Dynamic structure factors of the spin-1/2 $XX$ chain with Dzyaloshinskii-Moriya interaction

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Abstract

We consider the spin-1/2 isotropic $XY$ chain in a ($z$) transverse magnetic field with the Dzyaloshinskii-Moriya interaction directed along the $z$-axis in spin space and examine the effects of the latter interaction on the $zz$, $xx$ ($yy$) and $xy$ ($yx$) dynamic structure factors. The Dzyaloshinskii-Moriya interaction does not manifest itself in the $zz$ dynamic quantities. In contrast, the $xx$ ($yy$) and $xy$ ($yx$) dynamic structure factors show dramatical changes owing to the Dzyaloshinskii-Moriya interaction. Implications of our results for electron spin resonance experiments are briefly discussed.

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1 Introductory remarks

Magnetism in low-dimensional compounds which are modeled by quantum spin systems has been a subject of intense study in recent years. Among the experimental techniques which are used to probe various characteristics of magnetic systems the dynamic experiments are very important. Due to their high sensitivity and resolution they are among the basic tools to determine the detailed magnetic interactions. However, the correct interpretation of the experimental data requires a corresponding theoretical background. Usually the theories based on mean-field approximation or classical spin picture are not sufficient to explain dynamic phenomena in low-dimensional quantum spin systems in which quantum fluctuations may be very strong (see e.g. [1–5]).

In the present work we examine rigorously the dynamic properties of a quantum spin chain with the Dzyaloshinskii-Moriya interaction. The latter interaction is often present in low-dimensional magnetic insulators. Although its value is usually small it may cause noticeable changes in different observable characteristics of magnetic systems (see e.g. [6]). In our study we restrict ourselves to the spin-1/2 isotropic $XY$ (i.e. $XX$ or $X0$) chain in a ($z$) transverse magnetic field with the Dzyaloshinskii-Moriya interaction directed along $z$-axis in spin space [7,8]. That model is equivalent to a chain of free spinless fermions. In fermionic language, the Ising component of exchange coupling (or other components of the Dzyaloshinskii-Moriya interaction as well as the external magnetic field directed along other axes.


in spin space) corresponds to interaction between spinless fermions and makes the problem much more complicated. Although the spin-1/2 XY chain can be mapped onto a free spinless fermion chain, the analysis of the dynamic characteristics of the spin model is not trivial at all. The $zz$ spin correlation function corresponds to the density-density correlation function for spinless fermions and its calculation is relatively easy [9, 10]. In contrast, the other ($xx$, $yy$, $xy$, $yx$) spin correlation functions are more complicated quantities due to the nonlocal character of the Jordan-Wigner relation between the spin raising/lowering operators and the creation/annihilation fermion operators. The explicit analytical results for them are available in the high-temperature limit [11] and in the ground state for strong fields [12]. From Refs. [13, 14] we know also the asymptotic behavior of some time-dependent spin correlation functions in particular limiting cases. On the other hand, the time-dependent spin correlation functions (and the related dynamic structure factors and dynamic susceptibilities) can be computed numerically [15–17].

In the present paper, we employ the Jordan-Wigner fermionization supplemented by further analytical and numerical calculations to perform a comprehensive analysis of the effect of the Dzyaloshinskii-Moriya interaction on the dynamic structure factors of the spin-1/2 XX chain in a transverse field. The previous studies of the effect of the Dzyaloshinskii-Moriya interaction were restricted to transverse ($zz$) dynamics [18, 19] and to the dynamics of correlations between $x$ and $y$ spin components at infinite temperature [20]. In particular, the transverse dynamic susceptibility $\chi_{zz}(\kappa, \omega)$ was found at $\kappa = 0$ [18] and $\kappa \neq 0$ [19]. We also notice that a relation between the XY chains without and with the Dzyaloshinskii-Moriya interaction on the grounds of symmetry was discussed in [21]. However, the transverse dynamics was not discussed in the context of the two-fermion excitation continuum [10]. Moreover, to our best knowledge, the effect of the Dzyaloshinskii-Moriya interaction on the $xx$, $yy$, $xy$, $yx$ dynamic structure factors away from the infinite temperature limit has never been studied before. We must note here that the dynamic properties of a more general model, the spin-1/2 antiferromagnetic XXX Heisenberg chain, with the Dzyaloshinskii-Moriya interaction were explored in Refs. [22, 23]. Thus, in Ref. [22], using symmetry arguments it is 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 Ref. [23], the spin correlation functions / dynamic susceptibilities of the chain with the Dzyaloshinskii-Moriya interaction are expressed in terms of such quantities of a $XXZ$ chain. However, the results for the latter chain are restricted to the limit of wavevectors close to $\pi$, low energies and low temperatures.

The outline of this paper is as follows. In the next section (Sec. 2) we introduce the model, define the quantities of interest and make some remarks on symmetry. Then, in the next two sections (Secs. 3 and 4) we analyze the $zz$ dynamic structure factor and the $xx$ ($yy$, $xy$, $yx$) dynamic structure factors, respectively. In Sec. 5 we discuss the effect of the Dzyaloshinskii-Moriya interaction on the electron spin resonance absorption spectrum. In the last section (Sec. 6) we briefly summarize our findings. Some preliminary results of the present paper are reported in the conference papers [24].

### 2 The model and its symmetries

The model to be studied is a one-dimensional lattice of $N \to \infty$ spins $1/2$. The Hamiltonian of the model is given by

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

where $s^{\alpha}$ are the halves of the Pauli matrices, $J$ is the $XX$ exchange interaction, $D$ is the Dzyaloshinskii-Moriya interaction, and $h$ is the transverse magnetic field. We imply in both periodic boundary condi-
tions (in analytical computations) and open boundary conditions (in numerical computations) bearing in mind that the results which pertain to the thermodynamic limit \( N \to \infty \) are insensitive to the boundary conditions imposed. We are interested in the dynamic structure factors of the model (1) which can be expressed through the time-dependent spin correlation functions as follows

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

Here \( \langle \ldots \rangle = \frac{\text{Tr}(\exp(-\beta H)\langle \ldots \rangle)}{\text{Tr}\exp(-\beta H)} \) denotes the canonical thermodynamic average and \( s_{\alpha}^{n}(t) = \exp(iHt)s_{\alpha}^{n}\exp(-iHt) \) is the Heisenberg representation of the operator \( s_{\alpha}^{n} \). Note that the diagonal components of \( S_{\alpha\beta}(\kappa, \omega) \), \( S_{\alpha\alpha}(\kappa, \omega) \), are real and nonnegative but the off-diagonal components of \( S_{\alpha\beta}(\kappa, \omega) \), \( \alpha \neq \beta \) should not necessarily be real.

First of all we note that the spin model (1) possesses a number of symmetries which permit to reduce the range of parameters and simplify studies of the properties of the model. After performing a \( \pi/2 \)-rotation of all spins about the \( z \)-axis we conclude that \( S_{xx}(\kappa, \omega) = S_{yy}(\kappa, \omega) \) and \( S_{xy}(\kappa, \omega) = -S_{yx}(\kappa, \omega) \) and therefore, the only dynamic structure factors which remain to examine are \( S_{zz}(\kappa, \omega) \) and \( S_{zz}(\kappa, \omega) \). We also note, that making use of the transformation \( \tilde{s}_{\alpha}^{n} = s_{\alpha}^{n} \), \( \tilde{s}_{\alpha}^{n} = -s_{\alpha}^{n} \), \( \tilde{s}_{\alpha}^{n} = -s_{\alpha}^{n} \) we arrive at (1) with the parameters \( J, -D, -h \) and as a result, \( S_{\alpha\alpha}(\kappa, \omega) |_{D,h} = S_{\alpha\alpha}(\kappa, \omega) |_{-D,-h} \), \( \alpha = x, y, z \) but \( S_{xy}(\kappa, \omega) |_{D,h} = -S_{yx}(\kappa, \omega) |_{-D,-h} \). A similar transformation, \( \tilde{s}_{\alpha}^{n} = (-1)^{n}s_{\alpha}^{n} \), \( \tilde{s}_{\alpha}^{n} = (-1)^{n}s_{\alpha}^{n} \), \( \tilde{s}_{\alpha}^{n} = s_{\alpha}^{n} \), yields (1) with the parameters \( -J, -D, h \); this symmetry implies that \( S_{\alpha\alpha}(\kappa, \omega) |_{-J,-D} = S_{\alpha\alpha}(\kappa, \omega) |_{J,D} \). Finally, the renumbering of sites \( j \to N-j+1 \), \( j = 1, \ldots, N \) gives again (1) with the parameters \( J, -D, h \) and hence \( S_{\alpha\beta}(\kappa, \omega) |_{D} = S_{\alpha\beta}(\kappa, \omega) |_{-D} \), \( \alpha, \beta = x, y, z \).

In our study an important role is played by a gauge transformation that eliminates the Dzyaloshinskii-Moriya interaction from the Hamiltonian (1) at the expense of renormalized \( XX \) exchange interaction (see e.g. [6, 21–23, 25, 26]). Explicitly, this spin coordinate transformation reads

\[
\tilde{s}_{\alpha}^{n} = s_{\alpha}^{n} \cos \phi_{n} + s_{\alpha}^{n} \sin \phi_{n}, \quad \tilde{s}_{\alpha}^{n} = -s_{\alpha}^{n} \sin \phi_{n} + s_{\alpha}^{n} \cos \phi_{n}, \quad \tilde{s}_{\alpha}^{n} = s_{\alpha}^{n}, \quad \phi_{n} = (n-1)\varphi, \quad \tan \varphi = \frac{D}{J}. \tag{3}
\]

With the aid of (3) we find that the Hamiltonian (1) becomes

\[
H = \sum_{n=1}^{N} \tilde{J} \left( \tilde{s}_{\alpha}^{n} \tilde{s}_{\alpha}^{n+1} + \tilde{s}_{\alpha}^{n} \tilde{s}_{\alpha}^{n+1} \right) - \sum_{n=1}^{N} h \tilde{s}_{\alpha}^{n}, \quad \tilde{J} = \text{sgn}(J) \sqrt{J^{2} + D^{2}}. \tag{4}
\]

Eq. (4) corresponds to the model without the Dzyaloshinskii-Moriya interaction, however, with the renormalized \( XX \) exchange interaction \( \tilde{J} \). In what follows we use the large body of existing knowledge about the model (1) to obtain the properties of the model with the Dzyaloshinskii-Moriya interaction (1) exploiting the transformation (3). In principle, no new calculations (in comparison with those reported in [17]) are needed. Moreover, in Sec. 3 we make use of the results for \( S_{xy}(\kappa, \omega) \) obtained in Ref. [17], the physical meaning of which were nebulous and not obvious earlier. To close this section, we note that the Dzyaloshinskii-Moriya interaction cannot be detected from measurements of the thermodynamic quantities since these quantities cannot distinguish between the models (1) and (4) related through the unitary transformation (3). However, as we shall see below, the Dzyaloshinskii-Moriya interaction can be determined from some of the dynamic quantities.

### 3: \( \text{zz} \) Dynamic structure factor

We start with the transverse dynamic structure factor. Since the spin rotations (3) do not affect the \( z \) spin component we immediately obtain the following expression for the transverse dynamic structure
factor of the spin chain (1)

\[
S_{zz}(\kappa, \omega) = \int_{-\pi}^{\pi} d\kappa \, n_{\kappa} \, (1 - n_{\kappa + \kappa}) \, \delta (\omega + \Lambda_{\kappa} - \Lambda_{\kappa + \kappa}),
\]

\[
\Lambda_{\kappa} = -h + J \cos \kappa, \quad n_{\kappa} = \frac{1}{1 + \exp (\beta \Lambda_{\kappa})}
\]

(5)

(see [10] and references therein).

As can be seen from Eq. (5), the transverse dynamics is conditioned by a continuum of two-fermion (particle-hole) excitations. The properties of the two-fermion excitation continuum were studied in detail in Refs. [10, 27]. We need these results in what follows and therefore present them here for easy reference. For later convenience we introduce the following characteristic lines in the \(\kappa-\omega\) plane

\[
\frac{\omega^{(1)}(\kappa)}{\sqrt{J^2 + D^2}} = 2 \left| \sin \frac{\kappa}{2} \sin \left( \frac{|\kappa|}{2} - \alpha \right) \right|,
\]

\[
\frac{\omega^{(2)}(\kappa)}{\sqrt{J^2 + D^2}} = 2 \left| \sin \frac{\kappa}{2} \sin \left( \frac{|\kappa|}{2} + \alpha \right) \right|,
\]

\[
\frac{\omega^{(3)}(\kappa)}{\sqrt{J^2 + D^2}} = 2 \left| \sin \frac{\kappa}{2} \right|,
\]

(6) (7) (8)

where the parameter \(\alpha = \arccos (|h|/\sqrt{J^2 + D^2})\) varies from \(\pi/2\) when \(h = 0\) to \(0\) when \(|h| = \sqrt{J^2 + D^2}\).

(We notice that the authors of Ref. [27] used another parameter \(\sigma, \pi\sigma = \pi/2 - \alpha\).)

The ground-state transverse dynamic structure factor does not vanish until \(|h| < \sqrt{J^2 + D^2}\) and may have nonzero values only within a restricted region of the \(\kappa-\omega\) plane (\(|\kappa| \leq \pi, \omega \geq 0\)) with the lower boundary \(\omega_l(\kappa) = \omega^{(1)}(\kappa)\) and the upper boundary \(\omega_u(\kappa) = \omega^{(2)}(\kappa)\) if \(0 \leq |\kappa| \leq \pi - 2\alpha\) or \(\omega_u(\kappa) = \omega^{(3)}(\kappa)\) if \(\pi - 2\alpha \leq |\kappa| \leq \pi\). As it follows from (6), the soft modes occur at \(|\kappa_0| = 0, 2\alpha\).

Moreover, the transverse dynamic structure factor exhibits a finite jump along the middle boundary \(\omega_m(\kappa) = \omega^{(2)}(\kappa), \pi - 2\alpha \leq |\kappa| \leq \pi\). Finally, \(S_{zz}(\kappa, \omega)\) diverges along the curve \(\omega_s(\kappa) = \omega^{(3)}(\kappa)\). This is the van Hove density-of-states effect in one dimension. With growing temperature the lower boundary becomes smeared out and finally disappears. The upper boundary at nonzero temperatures is given by \(\omega^{(3)}(\kappa)\) (8) and \(S_{zz}(\kappa, \omega)\) exhibits the one-dimensional van Hove singularity along this boundary. The transverse dynamic structure factor becomes field-independent in the high-temperature limit.

Clearly, the Dzyaloshinskii-Moriya interaction does not manifest itself in the transverse dynamics. Again we cannot distinguish the quantities probing transverse spin dynamics for the spin-1/2 XX chain with the Dzyaloshinskii-Moriya interaction and for the spin-1/2 XX chain without the Dzyaloshinskii-Moriya interaction but with renormalized XX exchange interaction. In the next section we show what particular dynamic characteristics can unambiguously indicate the presence of the Dzyaloshinskii-Moriya interaction.

4 \(xx\) and \(xy\) dynamic structure factors

We turn to the remaining dynamic structure factors. Exploiting the transformation (3) one finds the relations between the \(xx\) and \(xy\) dynamic structure factors (2) of the model (1) (the l.h.s. of Eqs. (9), (10)) and the \(xx\) and \(xy\) dynamic structure factors (2) of the model (4) (the r.h.s. of Eqs. (9), (10))

\[
S_{xx}(\kappa, \omega) = \frac{1}{2} \left( S_{xx}(\kappa - \varphi, \omega) |j\rangle + S_{xx}(\kappa + \varphi, \omega) |j\rangle + i (S_{xy}(\kappa - \varphi, \omega) |j\rangle - S_{xy}(\kappa + \varphi, \omega) |j\rangle) \right),
\]

(9)
Thus, in the high-temperature limit derived earlier by direct calculation [20] (see Eq. (4.8) of that paper). Since the result for the model (1), which follows by symmetry from the results for the model (4), was also derived earlier by direct calculation [20] (see Eq. (4.8) of that paper). Since the xx and xy dynamic structure factors do not depend on \( \kappa \) the Dzyaloshinskii-Moriya interaction in accordance with (9), (10) changes only the energy scale for these dynamic structure factors in the high-temperature limit \( \beta = 0 \).

Explicitly, the closed-form expressions for these quantities read

\[
S_{xx}(\kappa, \omega) = \sqrt{\frac{\pi}{4J}} \left( \exp\left(-\frac{(\omega + h)^2}{J^2}\right) + \exp\left(-\frac{(\omega - h)^2}{J^2}\right) \right) \tag{11}
\]

and

\[
iS_{xy}(\kappa, \omega) = \sqrt{\frac{\pi}{4J}} \left( \exp\left(-\frac{(\omega + h)^2}{J^2}\right) - \exp\left(-\frac{(\omega - h)^2}{J^2}\right) \right) \tag{12}
\]

Thus, in the high-temperature limit \( \beta = 0 \) the xx and xy dynamic structure factors are \( \kappa \)-independent and display a single Gaussian ridge at \( \omega = |h| \).

In the case of finite temperatures \( 0 < \beta < \infty \) we do not have analytical expressions for the dynamic structure factors \( S_{xx}(\kappa, \omega)|_j \) and \( S_{xy}(\kappa, \omega)|_j \) of the model (1) but these can be found numerically for chains of several hundreds of sites. Following the lines explained in detail in Refs. [15, 17] we perform the numerical calculations for a chain of \( N = 400 \) sites [28]. We consider the antiferromagnetic sign of the XX exchange interaction and fix the units putting \( J = 1 \). Our results refer to the low temperature \( \beta = 20 \) and they pertain to the thermodynamic limit. In Figs. 1 and 2 we show gray-scale plots for \( S_{xx}(\kappa, \omega) \) and \( iS_{xy}(\kappa, \omega) \), respectively. The reported data refer to representative sets of the Hamiltonian parameters \( D = 0, 1, h = 0.001, 0.5, 1 \). As is nicely seen in Figs. 1 and 2 the xx and xy dynamic structure factors are concentrated mostly along certain lines in the \( \kappa - \omega \) plane which are connected with the characteristic lines of the two-fermion excitation continuum [6], [7], [8]. Let us recall that in the case \( D = 0 \) and \( J < 0 \) the xx and xy dynamic structure factors are concentrated roughly along the boundaries of the two-fermion excitation continuum \( \omega_l(\kappa), \omega_m(\kappa), \omega_u(\kappa) \) [17]. In the case \( D = 0 \) and \( J > 0 \) (see the left panels in Figs. 1 and 2) the symmetry relation mentioned in Sec. 2 implies that these dynamic structure factors should be concentrated roughly along the lines \( \omega_l(\kappa') = \omega_l(\kappa \pm \pi), \omega_m(\kappa') = \omega_m(\kappa \pm \pi), \omega_u(\kappa') = \omega_u(\kappa \pm \pi) \). That is really the case as can be seen in the left panels in Figs. 1 and 2. In the presence of the Dzyaloshinskii-Moriya interaction \( D \neq 0 \) this simple correspondence is violated becoming more intricate. Namely, the two-fermion excitation continuum splits into two continua, the “left” one (with the boundaries \( \omega_l(\kappa' - \varphi), \omega_m(\kappa' - \varphi), \omega_u(\kappa' - \varphi) \)) and the “right” one (with the boundaries \( \omega_l(\kappa' + \varphi), \omega_m(\kappa' + \varphi), \omega_u(\kappa' + \varphi) \)); these continua are connected by the symmetry operations discussed in Sec. 2. The larger \( D \) is the larger is the splitting controlled by the value of \( \varphi \). At fixed \( D \neq 0 \) and \( h = 0 \) the spectral weight is equally distributed between the left and the right continua, resulting in a symmetry with respect to \( \kappa \rightarrow -\kappa \) (Figs. 11 and 22). Asymmetry with respect to \( \kappa \rightarrow -\kappa \) arises as \( h \) deviates from zero. While \( |h| \) increases from 0 to \( \sqrt{J^2 + D^2} \) the spectral weight “moves” from the left
Figure 1: $S_{xx}(\kappa, \omega)$ (gray-scale plots) for the chain with $J = 1, D = 0$ (left panels a, b, c) and $D = 1$ (right panels d, e, f), $h = 0.001$ (a, d), $h = 0.5$ (b, e), $h = 1$ (c, f) at the low temperature $\beta = 20$. We have also plotted the boundaries $\omega^{(1)}(\kappa' \pm \varphi)$, $\omega^{(2)}(\kappa' \pm \varphi)$ (dotted and short-dashed curves) and $\omega^{(3)}(\kappa' \pm \varphi)$ (dashed curves).
Figure 2: The positive (a, g, c, i, e, k) and negative (b, h, d, j, f, l) parts of $iS_{xy}(\kappa, \omega)$ (gray-scale plots) for the chain (1) with $J = 1$, $D = 0$ (left panels a, b, c, d, e, f) and $D = 1$ (right panels g, h, i, j, k, l), $h = 0.001$ (a, b, g, h), $h = 0.5$ (c, d, i, j), $h = 1$ (e, f, k, l) at the low temperature $\beta = 20$. Note that $S_{xy}(\kappa, \omega) = 0$ at $D = 0$, $h = 0$ (see panels a and b) and $iS_{xy}(\kappa, \omega)$ becomes purely negative in the high-field limit (see panels e, f). We have also plotted the boundaries $\omega(1)(\kappa' \pm \phi)$ (dotted and short-dashed curves) and $\omega(2)(\kappa' \pm \phi)$ (7) (dotted and short-dashed curves) and $\omega(3)(\kappa' \pm \phi)$ (8).
continuum to the right one and all the spectral weight becomes concentrated along the boundaries of the right continuum as $|\hbar|$ approaches $\sqrt{J^2 + D^2}$ (Figs. 1 and 2). The presence of the Dzyaloshinskii-Moriya interaction produces a number of specific changes nicely seen in the right panels in Figs. 1, 2. For example, the field-independent modes at $\pm \pi$ shift to $\pm \pi \pm \varphi$. One can also see noticeable changes in the frequency profiles for fixed value of the wavevector (say, $\kappa = 0$ or $\kappa = \pm \pi$).

Finally, we turn to the case of zero temperature $\beta \to \infty$. In this case the exact result for strong fields, $|\hbar| > \sqrt{J^2 + D^2}$ is known [12]. Since the ground state is completely polarized (i.e., completely empty/filled in fermionic language) the time-dependent spin correlation functions $\langle s_n^x(t)s_n^x \rangle_f |_j$ and $\langle s_n^y(t)s_n^y \rangle_f |_j$ can be easily calculated [12]. That yields the following results for the dynamic structure factors $\langle 2 \rangle$ of the model (1) in this limit

$$S_{xx}(\kappa, \omega) = -\text{sgn}(\hbar) i S_{xy}(\kappa, \omega) = \frac{\pi}{2} \delta \left( \omega - |\hbar| - J 2 \cos(\kappa + \text{sgn}(\hbar)\varphi) \right).$$

(13)

In accordance with Eq. 13 $\text{sgn}(i S_{xy}(\kappa, \omega)) = -\text{sgn}(\hbar)$ and $i S_{xy}(\kappa, \omega) < 0$ for positive $\hbar$ (actually for $\hbar > \sqrt{J^2 + D^2}$) (see the low-temperature data in Fig. 2, panels e, f). Further, all of the spectral weight for both dynamic quantities is concentrated along the curve

$$\frac{\omega^* (\kappa)}{\sqrt{J^2 + D^2}} = \frac{|\hbar|}{\sqrt{J^2 + D^2}} + \text{sgn}(J) \cos (\kappa + \text{sgn}(\hbar)\varphi).$$

(14)

As $|\hbar| \to \sqrt{J^2 + D^2}$ the r.h.s. of Eq. 14 transforms either into $2 \cos((\kappa + \text{sgn}(\hbar)\varphi)/2)$ if $J > 0$ (compare with the low-temperature data reported in Figs. 1 and 2) or into $2 \sin^2((\kappa + \text{sgn}(\hbar)\varphi)/2)$ if $J < 0$.

Having calculated (partly analytically and partly numerically) the $xx$ and $xy$ dynamic structure factors of the model (1), we conclude that these dynamic quantities away from the infinite temperature limit $\beta = 0$ exhibit a number of peculiar features, namely, asymmetry with respect to $\kappa \to -\kappa$ at $\hbar \neq 0$, specific structure of frequency profiles at fixed values of $\kappa$, field-independent positions of soft modes, which can be used for unambiguous determination of the Dzyaloshinskii-Moriya interaction.

5 ESR absorption spectrum in the presence of Dzyaloshinskii-Moriya interaction

Our results for the dynamic structure factors may be used to discuss the effect of the Dzyaloshinskii-Moriya interaction on the energy absorption in electron spin resonance (ESR) experiments. We notice, a similar analysis of ESR in the spin-1/2 XX chain is reported in [4]. Clearly, that kind of analysis can be extended to the case when the Dzyaloshinskii-Moriya interaction is present.

Consider an ESR experiment, in which the static magnetic field directed along the $z$ axis and the electromagnetic wave with the polarization in the $x \perp z$ direction (say, $\alpha = x$) are applied to a magnetic system which is described as a spin-1/2 XX chain with Dzyaloshinskii-Moriya interaction (ESR experiment in the standard Faraday configuration). In such an ESR experiment one measures the intensity of the radiation absorption $I(\omega)$ as a function of frequency $\omega > 0$ of the electromagnetic wave. Within the linear response theory the absorption intensity is written as

$$I(\omega) \propto \omega \Im \chi_{\alpha \alpha}(0, \omega),$$

(15)

where $\Im \chi_{\alpha \alpha}(0, \omega)$ is the imaginary part of the $(\alpha \alpha)$ diagonal component of the dynamic susceptibility

$$\chi_{\alpha \beta}(\kappa, \omega) = \sum_{m=1}^N \exp(-i\kappa m) \int_0^\infty dt \exp(i(\omega + \kappa \epsilon) t) \langle \left[ s_n^\alpha(t), s_m^\beta \right] \rangle, \quad \epsilon \to +0$$

(16)
Figure 3: The low-temperature (left column a, b, c) and the intermediate-temperature (right column d, e, f) absorption intensity $I$ \cite{15}, \cite{17} at different frequencies $\omega$ and magnetic fields $h$ for the spin-1/2 $XX$ chain with the Dzyaloshinskii-Moriya interaction. $J = 1$, $D = 0$ (a, d), $D = 0.5$ (b, e), $D = 1$ (c, f), $\beta = 5$ (left panels a, b, c), $\beta = 1$ (right panels d, e, f).

at zero wavevector $\kappa = 0$ (see e.g. \cite{3}). We notice that

$$\Im \chi_{\alpha\alpha}(0, \omega) = \frac{1 - \exp(-\beta \omega)}{2} S_{\alpha\alpha}(0, \omega),$$  \hspace{1cm} (17)$$

where $S_{\alpha\alpha}(0, \omega)$ is given by \cite{2} (see \cite{4,9}) and hence our findings for $S_{xx}(\kappa, \omega)$ are directly related to the ESR absorption $I(\omega)$ for the spin-1/2 $XX$ chain with the Dzyaloshinskii-Moriya interaction. Further we restrict ourselves to the antiferromagnetic sign of the $XX$ exchange interaction $J > 0$. In Fig. 3 we report a typical dependence of the absorption intensity $I$ \cite{15}, \cite{17} at fixed frequency $\omega$ on the applied static magnetic field $h$ (three-dimensional plots) obtained numerically for a chain of $N = 400$ sites \cite{30}. The results refer to low (left) and intermediate (right) temperatures. They demonstrate the changes in the absorption intensity as $D$ increases (from top to bottom).

We now discuss the effect of the Dzyaloshinskii-Moriya interaction on the ESR absorption intensity for the spin-1/2 $XX$ antiferromagnetic chain. We start from the strong-field limit $h > \sqrt{J^2 + D^2}$ when all interspin interactions can be regarded as perturbations. At zero temperature according to \cite{15},
we have \( I(\omega) \propto (\pi/4)\omega \delta (\omega - h - J) \). Thus, for \( h > \sqrt{J^2 + D^2} \) and \( \beta \to \infty \) the resonance is completely sharp and located exactly at \( h + J \). Remarkably, the Dzyaloshinskii-Moriya interaction drops out of the absorption intensity! The behavior of the absorption intensity in the strong-field limit for low and intermediate temperatures can be read off the left and right panels in Fig. 9 respectively. For the infinite-temperature limit \( \beta = 0 \) we have (for arbitrary fields) \( I(\omega) \propto (1/2) (\beta \omega^2 + O(\beta^2)) S_{xx}(0, \omega) \) with \( S_{xx}(0, \omega) \) given by Eq. (11) and hence \( I \) displays a Gaussian peak at \( \omega = h \).

The simple picture valid in the strong-field limit breaks down below the saturation field \( 0 < h < \sqrt{J^2 + D^2} \). In this case the interspin interactions become important and we find more complicated behaviors (see Fig. 3). In particular, in the presence of the Dzyaloshinskii-Moriya interaction the \( h \)-dependence of the absorption intensity at low temperatures in a certain frequency range may show a two-peak structure (compare Figs. 3a, 3b, 3c). This is clearly connected to the above discussed splitting of the two-fermion excitation continuum, along the characteristic lines of which the \( xx \) dynamic structure factor is mostly concentrated.

Obviously, one may perform an exhaustive analysis of the ESR absorption examining the detailed structure of the frequency/field profiles, the resonant shift, the linewidth etc. A complete theoretical description of ESR in the spin-1/2 \( XX \) chain with the Dzyaloshinskii-Moriya interaction is left for further studies. Unfortunately, we are not aware of ESR experiments on spin-1/2 \( XX \) chain materials. However, there are now several suitable magnetic materials (see e.g. [31, 32] and also [33–35]) in which the presence of the Dzyaloshinskii-Moriya interaction cannot \( a \ priori \) be excluded and hence we may expect that some features described above may be observed in future ESR experiments. We hope the present work to stimulate further theoretical and experimental studies on this subject.

6 Concluding remarks

To summarize, we have presented a comprehensive treatment of all dynamic structure factors of the spin-1/2 \( XX \) chain in a transverse field with the Dzyaloshinskii-Moriya interaction providing explicit analytical expressions and high-precision numerical data. We have shown that the \( xx \) (\( yy \)), \( xy \) (\( yx \)) dynamic quantities may be used for determining the value of the Dzyaloshinskii-Moriya interaction. We have discussed briefly the ESR absorption spectrum for the spin-1/2 \( XX \) chain with the Dzyaloshinskii-Moriya interaction.

In recent years, following the progress in material sciences the interest in quantum spin chain compounds has noticeably increased. We notice that some of those compounds are good realizations of the one-dimensional spin-1/2 \( XX \) model (e.g. \( \text{Cs}_2\text{CoCl}_4 \) has been proposed as a possible quasi-one-dimensional \( XY \)-like magnet) [31–35]. Dynamic experiments are an important tool to investigate these compounds. Neutron scattering, ESR, NMR (see e.g. the recent paper [36]) etc. yield experimental probes of the dynamic properties which have to be compared with theoretical predictions. In the present work within the frame of the simple model we follow rigorously how the Dzyaloshinskii-Moriya interaction manifests itself in the quantities accessible to experimental investigation.

As a final remark, we emphasize that the dynamics of the spin-1/2 anisotropic \( XY \) chain with the Dzyaloshinskii-Moriya interaction is much more involved [37] since the Dzyaloshinskii-Moriya interaction cannot be eliminated by a spin axes transformation. The detailed study of the effects of the Dzyaloshinskii-Moriya interaction on the dynamic quantities in the presence of anisotropy of the \( XY \) exchange interaction is in progress.
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