been reported so far. We compare different two-fermion dynamic quantities contrasting their generic and specific features.

Key words: *quantum spin chains, dynamic structure factors*

PACS: *75.10.-b*

The subject of analysis of the dynamic properties of low-dimensional quantum spin systems has attracted considerable interest for the recent years. On the one hand, quite often the relevant quantities can be examined rigorously, especially if the space dimension is equal to one. This is important even if the models in question are simplified since conventional approximations usually fail after being applied to low-dimensional quantum spin systems. On the other hand, material science provides a number of magnetic materials which can be modelled using the spin-1/2 XXZ Heisenberg chains. Therefore, to interpret the experimental data obtained in neutron scattering experiments or resonance experiments for such compounds one needs a corresponding theory of the dynamic properties. A particular case of the spin-1/2 XXZ Heisenberg chain, the XY chain, owing to the Jordan-Wigner fermionization trick can be investigated analytically, thus shedding light on the physical effects that may be observed in less tractable cases.

In what follows, we consider the one-dimensional spin-1/2 XY model in a transverse ($\parallel z$) external field [1] defined by the Hamiltonian

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

Here J is the exchange interaction constant (we will set further $J=-1$), Ω is the external magnetic field, $s^\alpha=1/2\cdot\sigma^\alpha$, σ^α with $\alpha=x,y,z$ are the Pauli matrices, and $N\to\infty$ is the number of sites. We imposed periodic boundary conditions in (1). After exploiting the Jordan-Wigner transformation the considered spin model can be presented in terms of noninteracting spinless fermions with the Hamiltonian

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

Here periodic boundary conditions are implied (the so-called boundary term is not important for the dynamic quantities examined below) and κ is the quasi-momentum which takes N values in the region from $-\pi$ to π.

Important information about the behavior of the system under small perturbations follows from the dynamic susceptibilities [2]

$$\begin{aligned}\chi_{AB}(\kappa,\omega)\ &=\ \sum_{n=1}^{N}\exp\left(-\mathrm{i}\kappa n\right)\int_0^\infty \mathrm{d}t\exp\left(\mathrm{i}\left(\omega+\mathrm{i}\epsilon\right)t\right)\frac{1}{\mathrm{i}}\left\langle\left[A_j(t),B_{j+n}(0)\right]\right\rangle,\\ \epsilon\ &\to\ +0.\end{aligned} \tag{3}$$

Here A_m, B_m are the local operators attached to the site m (for example, the spin operators s_m^x, s_m^y, s_m^z, the dimer operator $D_m=s_m^x s_{m+1}^x+s_m^y s_{m+1}^y$ or the trimer operator $T_m=s_m^x s_{m+2}^x+s_m^y s_{m+2}^y$ [3–8]). Another quantities which reflect the dynamic properties of the system are the dynamic structure factors

$$S_{AB}(\kappa,\omega)=\sum_{n=1}^{N}\exp\left(-\mathrm{i}\kappa n\right)\int_{-\infty}^{\infty}\mathrm{d}t\exp\left(\mathrm{i}\omega t\right)\left\langle A_j(t)B_{j+n}(0)\right\rangle. \tag{4}$$

$S_{AB}(\kappa,\omega)$ is connected to the imaginary part of $\chi_{AB}(\kappa,\omega)$ through the fluctuation-dissipation theorem. The imaginary and real parts of $\chi_{AB}(\kappa,\omega)$ are connected by the

Kramers-Kronig transformation. In what follows we focus on the dynamic structure factors (4).

Introducing the fermionic representation (2) and exploiting the Wick-Bloch-de Dominicis theorem we easily calculate the two-spin correlation functions entering equations (3), (4)

$$
\begin{aligned}
\langle s_n^z(t)s_{n+l}^z(0)\rangle - \langle s^z\rangle^2 &= \frac{1}{N^2}\sum_{\kappa_1,\kappa_2}\exp\left(-\mathrm{i}\left(\kappa_1-\kappa_2\right)l\right)\exp\left(\mathrm{i}\left(\Lambda_{\kappa_1}-\Lambda_{\kappa_2}\right)t\right)\\
&\quad\times n_{\kappa_1}\left(1-n_{\kappa_2}\right), \qquad (5)\\
\langle s_n^z(t)D_{n+l}(0)\rangle - \langle s^z\rangle\langle D\rangle &= \frac{1}{N^2}\sum_{\kappa_1,\kappa_2}\frac{\exp(-\mathrm{i}\kappa_1)+\exp(\mathrm{i}\kappa_2)}{2}\exp\left(-\mathrm{i}\left(\kappa_1-\kappa_2\right)l\right)\\
&\quad\times\exp\left(\mathrm{i}\left(\Lambda_{\kappa_1}-\Lambda_{\kappa_2}\right)t\right)n_{\kappa_1}\left(1-n_{\kappa_2}\right), \qquad (6)\\
\langle D_n(t)D_{n+l}(0)\rangle - \langle D\rangle^2 &= \frac{1}{N^2}\sum_{\kappa_1,\kappa_2}\cos^2\frac{\kappa_1+\kappa_2}{2}\exp\left(-\mathrm{i}\left(\kappa_1-\kappa_2\right)l\right)\\
&\quad\times\exp\left(\mathrm{i}\left(\Lambda_{\kappa_1}-\Lambda_{\kappa_2}\right)t\right)n_{\kappa_1}\left(1-n_{\kappa_2}\right), \qquad (7)
\end{aligned}
$$

where $n_\kappa = \left(1+\exp\left(\beta\Lambda_\kappa\right)\right)^{-1}$ is the Fermi function and

$$
\begin{aligned}
\langle s^z\rangle &= \frac{1}{N}\sum_{n=1}^{N}\langle s_n^z\rangle = -\frac{1}{2N}\sum_\kappa\tanh\frac{\beta\Lambda_\kappa}{2},\\
\langle D\rangle &= \frac{1}{N}\sum_{n=1}^{N}\langle D_n\rangle = -\frac{1}{2N}\sum_\kappa\cos\kappa\tanh\frac{\beta\Lambda_\kappa}{2}.
\end{aligned}
$$

The associated dynamic structure factors are obtained from equations (5)–(7) by Fourier transform. The resulting expressions for $N\to\infty$ can be brought into the form

$$
\begin{aligned}
S_{zz}(\kappa,\omega) - 2\pi N\delta_{\kappa,0}\delta(\omega)\langle s^z\rangle^2 &= \int_{-\pi}^{\pi}\mathrm{d}\kappa_1 n_{\kappa_1}\left(1-n_{\kappa_1+\kappa}\right)\delta\left(\omega+\Lambda_{\kappa_1}-\Lambda_{\kappa_1+\kappa}\right)\\
&= \sum_{\kappa^\star}\frac{n_{\kappa^\star}\left(1-n_{\kappa+\kappa^\star}\right)}{2|J\sin\frac{\kappa}{2}\cos\left(\frac{\kappa}{2}+\kappa^\star\right)|}, \qquad (8)\\
S_{z\mathrm{D}}(\kappa,\omega) - 2\pi N\delta_{\kappa,0}\delta(\omega)\langle s^z\rangle\langle D\rangle &= \exp\left(\mathrm{i}\frac{\kappa}{2}\right)\sum_{\kappa^\star}\frac{\cos\left(\frac{\kappa}{2}+\kappa^\star\right)n_{\kappa^\star}\left(1-n_{\kappa+\kappa^\star}\right)}{2|J\sin\frac{\kappa}{2}\cos\left(\frac{\kappa}{2}+\kappa^\star\right)|}, \qquad (9)\\
S_{\mathrm{D}z}(\kappa,\omega) &= \left(S_{z\mathrm{D}}(\kappa,\omega)\right)^\star, \qquad (10)\\
S_{\mathrm{DD}}(\kappa,\omega) - 2\pi N\delta_{\kappa,0}\delta(\omega)\langle D\rangle^2 &= \sum_{\kappa^\star}\frac{\cos^2\left(\frac{\kappa}{2}+\kappa^\star\right)n_{\kappa^\star}\left(1-n_{\kappa+\kappa^\star}\right)}{2|J\sin\frac{\kappa}{2}\cos\left(\frac{\kappa}{2}+\kappa^\star\right)|}, \qquad (11)
\end{aligned}
$$

where $-\pi\leqslant\kappa^\star\leqslant\pi$ are the solutions of the equation

$$
\omega = -2J\sin\frac{\kappa}{2}\sin\left(\frac{\kappa}{2}+\kappa^\star\right). \qquad (12)
$$

We can combine formulas (8)–(11) rewriting them in the form

$$
\begin{aligned}
& S_{AB}(\kappa,\omega) - 2\pi N\delta_{\kappa,0}\delta(\omega)\langle A\rangle\langle B\rangle \\
& \qquad = \int_{-\pi}^{\pi} \mathrm{d}\kappa_1 \mathrm{d}\kappa_2 C_{AB}^{(2)}(\kappa_1,\kappa_2) n_{\kappa_1}\left(1-n_{\kappa_2}\right)\delta\left(\omega+\Lambda_{\kappa_1}-\Lambda_{\kappa_2}\right)\delta_{\kappa+\kappa_1-\kappa_2,0} \\
& \qquad = \sum_{\kappa^\star} \frac{\mathcal{C}_{AB}^{(2)}(\kappa,\kappa^\star) n_{\kappa^\star}\left(1-n_{\kappa+\kappa^\star}\right)}{2\left|J\sin\frac{\kappa}{2}\cos\left(\frac{\kappa}{2}+\kappa^\star\right)\right|} \qquad (13)
\end{aligned}
$$

with

$$
\begin{aligned}
\mathcal{C}_{zz}^{(2)}(\kappa,\kappa^\star) &= 1, & (14)\\
\mathcal{C}_{z\mathrm{D}}^{(2)}(\kappa,\kappa^\star) &= \exp\left(\mathrm{i}\frac{\kappa}{2}\right)\cos\left(\frac{\kappa}{2}+\kappa^\star\right), & (15)\\
\mathcal{C}_{\mathrm{D}z}^{(2)}(\kappa,\kappa^\star) &= \left(\mathcal{C}_{z\mathrm{D}}^{(2)}(\kappa,\kappa^\star)\right)^\star, & (16)\\
\mathcal{C}_{\mathrm{DD}}^{(2)}(\kappa,\kappa^\star) &= \cos^2\left(\frac{\kappa}{2}+\kappa^\star\right). & (17)
\end{aligned}
$$

The dynamic transverse structure factor $S_{zz}(\kappa,\omega)$ was obtained by Th. Niemeijer (see [9]), the dynamic dimer structure factor $S_{\mathrm{DD}}(\kappa,\omega)$ was examined in [3–5].

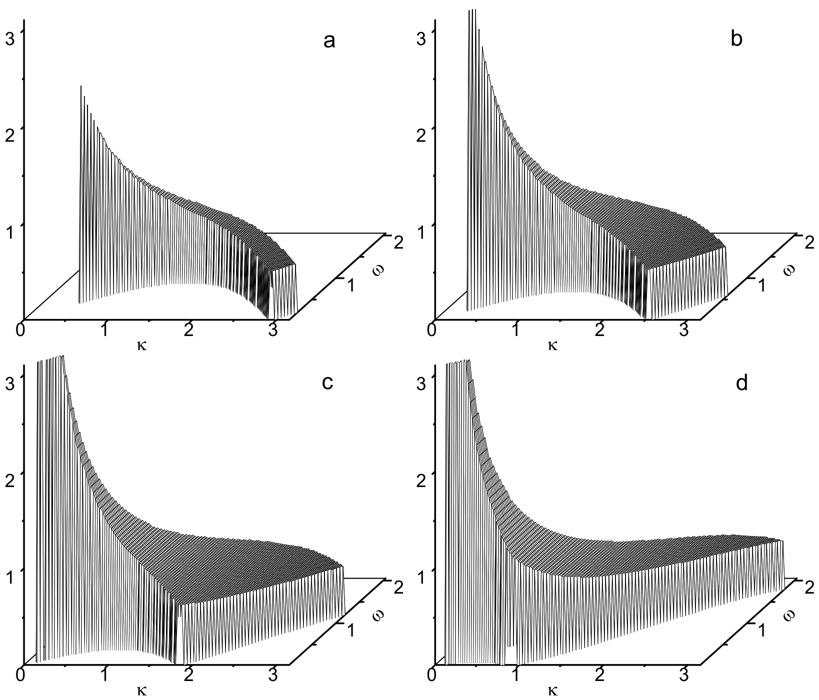

Figure 1. The l. h. s. of equation (9) multiplied by $\exp\left(-\mathrm{i}[\kappa/2]\right)$ for the spin chain (1) with $J=-1$ and $\Omega=0.1$ (a), $\Omega=0.3$ (b), $\Omega=0.6$ (c), $\Omega=0.9$ (d) at zero temperature $\beta\to\infty$.

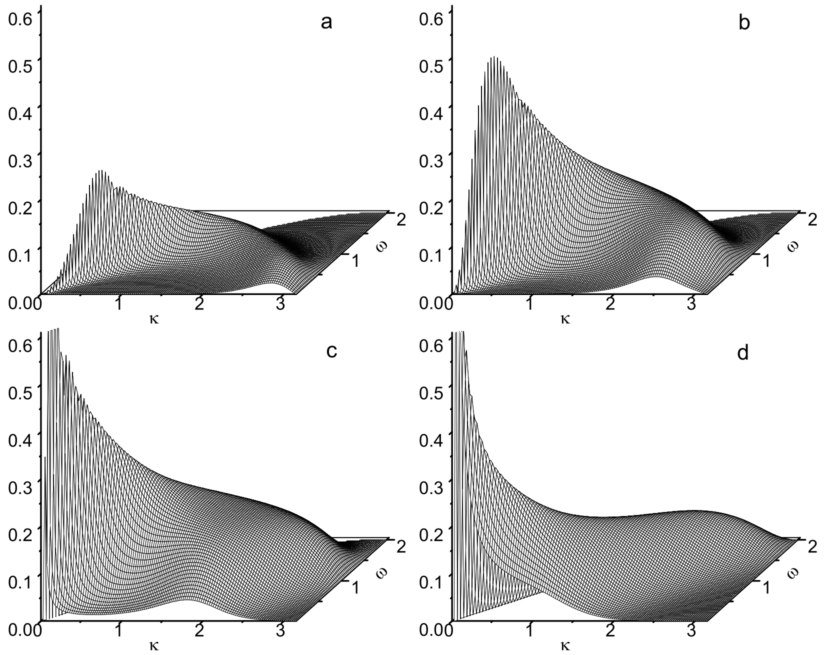

Figure 2. The same as in figure 1 at $\beta = 10$. Note the different vertical scales in figure 1 and figure 2.

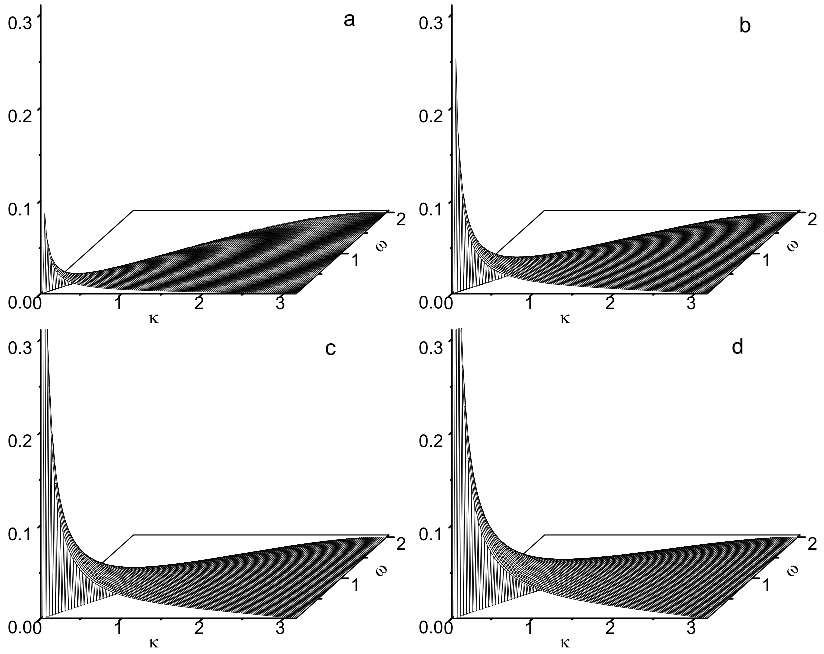

Figure 3. The same as in figure 1 at $\beta = 1$. Note the different vertical scales in figure 1 and figure 3.

To the best of our knowledge, the dynamic structure factor $S_{z\mathrm{D}}(\kappa,\omega) = (S_{\mathrm{D}z}(\kappa,\omega))^{\star}$ has not been discussed so far.

In figures 1–3 we plot the dynamic structure factor $S_{z\mathrm{D}}(\kappa,\omega)$ at different temperatures. These plots demonstrate not only the specific features of the dynamic structure factor $S_{z\mathrm{D}}(\kappa,\omega)$ but also the generic features of all two-fermion dynamic structure factors (13).

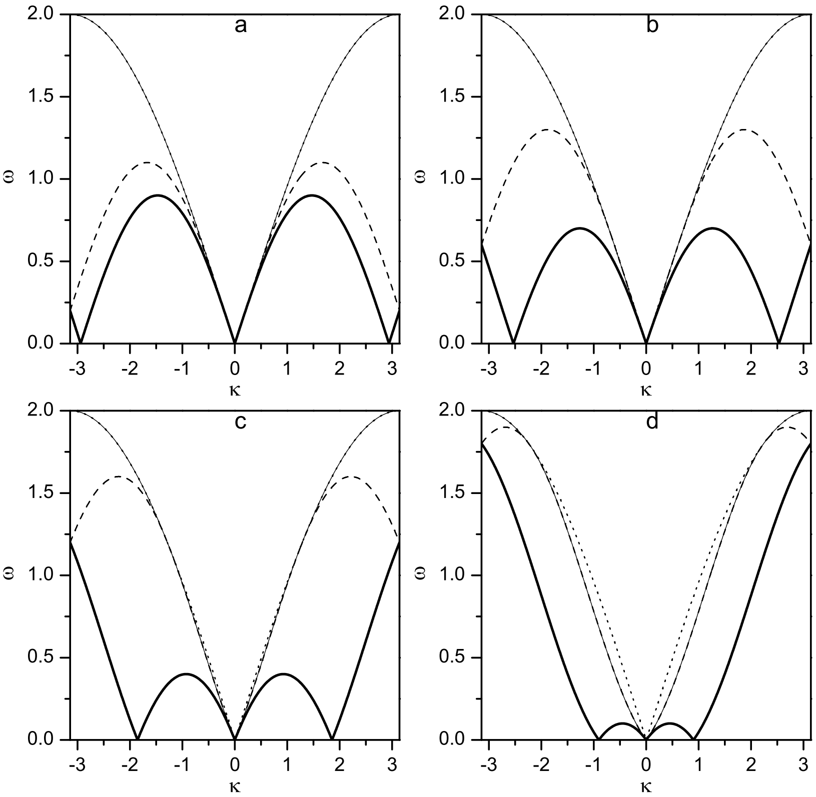

Figure 4. Two-fermion excitation continuum which governs the ground-state dynamic structure factors (13). We set $|J|=1$ and $\Omega=0.1$ (a) $\Omega=0.3$ (b), $\Omega=0.6$ (c), $\Omega=0.9$ (d). The lower boundary (18) (bold lines), the middle boundary (19) (dashed lines), the upper boundary (20) (thin lines), the line of potential singularities (21) (dotted lines).

From equation (13) it is clearly seen that the dynamic structure factors (8), (9), (10), (11) are governed entirely by the two-fermion (particle-hole) excitation continuum the properties of which were examined in [9,10]. Hereinafter we briefly account for these results. At zero temperature $\beta\to\infty$ the two-fermion excitation continuum exists only if $|\Omega|<|J|$ and has the following lower, middle and upper boundaries in the plane wave-vector κ – frequency ω

$$\frac{\omega_l}{|J|} = 2\sin\frac{|\kappa|}{2}\left|\sin\left(\frac{|\kappa|}{2}-\alpha\right)\right|, \tag{18}$$

$$\frac{\omega_m}{|J|} = 2\sin\frac{|\kappa|}{2}\sin\left(\frac{|\kappa|}{2}+\alpha\right), \tag{19}$$

$$\frac{\omega_u}{|J|} = \begin{cases} 2\sin\frac{|\kappa|}{2}\sin\left(\frac{|\kappa|}{2}+\alpha\right), & \text{if} \quad 0 \leqslant |\kappa| \leqslant \pi - 2\alpha, \\ 2\sin\frac{|\kappa|}{2}, & \text{if} \quad \pi - 2\alpha \leqslant |\kappa| \leqslant \pi, \end{cases} \tag{20}$$

respectively; here we have introduced the parameter $\alpha = \arccos(\Omega/|J|)$ which varies from π when $\Omega = -|J|$ to 0 when $\Omega = |J|$. The region $\omega_l \leqslant \omega \leqslant \omega_m$ corresponds to the lower two-fermion excitation continuum, whereas the region $\omega_m \leqslant \omega \leqslant \omega_u$ corresponds to the upper two-fermion excitation continuum. The ω-profiles at fixed κ of the two-fermion dynamic structure factors (13) may exhibit Van Hove's singularities (as the density of one-particle states in one dimension) when $\omega \to \omega_s - 0$,

$$\frac{\omega_s}{|J|} = 2\sin\frac{|\kappa|}{2}. \tag{21}$$

Figure 4 shows expressions (18)–(21) plotted for $|J| = 1$ and various Ω. As temperature increases the lower boundary of the two-fermion excitation continuum smears out, i.e. $\omega_l = 0$, and the upper boundary becomes $\omega_u = 2|J|\sin(|\kappa|/2)$.

The specific features of different dynamic structure factors are connected with the explicit form of the function $\mathcal{C}^{(2)}_{AB}(\kappa,\kappa^\star)$ (14)–(17). Thus, the dynamic dimer structure factor vanishes (and hence does not diverge) along ω_s (21) since $\mathcal{C}^{(2)}_{\mathrm{DD}}(\kappa,\kappa^\star)$ (17) cancels the zero in the denominator in equation (13). This is contrary to the case of the dynamic transverse structure factor with $\mathcal{C}^{(2)}_{zz}(\kappa,\kappa^\star)$ (14). Moreover, the zero-temperature dynamic structure factor $S_{z\mathrm{D}}(\kappa,\omega)$ is zero in the upper two-fermion excitation continuum, i.e. for $\omega_m \leqslant \omega \leqslant \omega_u$. For this region of the κ–ω plane the two roots $\kappa_1^\star$ and $\kappa_2^\star$ of equation (12) yield in equation (13) two contributions of the same value but with opposite signs. At nonzero temperatures the values of these contributions become different and $S_{z\mathrm{D}}(\kappa,\omega)$ deviates from zero in the upper two-fermion excitation continuum. In the lower two-fermion excitation continuum one of the roots does not contribute at zero temperature due to the Fermi functions in equation (13). However, when temperature tends to infinity $\beta \to 0$ the restrictions owing to the Fermi functions in equation (13) disappear and two roots $\kappa_1^\star$ and $\kappa_2^\star$ come into play for all $0 \leqslant \omega \leqslant \omega_u$. They again have the same value but opposite signs and as a result, $S_{z\mathrm{D}}(\kappa,\omega)$ disappears within the whole two-fermion excitation continuum in the κ–ω plane. This behavior is illustrated in figures 1–3.

Thus, all the considered dynamic quantities exhibit the same generic properties controlled by the δ-functions and the Fermi functions in equation (13) (lower, middle and upper boundaries, soft modes, Van Hove's singularities) and some specific properties controlled by the function $\mathcal{C}^{(2)}_{AB}(\kappa,\kappa^\star)$ (zero values in the accessible region of the κ–ω plane, disappearance of Van Hove's singularities). Our results may be important from the theoretical point of view helping to understand the dynamic properties of quantum spin chains. Thus, equation (13) gives a hint to the form of multi-fermion excitation continua contributions to dynamic quantities (see [7,8]). On the other hand, we note that spin-1/2 XY chains are realized in some quasi-one-dimensional magnetic insulators [11,12], and hence our findings may have a relation to the experimental data obtained in dynamic experiments.

This study was supported by the STCU under the project #1673. The authors thank Prof. Joachim Stolze and Prof. Gerhard Müller for collaboration on closely related subjects [7,8]. The paper was partially presented at the International Conference on Strongly Correlated Electron Systems (Vienna, July 26 - 30, 2005). O. D. and T. K. thank the Organizing Committee of the SCES'05 for the support to attend the conference.

References

1. Lieb E., Schultz T., Mattis D., Ann. Phys. (N.Y.), 1961, **16,** 407.
2. Zubarev D.N. Njeravnovjesnaja Statistichjeskaja Tjermodinamika. Nauka, Moskva, 1971 (in Russian).
3. Suzuura H., Yasuhara H., Furusaki A., Nagaosa N., Tokura Y., Phys. Rev. Lett., 1996, **76,** 2579.
4. Yongmin Yu, Müller G., Viswanath V.S., Phys. Rev. B, 1996, **54,** 9242.
5. Lorenzana J., Eder R., Phys. Rev. B, 1997, **55,** R3358.
6. Werner R., Phys. Rev. B, 2001, **63,** 174416.
7. Derzhko O., Krokhmalskii T., Stolze J., Müller G., Phys. Rev. B, 2005, **71,** 104432.
8. Derzhko O., Krokhmalskii T., Stolze J., Müller G., to appear in Physica B, 2005.
9. Müller G., Thomas H., Beck H., Bonner J.C., Phys. Rev. B, 1981, **24,** 1429.
10. Taylor J.H., Müller G., Physica A, 1985, **130,** 1.
11. Kenzelmann M., Coldea R., Tennant D.A., Visser D., Hofmann M., Smeibidl P., Tylczynski Z., Phys. Rev. B, 2002, **65,** 144432.
12. Rainford B.D., private communication (2005).

Динаміка флуктуацій димерного оператора і оператора z спінової компоненти у спін-$1/2$ XY ланцюжку

О.Держко, Т.Крохмальський, П.Глушак

Інститут фізики конденсованих систем НАН України,
79011 Львів, вул. Свєнціцького, 1

Отримано 15 серпня 2005 р.

Одновимірні квантові спін-$1/2$ XY моделі допускають строгий аналіз не лише їх статичних властивостей (тобто термодинамічних величин і однаковочасових спінових кореляційних функцій), але також і їх динамічних властивостей (тобто різночасових спінових кореляційних функцій, динамічних сприйнятливостей, динамічних структурних факторів). Це стає можливим після використання перетворення Йордана-Вігнера, яке зводить спінову модель до моделі безспінових невзаємодіючих ферміонів. Ряд динамічних величин (наприклад, пов'язаних з флуктуаціями оператора поперечної спінової компоненти чи димерного оператора) цілком визначаються двоферміонними збудженнями і можуть бути детально вивчені. Ми розглядаємо спін-$1/2$ XY ланцюжок у поперечному ($\parallel z$) магнітному полі з гамільтоніаном

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

і обчислюємо динамічні структурні фактори

$$S_{AB}(\kappa,\omega)=\sum_n \exp\left(-\mathrm{i}\kappa n\right)\int_{-\infty}^{\infty}\mathrm{d}t\exp\left(\mathrm{i}\omega t\right)\left\langle A_j(t)B_{j+n}(0)\right\rangle$$

для локальних спінових операторів $\{A_m,B_m\}=\left\{s_m^z,D_m\right\}$, де $D_m=s_m^x s_{m+1}^x+s_m^y s_{m+1}^y$ є димерним оператором. Результати для динамічного поперечного структурного фактора $S_{zz}(\kappa,\omega)$ і для динамічного димерного структурного фактора $S_{\mathrm{DD}}(\kappa,\omega)$ є відомі, тоді ж як динамічний структурний фактор $S_{z\mathrm{D}}(\kappa,\omega)=\left(S_{\mathrm{D}z}(\kappa,\omega)\right)^{\star}$ досі не був проаналізований. Ми порівнюємо різні двоферміонні динамічні величини, співставляючи їхні загальні і специфічні властивості.

Ключові слова: *квантові спінові ланцюжки, динамічні структурні фактори*

PACS: *75.10.-b*