Jordan–Wigner Fermions and Dynamic Probes of Quantum Spin Chains

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With the help of the Jordan–Wigner transformation the spin-$\frac{1}{2}$ XY chains can be reformulated in terms of noninteracting spinless fermions and, as a result, many statistical-mechanics calculations can be performed rigorously, i.e. without making any simplifying approximations. We are interested in dynamic properties of such chains (time-dependent spin correlation functions, dynamic structure factors, dynamic susceptibilities) which are of great importance for interpretation of experimental data. We have worked out a number of dynamic quantities explicitly as well as have performed a general analysis of the two-fermion continua which are relevant for different dynamic quantities.

1 Introductory remarks

The spin-$\frac{1}{2}$ XY chains are known as a simplest quantum interacting system for which a lot of statistical-mechanics calculations can be performed exactly [1]. The properties of such quantum spin chains were studied intensively during last more than forty years and the interest in such models may be renewed owing to a discovery of almost spin-$\frac{1}{2}$ XY chain compounds (see e.g. [2, 3]). On the other hand, such studies are interesting in their own rights since they provide a set of reference results which may be useful for understanding the much more common Heisenberg chains.

In what follows we consider the spin-$\frac{1}{2}$ anisotropic XY chain in a transverse field with an additional Dzyaloshinskii–Moriya interaction directed along z-axis in spin space to elucidate the effects of the Dzyaloshinskii–Moriya interaction on the dynamic properties of quantum spin chains. The Dzyaloshinskii–Moriya interaction plays important role in a number of quasi-one-dimensional materials and although it is generally small, its effects could be very important [4–6]. The Dzyaloshinskii–Moriya interaction also arises in description of the nonequlibrium steady states of spin chains [7]. Let us recall what is known about the dynamics of the considered quantum spin chains. The spin-$\frac{1}{2}$ XY chain with the Dzyaloshinskii–Moriya interaction was introduced in Ref. [8] (see also Ref. [9]) and the effects of this interaction on the zz dynamics were analyzed in Refs. [10, 11]. In particular, the zz dynamic susceptibility $\chi_{zz}(\kappa, \omega)$ of the spin-$\frac{1}{2}$ anisotropic XY chain with the Dzyaloshinskii–Moriya interaction was derived explicitly for $\kappa = 0$ [10] and $\kappa \neq 0$ [11]. Nevertheless, the effects of the Dzyaloshinskii–Moriya interaction on the two-fermion excitation continuum which governs zz dynamics [12, 13] have not been examined yet. There are notorious difficulties in calculations of the xx, xy, yx, yy dynamic quantities (for references see [14]), and to our best knowledge the effects of the Dzyaloshinskii–Moriya interaction on such quantities have not been reported until now. On the other hand, we should mentioned here the recent papers on the Heisenberg chains with the Dzyaloshinskii–Moriya interaction [15, 16]. Thus, using the symmetry arguments for the antiferromagnetic isotropic Heisenberg (XXX) chain with the Dzyaloshinskii–Moriya term directed along z-axis in spin space it was shown that although the Dzyaloshinskii–Moriya interaction may leave the spectrum of the problem unchanged, it can essentially influence the spin correlations / dynamic susceptibilities. In what follows we also derive such a conclusion in the case of the isotropic XY (i.e. $XX0$) chain, however, calculated different dynamic structure factors explicitly.

In the present paper we report the first results for the Dzyaloshinskii–Moriya effects on the two-fermion excitation continuum, which governs the zz dynamics of spin-$\frac{1}{2}$ XY chains and on the xx, xy, yx, yy dynamics of such chains. We start with presenting the basic formulas of the Jordan–Wigner fermionization approach (Section 2). Then we consider the case of isotropic XY exchange interaction. This case is essentially simpler than the case of anisotropic XY exchange interaction since the Dzyaloshinskii–Moriya interaction can be eliminated by a spin axes rotation. As a result, we can examine the dynamic structure factors of the chain with the Dzyaloshinskii–Moriya interaction using the obtained earlier results for such a chain without the Dzyaloshinskii–Moriya interaction (Section 3). Finally, we summarize our results (Section 4).

2 Dzyaloshinskii–Moriya interaction and Jordan–Wigner fermions

In what follows we consider $N \to \infty$ spins $\frac{1}{2}$ arranged in a circle and governed by the Hamiltonian

$$
\begin{aligned}
H &= \sum_{n=1}^{N} \Omega s_n^z + \sum_{n=1}^{N} \left(J^x s_n^x s_{n+1}^x + J^y s_n^y s_{n+1}^y \right) + \sum_{n=1}^{N} D \left(s_n^x s_{n+1}^y - s_n^y s_{n+1}^x \right) \\
&= \sum_{n=1}^{N} \Omega \left(s_n^+ s_n^- - \frac{1}{2} \right) + \frac{1}{2} \sum_{n=1}^{N} \left(\left(I^+ + iD \right) s_n^+ s_{n+1}^- \right. \\
&\quad + \left(I^+ - iD \right) s_n^- s_{n+1}^+ + I^- \left(s_n^+ s_{n+1}^+ + s_n^- s_{n+1}^- \right) \right).
\end{aligned}
\tag{1}
$$

Here $J^\alpha = 2I^\alpha$, $\alpha = x, y$ is the anisotropic XY exchange interaction, $I^\pm = I^x \pm I^y$, D is the Dzyaloshinskii–Moriya interaction and Ω is the transverse field. It is worthwhile to note that making use of the transformation $\tilde{s}_n^x = s_n^x$, $\tilde{s}_n^y = -s_n^y$, $\tilde{s}_n^z = -s_n^z$ (a π rotation of all spins about the x-axis) one gets again (1) with the parameters $-\Omega$, J^x, J^y, $-D$, whereas a similar transformation, $\tilde{s}_n^x = (-1)^n s_n^x$, $\tilde{s}_n^y = (-1)^n s_n^y$, $\tilde{s}_n^z = s_n^z$, yields (1) with the parameters Ω, $-J^x$, $-J^y$, $-D$. The renumbering of sites $j \to N - j + 1$, $j = 1, 2, \ldots, N$ in (1) yields again (1) with the parameters Ω, J^x, J^y, $-D$. These symmetry remarks permit to reduce the range of parameters for a study of the properties of the model.

We are interested in dynamics of quantum spin chain (1). For this purpose we need the two-spin time-dependent correlation functions, $\left\langle s_n^\alpha(t) s_{n+m}^\beta(0) \right\rangle$, $\alpha, \beta = x, y, z$, the angular brackets denote the canonical thermodynamic averaging, which yield the dynamic structure factors

$$
S_{\alpha\beta}(\kappa, \omega) = \sum_{m=1}^{N} \exp\left(i\kappa m \right) \int_{-\infty}^{\infty} dt \exp\left(i\omega t \right) \left\langle s_n^\alpha(t) s_{n+m}^\beta(0) \right\rangle.
\tag{2}
$$

Another dynamic quantity, the dynamic susceptibility $\chi_{\alpha\beta}(\kappa, \omega)$, can be obtained from the dynamic structure factor (2) using the fluctuation-dissipation theorem and the Kramers–Kronig transformation.

To derive the statistical-mechanics quantities of the spin model (1) we first use the Jordan–Wigner transformation

$$
\begin{aligned}
c_1^+ &= s_1^+, \quad c_1 = s_1^-, \quad c_n^+ = \left(-2s_1^z \right) \ldots \left(-2s_{n-1}^z \right) s_n^+, \\
c_n &= \left(-2s_1^z \right) \ldots \left(-2s_{n-1}^z \right) s_n^-, \quad n = 2, \ldots, N
\end{aligned}
\tag{3}
$$

to express the spin Hamiltonian in fermionic language

$$H = \sum_{n=1}^{N} \Omega \left(c_n^+ c_n - \frac{1}{2} \right)$$
$$+ \frac{1}{2} \sum_{n=1}^{N} \left((I^+ + iD) c_n^+ c_{n+1} - (I^+ - iD) c_n c_{n+1}^+ + I^- \left(c_n^+ c_{n+1}^+ - c_n c_{n+1} \right) \right). \tag{4}$$

Here the periodic boundary conditions are implied (the boundary term not important for further calculations when $N \to \infty$ has been omitted). Then we perform the Fourier transformation

$$c_n^+ = \frac{1}{\sqrt{N}} \sum_{\kappa} \exp(i\kappa n) c_\kappa^+, \qquad c_n = \frac{1}{\sqrt{N}} \sum_{\kappa} \exp(-i\kappa n) c_\kappa,$$
$$c_\kappa^+ = \frac{1}{\sqrt{N}} \sum_{n} \exp(-i\kappa n) c_n^+, \qquad c_\kappa = \frac{1}{\sqrt{N}} \sum_{n} \exp(i\kappa n) c_n \tag{5}$$

with $\kappa = \frac{2\pi}{N} n$ and $n = -\frac{N}{2}, -\frac{N}{2} + 1, \ldots, \frac{N}{2} - 1$ (if N is even) or $n = -\frac{N-1}{2}, -\frac{N-1}{2} + 1, \ldots, \frac{N-1}{2}$ (if N is odd) and the Bogolyubov transformation

$$\begin{pmatrix} \beta_\kappa \\ \beta_{-\kappa}^+ \end{pmatrix} = \begin{pmatrix} iu_\kappa & v_\kappa \\ v_\kappa & iu_\kappa \end{pmatrix} \begin{pmatrix} c_\kappa \\ c_{-\kappa}^+ \end{pmatrix}, \qquad u_\kappa = \mathrm{sgn}\left(I^- \sin\kappa \right) \frac{1}{\sqrt{2}} \sqrt{1 + \frac{\Omega + I^+ \cos\kappa}{\lambda_\kappa}},$$
$$v_\kappa = \frac{1}{\sqrt{2}} \sqrt{1 - \frac{\Omega + I^+ \cos\kappa}{\lambda_\kappa}}, \qquad \lambda_\kappa = \sqrt{(\Omega + I^+ \cos\kappa)^2 + (I^- \sin\kappa)^2} \tag{6}$$

to get instead of (4) the final fermionic Hamiltonian

$$H = \sum_{\kappa} \left(-\frac{\Omega}{2} + (\Omega + I^+ \cos\kappa + D \sin\kappa) c_\kappa^+ c_\kappa - i\frac{1}{2} I^- \sin\kappa \left(c_\kappa^+ c_{-\kappa}^+ + c_\kappa c_{-\kappa} \right) \right)$$
$$= {\sum_{\kappa}}' \left(\left(c_\kappa^+ \quad c_{-\kappa} \right) \begin{pmatrix} \Omega + I^+ \cos\kappa + D \sin\kappa & -iI^- \sin\kappa \\ iI^- \sin\kappa & -\Omega - I^+ \cos\kappa + D \sin\kappa \end{pmatrix} \right.$$
$$\times \left. \begin{pmatrix} c_\kappa \\ c_{-\kappa}^+ \end{pmatrix} - D \sin\kappa \right)$$
$$= {\sum_{\kappa}}' \left(\left(\beta_\kappa^+ \quad \beta_{-\kappa} \right) \begin{pmatrix} D \sin\kappa + \lambda_\kappa & 0 \\ 0 & D \sin\kappa - \lambda_\kappa \end{pmatrix} \begin{pmatrix} \beta_\kappa \\ \beta_{-\kappa}^+ \end{pmatrix} - D \sin\kappa \right)$$
$$= {\sum_{\kappa}}' \left(D \sin\kappa \left(\beta_\kappa^+ \beta_\kappa + \beta_{-\kappa} \beta_{-\kappa}^+ - 1 \right) + \lambda_\kappa \left(\beta_\kappa^+ \beta_\kappa - \beta_{-\kappa} \beta_{-\kappa}^+ \right) \right)$$
$$= \sum_{\kappa} (D \sin\kappa + \lambda_\kappa) \left(\beta_\kappa^+ \beta_\kappa - \frac{1}{2} \right) = \sum_{\kappa} \Lambda_\kappa \left(\beta_\kappa^+ \beta_\kappa - \frac{1}{2} \right). \tag{7}$$

Here the prime denotes that κ varies (when $N \to \infty$) from 0 to π and the elementary excitations energies are given by

$$\Lambda_\kappa = D \sin\kappa + \lambda_\kappa = D \sin\kappa + \sqrt{(\Omega + I^+ \cos\kappa)^2 + (I^- \sin\kappa)^2} \neq \Lambda_{-\kappa}. \tag{8}$$

It should be noted here that the Bogolyubov transformation (6) does not depend on the Dzyaloshinskii–Moriya interaction D.

3 Isotropic XY chain

The isotropic case $J^x = J^y = J$ is essentially simpler than a general anisotropic case $J^x \neq J^y$ since the Dzyaloshinskii–Moriya interaction can be eliminated from the Hamiltonian (1) by a simple spin axes rotation (see, e.g. [4]). Really, introducing new spin variables

$$\tilde{s}_n^x = s_n^x \cos \phi_n + s_n^y \sin \phi_n, \qquad \tilde{s}_n^y = -s_n^x \sin \phi_n + s_n^y \cos \phi_n, \qquad \tilde{s}_n^z = s_n^z,$$

$$\phi_n = (n-1)\varphi, \qquad \tan \varphi = \frac{D}{J} \tag{9}$$

one finds that

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

$$= \sum_{n=1}^{N} \Omega \tilde{s}_n^z + \sum_{n=1}^{N} \text{sgn}(J)\sqrt{J^2 + D^2} \left(\tilde{s}_n^x \tilde{s}_{n+1}^x + \tilde{s}_n^y \tilde{s}_{n+1}^y \right). \tag{10}$$

Obviously, the thermodynamic properties of the model with Dzyaloshinskii–Moriya interaction are the same as of the model without such interaction, but with renormalized isotropic exchange interaction $|J| \rightarrow \sqrt{J^2 + D^2}$. As a result, the Dzyaloshinskii–Moriya interaction cannot be revealed from the measurements of thermodynamic quantities. Let us pass to the dynamic quantities.

3.1 zz dynamics and two-fermion excitation continuum

The spin rotations (9) do not effect the z spin component and therefore

$$\left\langle s_n^z(t)s_{n+m}^z(0)\right\rangle\big|_{J,D} = \left\langle \tilde{s}_n^z(t)\tilde{s}_{n+m}^z(0)\right\rangle\big|_{\text{sgn}(J)\sqrt{J^2+D^2},0}. \tag{11}$$

As a result we may use the long-known results for the zz dynamics (see, e.g. [12, 13])

$$S_{zz}(\kappa,\omega)\big|_{J,D} = S_{zz}(\kappa,\omega)\big|_{\text{sgn}(J)\sqrt{J^2+D^2},0}$$

$$= \int_{-\pi}^{\pi} d\kappa_1 n_{\kappa_1} \left(1 - n_{\kappa_1-\kappa}\right) \delta\left(\omega + \Lambda_{\kappa_1} - \Lambda_{\kappa_1-\kappa}\right). \tag{12}$$

Here $\Lambda_\kappa = \Omega + \text{sgn}(J)\sqrt{J^2 + D^2}\cos \kappa$ is the elementary excitation energy and $n_\kappa = \frac{1}{1+\exp(\beta\Lambda_\kappa)}$ is the Fermi function. From Refs. [12, 13] we know that the zz dynamic structure factor (12) is governed by the two-fermion excitation continuum. The lower, middle, and upper boundaries of the continuum in the plane wavevector κ – frequency ω are given by

$$\frac{\omega_l}{\sqrt{J^2 + D^2}} = 2\sin\frac{|\kappa|}{2}\left|\sin\left(\frac{|\kappa|}{2} - \alpha\right)\right|, \tag{13}$$

$$\frac{\omega_m}{\sqrt{J^2 + D^2}} = 2\sin\frac{|\kappa|}{2}\sin\left(\frac{|\kappa|}{2} + \alpha\right), \tag{14}$$

and

$$\frac{\omega_u}{\sqrt{J^2 + D^2}} = \begin{cases} 2\sin\dfrac{|\kappa|}{2}\sin\left(\dfrac{|\kappa|}{2} + \alpha\right), & \text{if} \quad 0 \leq |\kappa| \leq \pi - 2\alpha, \\[2mm] 2\sin\dfrac{|\kappa|}{2}, & \text{if} \quad \pi - 2\alpha \leq |\kappa| \leq \pi, \end{cases} \tag{15}$$

respectively; here $\alpha = \arccos \frac{\Omega}{\sqrt{J^2+D^2}}$. The soft modes (i.e. the values of κ at which $\omega_l = 0$) occur at $|\kappa_0| = 0,\ 2\alpha$. The zz dynamic structure factor may exhibit a one-dimensional Van Hove's singularity (i.e. $S_{zz}(\kappa, \omega = \omega_s - 0) \sim \frac{1}{\sqrt{\omega_s - \omega}}$) while approaching the curve

$$\frac{\omega_s}{\sqrt{J^2 + D^2}} = 2 \sin \frac{|\kappa|}{2}. \tag{16}$$

As temperature increases, the lower boundary of the continuum smears out, i.e. $\frac{\omega_l}{\sqrt{J^2+D^2}} = 0$, and the upper boundary becomes $\frac{\omega_u}{\sqrt{J^2+D^2}} = 2 \sin \frac{|\kappa|}{2}$. To conclude, the zz dynamics in the presence of the Dzyaloshinskii–Moriya interaction remains as for the chain without such interaction but with renormalized isotropic exchange interaction $|J| \to \sqrt{J^2 + D^2}$. As a result the Dzyaloshinskii–Moriya interaction does not manifest itself in the zz dynamic quantities.

3.2   *xx* and *xy* dynamics

Let us pass to the remaining spin correlation functions. Employing equation (9) one finds

$$\left\langle s_n^x(t) s_{n+m}^x \right\rangle \Big|_{J,D} = \cos \phi_n \cos \phi_{n+m} \left\langle \tilde{s}_n^x(t) \tilde{s}_{n+m}^x \right\rangle \Big|_{\mathrm{sgn}(J)\sqrt{J^2+D^2},0}$$
$$- \cos \phi_n \sin \phi_{n+m} \left\langle \tilde{s}_n^x(t) \tilde{s}_{n+m}^y \right\rangle \Big|_{\mathrm{sgn}(J)\sqrt{J^2+D^2},0}$$
$$- \sin \phi_n \cos \phi_{n+m} \left\langle \tilde{s}_n^y(t) \tilde{s}_{n+m}^x \right\rangle \Big|_{\mathrm{sgn}(J)\sqrt{J^2+D^2},0}$$
$$+ \sin \phi_n \sin \phi_{n+m} \left\langle \tilde{s}_n^y(t) \tilde{s}_{n+m}^y \right\rangle \Big|_{\mathrm{sgn}(J)\sqrt{J^2+D^2},0} \tag{17}$$

and similar formulas for $\left\langle s_n^x(t) s_{n+m}^y \right\rangle \big|_{J,D}$, $\left\langle s_n^y(t) s_{n+m}^x \right\rangle \big|_{J,D}$ and $\left\langle s_n^y(t) s_{n+m}^y \right\rangle \big|_{J,D}$. Using further the relations $\left\langle \tilde{s}_n^x(t) \tilde{s}_{n+m}^x \right\rangle \big|_{J,0} = \left\langle \tilde{s}_n^y(t) \tilde{s}_{n+m}^y \right\rangle \big|_{J,0}$, $\left\langle \tilde{s}_n^x(t) \tilde{s}_{n+m}^y \right\rangle \big|_{J,0} = - \left\langle \tilde{s}_n^y(t) \tilde{s}_{n+m}^x \right\rangle \big|_{J,0}$ one gets

$$S_{xx}(\kappa, \omega)\big|_{J,D} = \frac{1}{2} \left(S_{xx}(\kappa + \varphi, \omega)\big|_{\mathrm{sgn}(J)\sqrt{J^2+D^2},0} + S_{xx}(\kappa - \varphi, \omega)\big|_{\mathrm{sgn}(J)\sqrt{J^2+D^2},0} \right. \tag{18}$$
$$\left. + \mathrm{i} \left(S_{xy}(\kappa + \varphi, \omega)\big|_{\mathrm{sgn}(J)\sqrt{J^2+D^2},0} - S_{xy}(\kappa - \varphi, \omega)\big|_{\mathrm{sgn}(J)\sqrt{J^2+D^2},0} \right) \right) = S_{yy}(\kappa, \omega)\big|_{J,D}\,,$$

$$S_{xy}(\kappa, \omega)\big|_{J,D} = \frac{1}{2} \left(S_{xy}(\kappa + \varphi, \omega)\big|_{\mathrm{sgn}(J)\sqrt{J^2+D^2},0} + S_{xy}(\kappa - \varphi, \omega)\big|_{\mathrm{sgn}(J)\sqrt{J^2+D^2},0} \right. \tag{19}$$
$$\left. - \mathrm{i} \left(S_{xx}(\kappa + \varphi, \omega)\big|_{\mathrm{sgn}(J)\sqrt{J^2+D^2},0} - S_{xx}(\kappa - \varphi, \omega)\big|_{\mathrm{sgn}(J)\sqrt{J^2+D^2},0} \right) \right) = - S_{yx}(\kappa, \omega)\big|_{J,D}\,.$$

We may use now the results available for the isotropic XY chain without the Dzyaloshinskii–Moriya interaction to follow the effects of the latter interaction on xx (yy) and xy (yx) dynamics. We start from the exact analytical result for zero temperature $\beta = \infty$ and strong fields $\Omega > \sqrt{J^2 + D^2}$ [17, 14]. The ground-state is completely polarized $|\mathrm{GS}_s\rangle = \prod_n | \downarrow_n \rangle$ (in spin language) or completely empty $c_\kappa |\mathrm{GS}_c\rangle = 0$ (in fermionic language). Therefore, a crucial simplification occurs

$$s_m^+ |\mathrm{GS}_s\rangle = c_m^+ |\mathrm{GS}_c\rangle = \frac{1}{\sqrt{N}} \sum_\kappa \exp\left(\mathrm{i}\kappa m\right) c_\kappa^+ |\mathrm{GS}_c\rangle\,, \qquad s_m^- |\mathrm{GS}_s\rangle = 0. \tag{20}$$

As a result

$$\left\langle s_n^x(t) s_{n+m}^x \right\rangle \Big|_{\mathrm{sgn}(J)\sqrt{J^2+D^2},0} = \frac{1}{4} \left\langle \mathrm{GS}_s | s_n^-(t) s_{n+m}^+ | \mathrm{GS}_s \right\rangle$$
$$= \frac{1}{4N} \sum_\kappa \exp\left(\mathrm{i}\kappa m - \mathrm{i}\left(\Omega + \mathrm{sgn}(J)\sqrt{J^2+D^2} \cos\kappa\right) t\right)\,, \tag{21}$$

$$\left\langle s_n^x(t) s_{n+m}^y \right\rangle \Big|_{\mathrm{sgn}(J)\sqrt{J^2+D^2},0} = \frac{1}{4\mathrm{i}} \left\langle \mathrm{GS}_s | s_n^-(t) s_{n+m}^+ | \mathrm{GS}_s \right\rangle$$
$$= -\mathrm{i} \left\langle s_n^x(t) s_{n+m}^x \right\rangle \Big|_{\mathrm{sgn}(J)\sqrt{J^2+D^2},0}\,, \tag{22}$$
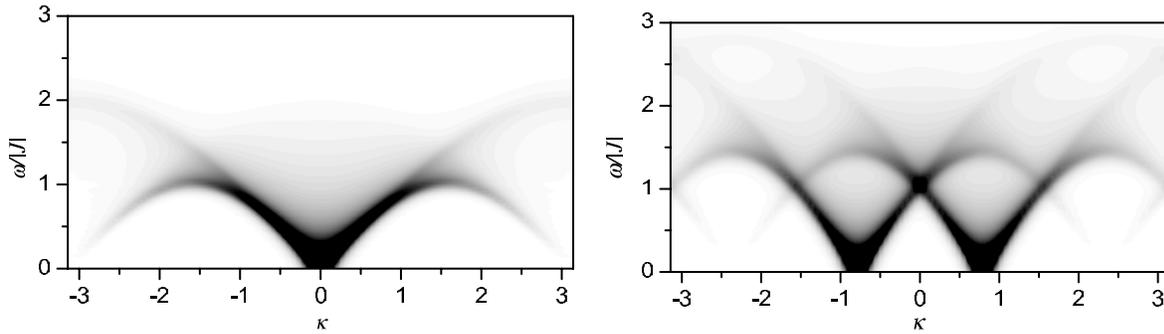
Figure 1. $S_{xx}(\kappa, \omega)$ for $\Omega = 0.001$, $J = -1$, $D = 0$ (left panel), $D = 1$ (right panel), $\beta = 20$.
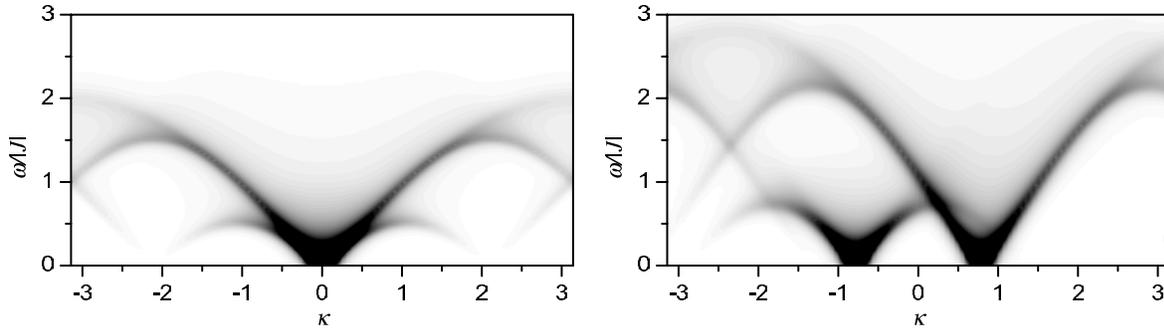

Figure 2. $S_{xx}(\kappa, \omega)$ for $\Omega = 0.5$, $J = -1$, $D = 0$ (left panel), $D = 1$ (right panel), $\beta = 20$.

and therefore

$$S_{xx}(\kappa, \omega)|_{J,D} = i\, S_{xy}(\kappa, \omega)|_{J,D} = \frac{\pi}{2}\delta\left(\omega - \Omega - \mathrm{sgn}(J)\sqrt{J^2 + D^2}\cos\left(\kappa + \varphi\right)\right). \tag{23}$$

If $\Omega < -\sqrt{J^2 + D^2}$ instead of (20) one has

$$s_m^+ |\mathrm{GS}_s\rangle = 0, \qquad s_m^- |\mathrm{GS}_s\rangle = (-1)^m\, c_m\, |\mathrm{GS}_c\rangle = \frac{1}{\sqrt{N}}\sum_\kappa \exp\left(-i\left(\kappa + \pi\right)m\right) c_\kappa\, |\mathrm{GS}_c\rangle. \tag{24}$$

As a result

$$\left\langle s_n^x(t) s_{n+m}^x \right\rangle\big|_{\mathrm{sgn}(J)\sqrt{J^2+D^2},0} = -i\left\langle s_n^x(t) s_{n+m}^y \right\rangle\big|_{\mathrm{sgn}(J)\sqrt{J^2+D^2},0} = \frac{1}{4}\left\langle \mathrm{GS}_s | s_n^+(t) s_{n+m}^- | \mathrm{GS}_s \right\rangle$$

$$= \frac{1}{4N}\sum_\kappa \exp\left(-i\left(\kappa + \pi\right)m + i\left(\Omega + \mathrm{sgn}(J)\sqrt{J^2 + D^2}\cos\kappa\right)t\right), \tag{25}$$

and therefore

$$S_{xx}(\kappa, \omega)|_{J,D} = -i\, S_{xy}(\kappa, \omega)|_{J,D} = \frac{\pi}{2}\delta\left(\omega + \Omega - \mathrm{sgn}(J)\sqrt{J^2 + D^2}\cos\left(\kappa - \varphi\right)\right). \tag{26}$$

Another exact analytical results may be obtained for infinite temperature $\beta = 0$.

Let us pass to the case of finite temperatures $0 < \beta < \infty$ (and $0 \le \Omega < \sqrt{J^2 + D^2}$). Unfortunately, in this case we can calculate the dynamic structure factors $S_{xx}(\kappa, \omega)$, $S_{xy}(\kappa, \omega)$ of the isotropic XY chain which enter (18), (19) only numerically. The xx dynamic structure factor (grey-scale plots) of the finite-size ($N = 400$) isotropic XY chain ($J = -1$) with the Dzyaloshinskii–Moriya interaction at low temperature ($\beta = 20$) for different strengths of the transverse field $\Omega = 0.001$ and $\Omega = 0.5$ can be seen in Fig. 1 and Fig. 2, respectively.

From the earlier studies for isotropic XY chains [14] we know that the xx dynamic structure factor at low temperatures is concentrated in the plane wavevector κ – frequency ω roughly along

the boundaries of the two-fermion continuum (13), (14), (15) (left panels in Figs. 1 and 2). If the Dzyaloshinskii–Moriya interaction is present it is not true any more (right panels in Figs. 1 and 2). The xx dynamic structure factor is concentrated mostly along the curves which correspond to the boundaries of two two-fermion continuum (13), (14), (15) which are shifted by $\pm\varphi$ along the wavevector axis κ and are renormalized $|J| \to \sqrt{J^2 + D^2}$ along the frequency axis ω. Thus, the correspondence between the xx and zz dynamic quantities becomes violated. From Figs. 1, 2 we can also see arising of the asymmetry in $S_{xx}(\kappa, \omega)$ with respect to the change $\kappa \to -\kappa$ owing to the Dzyaloshinskii–Moriya interaction as the transverse field deviates from zero. As Ω increases (at fixed D), a redistribution of a weight of $S_{xx}(\kappa, \omega)$ between "left" and "right" two-fermion continua takes place until the "left" one completely disappears as Ω exceeds $\sqrt{J^2 + D^2}$. (Obviously, we should change "left" to "right" and vice versa when Ω increases its value being negative.) It is important to note that the soft modes of "left" and "right" continua originating from the soft mode of the original continuum at $\kappa = 0$ occur at $\kappa = \pm\varphi$ and they are field independent; they can be used for determining of the value of the Dzyaloshinskii–Moriya interaction in the corresponding compounds. For electron-spin resonance experiments the frequency profiles of $S_{xx}(\kappa, \omega)$ at $\kappa = 0$ and $\kappa = \pi$ are relevant [18]. We see that both profiles change drastically if the Dzyaloshinskii–Moriya interaction is present. For example, the zero-frequency peak at $\kappa = 0$, which is relevant for the ferromagnetic case, moves towards higher frequency and its position is determined by the value of the Dzyaloshinskii–Moriya interaction. Similarly, the Dzyaloshinskii–Moriya interaction spectacularly changes the frequency profile at $\kappa = \pi$, which is relevant for the antiferromagnetic case. Obviously, these effects can be used for experimental determining of the value of the Dzyaloshinskii–Moriya interaction in the corresponding compounds.

4   Concluding remarks

To summarize, we have studied the xx (yy) and xy (yx) dynamic structure factors of the spin-$\frac{1}{2}$ isotropic XY chain with the Dzyaloshinskii–Moriya interaction and have demonstrated how the relation between these quantities and the zz dynamic structure factor is modified due to the Dzyaloshinskii–Moriya interaction. We have discussed how the Dzyaloshinskii–Moriya interaction may manifest itself in the dynamic experiments.

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