The effects of the symmetric and antisymmetric anisotropies on the dynamics of the spin-$\frac{1}{2}$ XY chain

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Abstract

The dynamic properties of the spin-$\frac{1}{2}$ anisotropic XY chain with the Dzyaloshinskii-Moriya (DM) interaction in a transverse field are investigated. Using the Jordan-Wigner transformation, the dynamic structure factors of the model are evaluated rigorously (partially analytically and partially numerically). The effects of the DM interaction on the frequency shapes of the dynamic structure factors are discussed.

Key words: quantum spin chains, Dzyaloshinskii-Moriya interaction, dynamic structure factors

PACS: 75.10.Jm

One-dimensional magnetic systems exhibit a variety of interesting phenomena which are the subject of intensified theoretical and experimental studies nowadays. In this paper, we study the dynamic properties of the spin-$\frac{1}{2}$ anisotropic XY chain with the Dzyaloshinskii-Moriya (DM) interaction directed along $z$-axis in spin space in a transverse (i.e. parallel to $z$-axis in spin space) magnetic field. The one-dimensional spin-$\frac{1}{2}$ XY model is related to some quasi-one-dimensional compounds (e.g. Cs$_2$CoCl$_4$ [1]). On the other hand, the DM interaction is often present in the models of many low-dimensional magnetic materials. Despite being small, this interaction is known to give rise to many spectacular features of such compounds. However, we do not intend to fit the spin model in question to some specific real systems. The merit of the considered model is exact solvability, i.e. the possibility to obtain for this model reliable conclusions avoiding different uncontrolled approximations.

To be specific, we consider $N \to \infty$ spins one-half governed by the Hamiltonian

\[
H = \sum_n \left( J^x s^x_n s^x_{n+1} + J^y s^y_n s^y_{n+1} \right) + D \left( s^x_n s^x_{n+1} - s^y_n s^y_{n+1} \right) + \sum_n \Omega s^z_n. \tag{1}
\]

This model was introduced in [2,3]. Some of its dynamic properties were examined in [4,5,6,7]. After applying the Jordan-Wigner transformation the spin system (1) can be mapped onto a system of noninteracting spinless fermions. In our calculations we impose both periodic and open boundary conditions for the spin model (1) bearing in mind that boundary conditions are irrelevant in the thermodynamic limit for bulk characteristics. The spinless fermions which represent the model (1) on a ring are governed by the Hamiltonian

\[
H = \sum_n \Lambda_\kappa \left( \beta^\dagger_n \beta_n - \frac{1}{2} \right), \quad \Lambda_\kappa = D \sin \kappa + \lambda_\kappa \tag{2}
\]

with $\lambda_\kappa = \sqrt{(\Omega + J \cos \kappa)^2 + \gamma^2 \sin^2 \kappa}$. Here $-\pi \leq \kappa < \pi$ denotes the quasimomentum which parameterizes the fermions, $J = \frac{1}{2} (J^x + J^y)$, $\gamma = \frac{1}{2} (J^x - J^y)$. From Eq. (2) one immediately concludes that the energy spectrum becomes gapless when i) $\gamma^2 \leq D^2$ and $\Omega^2 \leq J^2 + D^2 - \gamma^2$ or ii) $\gamma^2 > D^2$ and $\Omega^2 = J^2$. 

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In our calculations of the \(zz\) dynamic structure factor we follow the standard route (see, e.g., [8]) obtaining as a result

\[
S_{zz}(\kappa, \omega) = \sum_{j=1}^{3} \int_{-\pi}^{\pi} d\kappa_{1} B^{(j)} C^{(j)} \delta (\omega - E^{(j)}),
\]

(3)

where \(B^{(1)} = B^{(3)} = \frac{1}{2} (1 - f), \ B^{(2)} = \frac{1}{2} (1 + f), \ f\) is a certain function which depends on \(\kappa_{1}, \kappa, J, \gamma, \Omega\) (but not \(D\)) (see Eq. (4.3c) of [8]), \(C^{(1)} = \frac{\kappa_{1} - \kappa}{\kappa_{1} + \kappa}, \ C^{(2)} = \frac{\kappa_{1}}{\kappa_{1} + \kappa}, \ C^{(3)} = \frac{\kappa_{1}}{\kappa_{1} + \kappa}, \ n_{\kappa} = \frac{\exp(\beta \Lambda_{\kappa}) + 1}{\exp(\beta \Lambda_{\kappa}) - 1}\) is the Fermi function, \(n_{\omega} = 1 - n_{\kappa}, \ E^{(1)} = \Lambda_{\kappa} \gamma^{2} + \Lambda_{-\kappa} \gamma^{2}, \ E^{(2)} = \Lambda_{\kappa} + \Lambda_{-\kappa} \gamma^{2}, \ E^{(3)} = -\Lambda_{\kappa} + \Lambda_{-\kappa} \gamma^{2}\). In the limit of isotropic interaction \(\gamma = 0\) Eq. (3) yields the result reported earlier [7]. In the limit \(D = 0\) and \(T = 0\) Eq. (3) coincides with the expression obtained in [8]. In this case (and more generally for \(D^{2} < \gamma^{2}\)) only the two-fermion excitation continuum which corresponds to \(j = 1\) contributes in Eq. (3). In the case \(D^{2} > \gamma^{2}\) and \(T = 0\) (or \(T > 0\)) all three two-fermion excitation continua (which correspond to \(j = 1, 2, 3\)) come into play in Eq. (3). The properties of the two-fermion excitations which govern \(zz\) dynamics of the model (1) with \(D = 0\) were elaborated in [9,8]. The DM interaction essentially affects the two-fermion excitation continua; we will postpone a complete analysis of this issue to a later paper.

In our calculation of the \(xx\) and \(yy\) dynamic structure factors we follow the route described in [10]. Considering a chain of \(N = 400\) sites we first compute the time dependent correlation functions \(\langle s_{j}^{\sigma}(t) s_{j+n}^{\sigma}\rangle\) and then perform the Fourier transformations with respect to the time and space variables. To be sure that our results pertain to the thermodynamic limit we assess the finite-size effects performing many simulations similar to the ones described in [10].

We demonstrate the effects of the (weak) DM interaction on the dynamics of (weakly) anisotropic \(XY\) chain at low temperatures plotting in Fig. 1 the dependences \(S_{xx}(\kappa, \omega)\) vs. \(\omega\) at \(\kappa = 0\) and \(\kappa = \pi\). \(S_{xx}(\kappa, \omega)\) may have nonzero values only within a restricted frequency range in correspondence with the two-fermion excitation continua boundaries; moreover, it may diverge owing to the divergent density of two-fermion states (panels e, f). \(S_{xy}(\kappa, \omega)\) and \(S_{yy}(\kappa, \omega)\) are not restricted to the two-fermion excitations and involve excitations of many fermions. However, similarly to the cases \(\gamma = D = 0\) [10] and \(\gamma = 0, D \neq 0\) [7] their values are rather small outside the two-fermion excitation continua and are concentrated mainly along several washed-out excitation branches (sharp peaks in panels a - d). Our results may be of interest for interpreting of the data measured by neutron scattering or ESR techniques. Thus, the ESR absorption spectrum in Faraday configuration is related to \(S_{xx}(\kappa, \omega)\),

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig1}
\caption{The frequency profiles of \(xx\) (a,b), \(yy\) (c,d) and \(zz\) (e,f) dynamic structure factors at \(\kappa = 0\) (solid lines) and \(\kappa = \pi\) (dashed lines) for the spin chain (1) with \(J = 1, \gamma = 0.1, D = 0\) (thin lines), \(D = 0.2\) (bold lines), \(\Omega = 0\) (a,c,e), \(\Omega = 0.5\) (b,d,f) at low temperature \(\beta = 50\).}
\end{figure}

\begin{table}[h]
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\begin{tabular}{|c|c|}
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\(S_{yy}(\kappa, \omega)\) & [11]. The presented in Fig. 1 frequency shapes clearly demonstrate that the DM interaction can change dramatically the dynamic quantities observed experimentally on materials modeled by the spin-\(\frac{1}{2}\) \(XY\) chain.

T. V. acknowledges the kind hospitality of the University of Bayreuth in the spring and autumn of 2004. The paper was presented partially at the International Workshop on Collective quantum states in low-dimensional transition metal oxides (Dresden, February 22-25, 2005). O. D. thanks the MPIPKS, Dresden for the hospitality.

\begin{thebibliography}{99}
\bibitem{1} M. Kenzelmann et al., Phys. Rev. B 65 (2002) 144432.
\bibitem{2} V. M. Kontorovich and V. M. Tsukernik, ZhETF 52 (1967) 1446 (in Russian).
\bibitem{3} Th. J. Siskens et al., Physica A 79 (1975) 259.
\bibitem{4} Th. J. Siskens and H. W. Capel, Physica A 79 (1975) 296.
\bibitem{5} J. H. H. Perk and H. W. Capel, Physica A 92 (1978) 163.
\bibitem{6} O. Derzhko and A. Moina, Ferroelectrics 153 (1994) 49; Condens. Matter Phys. (L’viv) 3 (1994) 3.
\bibitem{7} O. Derzhko and T. Verkholyak, Czech. J. Phys. 54 (2004) 1535-361 (2005) 1403.
\bibitem{8} J. H. Taylor and G. Müller, Physica A 130 (1985) 1.
\bibitem{9} G. Müller et al., Phys. Rev. B 24 (1981) 1429.
\bibitem{10} O. Derzhko and T. Krokhmalskii, phys. stat. sol. (b) 208 (1998) 221; O. Derzhko, T. Krokhmalskii and J. Stolze, J. Phys. A 33 (2000) 3063; J. Phys. A 35 (2002) 3573.
\bibitem{11} Y. Maeda and M. Oshikawa, Phys. Rev. B 67 (2003) 224424.
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