Dynamic properties of quantum spin chains: Simple route to complex behavior

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We examine dynamic structure factors of spin-1/2 chains with nearest-neighbor interactions of *XX* and Dzyaloshinskii-Moriya type and with periodic and random changes in the sign of these interactions. This special kind of inhomogeneity can be eliminated from the Hamiltonian by suitable transformation of the spin variables. As a result, the dynamic structure factors of periodic or random chains can be computed from those of the uniform chains. Using the exact analytical and precise numerical results available for the uniform systems, we illustrate the effects of regular alternation or random disorder on dynamic structure factors of quantum spin chains.

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I. INTRODUCTION: JORDAN-WIGNER FERMIONS AND DYNAMIC QUANTITIES

Quantum spin chains have received much attention for more than 70 years for several reasons. First, they provide an excellent ground for studying rigorously quantum many-particle phenomena. Second, owing to the tremendous progress in material sciences (as well as the recent availability of optical lattices for trapping atoms in artificial crystals), many real-life systems, which can be modeled as quantum spin chains invented by theoreticians, have become available. This opens the possibility to compare the results of accurate theoretical calculations with experimental data. Dynamic quantities for quantum spin chains are of special interest and importance. On the one hand, their study, as a rule, is a harder problem in comparison with similar studies of static quantities. On the other hand, dynamic quantities are related to experimental data obtained in scattering and resonance experiments, which yield valuable information about the magnetic structure of materials provided that one has a reliable theory for their interpretation. Therefore, the theoretical analysis of the dynamic quantities for quantum spin chains is significant both from theoretical and/or academic and experimental and/or practical points of view.

Since the early 1930s, the Bethe ansatz has been known as a powerful method of exploring quantum spin chains. However, only recently it has become possible to calculate quantities such as norms of and matrix elements between Bethe ansatz states, which are necessary to calculate dynamic quantities. For recent Bethe ansatz results on the ground-state dynamic structure factors of the spin-1/2 *XXZ* Heisenberg chain, see Refs. 1–3. We also mention here the field-theoretical approaches for the evaluation of the dynamic quantities,[4] which, however, are restricted to low-energy physics only and therefore can only give the dynamic quantities in a small part of the plane wave vector κ–frequency ω (hereinafter the κ-ω plane). Traditionally, those calculations were performed for the Tomonaga-Luttinger model, which describes one-dimensional spinless fermions moving in a continuum, with linear dispersion relation. Recently, however, the curvature of the dispersion relation has been taken into account in calculating the properties of quantum wires.[5] The spin-1/2 *XXZ* chain is a lattice system closely related to these continuum models. The low-energy and long-wavelength limit of its ground-state *zz* dynamic structure factor was recently studied by combining several analytic and numeric techniques.[6] Recently,[7] an extension of the density-matrix renormalization group method was proposed, which allows for the calculation of real-time correlation functions of *XXZ* chains at arbitrary finite temperatures in the thermodynamic limit. However, numerical limitations presently restrict the time range over which results are reliable to values comparable to those reached in complete diagonalization studies.[8]

Another exactly solvable class of quantum spin chains are spin-1/2 *XY* chains. Rigorous analysis of these systems is based on exploiting the Jordan-Wigner transformation to spinless fermions.[9] [For a relation between the Bethe ansatz method and the Jordan-Wigner approach for the spin-1/2 *XX*0 (i.e., isotropic *XY*) chain, see Ref. 10.] Although after applying the Jordan-Wigner transformation to the spin-1/2 *XY* chains one faces a system of noninteracting spinless fermions, the calculation of the spin correlation functions is not a trivial problem because of the nonlocal character of the transformation. Thus, the *zz* spin correlations are related to the two-fermion (density-density) correlations, whereas, e.g., the *xx* spin correlations are related to many-fermion correlations. Accordingly, the *zz* dynamics is well studied,[11,12] whereas closed-form expressions, e.g., for the *xx* dynamic quantities, are rather scarce[13–15] (see also references in Ref. 16).

In the present paper, we consider several quantum spin chains with regular alternation or random disorder in the nearest-neighbor interactions and follow the effect of such modifications on the dynamic structure factors. The inhomogeneity introduced refers mainly to the sign of interactions and may mimic the ferromagnetic or antiferromagnetic types of nearest-neighbor exchange coupling. The interest in models of such a kind is not purely theoretical. Recently, some organic and inorganic magnets have been recognized as alternating-sign,[17] random-bond,[18] and alternating random-bond[19–21] antiferromagnetic spin chains. The dynamic study of the quantum spin chain material with bond randomness $BaCu_2(Si_{1-x}Ge_x)_2O_2$, $x=0.5$, using inelastic neutron scattering revealed that its dynamic structure factor can

be fitted by the Müller ansatz[12] surprisingly well.[18] The correspondence between the dynamic properties of the random-bond Heisenberg antiferromagnetic spin chain and the $BaCu_2(Si_{1-x}Ge_x)_2O_7$ compound has been confirmed numerically by the quantum Monte Carlo method.[22]

In our calculation of dynamic quantities, we use appropriate transformations to eliminate the inhomogeneity from the spin Hamiltonian arriving at the homogeneous model, the dynamic properties of which are well known. Thus, we reduce the complex behavior of dynamic quantities for periodic or random quantum spin chains to the known dynamic properties of the homogeneous model. In what follows, we deal with spin-1/2 isotropic *XY* (*XX* or *XX*0) chains since the dynamic quantities for the more general case of the *XXZ* Heisenberg exchange interaction are less known.

The paper is organized as follows. To the end of this section, we introduce the spin model and the quantities of interest and recall some results for the dynamic quantities obtained within the Jordan-Wigner fermionization approach, which are used in the following sections. In Sec. II, we consider the spin-1/2 *XX* chain with regularly alternating or random sign of the *XX* exchange interaction. In Sec. III, we consider the spin-1/2 *XX* chain with the Dzyaloshinskii-Moriya interaction, the sign of which may either vary regularly along the chain (or it has a regularly varying component in addition to a constant component) or may acquire its sign randomly. We summarize our findings in Sec. IV.

We consider the following Hamiltonian of a one-dimensional spin $s=1/2$ *XX* model with two-site interactions, which can be examined rigorously within the framework of the Jordan-Wigner approach,[9]

$$H=\sum_n [J_n(s_n^x s_{n+1}^x + s_n^y s_{n+1}^y) + D_n(s_n^x s_{n+1}^y - s_n^y s_{n+1}^x) + \Omega s_n^z]. \tag{1.1}$$

Here, J_n is the exchange *XX* interaction between neighboring sites n and $n+1$, D_n is the z component of the Dzyaloshinskii-Moriya interaction between these sites, and Ω is the external transverse (z) magnetic field. The sum in Eq. (1.1) runs over all N sites; the boundary conditions (periodic or open) are not essential for the quantities considered below which we calculate in the thermodynamic limit $N\to\infty$.

We are interested in the dynamic structure factors of the spin model [Eq. (1.1)] (defined most conveniently for periodic boundary conditions, so that $m=N$ is equivalent to $m=0$),

$$S_{\alpha\beta}(\kappa,\omega)=\frac{1}{N}\sum_{j=1}^{N}\sum_{m=1}^{N}\exp(-i\kappa m)\int_{-\infty}^{\infty}dt\exp(i\omega t)(\langle s_j^\alpha(t)s_{j+m}^\beta\rangle - \langle s_j^\alpha\rangle\langle s_{j+m}^\beta\rangle), \tag{1.2}$$

where $\alpha,\beta=x,y,z$. These experimentally accessible quantities contain important information about the spin model [Eq. (1.1)]. By symmetry arguments, $S_{xx}(\kappa,\omega)=S_{yy}(\kappa,\omega)$, $S_{xy}(\kappa,\omega)=-S_{yx}(-\kappa,\omega)$. Therefore, in what follows, we may focus only on $S_{xx}(\kappa,\omega)$, $S_{xy}(\kappa,\omega)$, and $S_{zz}(\kappa,\omega)$. Moreover, the model [Eq. (1.1)] implies that $\langle s_n^x\rangle=\langle s_n^y\rangle=0$ and hence the second term in the parentheses in Eq. (1.2) may be omitted if $\alpha,\beta=x,y$.

Consider first a uniform chain [Eq. (1.1)] with $J_n=J$, $D_n=0$. Again, by symmetry arguments, $S_{zz}(\kappa,\omega)$ is insensitive to a sign change of the exchange interaction $J\to -J$, whereas $S_{xx}(\kappa,\omega)\to S_{xx}(\kappa\mp\pi,\omega)$, $S_{xy}(\kappa,\omega)\to S_{xy}(\kappa\mp\pi,\omega)$. Next, from Refs. 11 and 12, we know that

$$S_{zz}(\kappa,\omega)=\int_{-\pi}^{\pi}d\kappa_1 n_{\kappa_1}(1-n_{\kappa+\kappa_1})\delta(\omega+\Lambda_{\kappa_1}-\Lambda_{\kappa+\kappa_1}), \tag{1.3}$$

where $\Lambda_\kappa=\Omega+J\cos\kappa$ is the elementary excitation energy of the Jordan-Wigner fermions and $n_\kappa=1/[1+\exp(\beta\Lambda_\kappa)]$ is the Fermi function. Obviously, the zz dynamic structure factor [Eq. (1.3)] is governed by a continuum of two-fermion (particle-hole) excitations.[12] Let us introduce the following characteristic lines in the κ-ω plane:

$$\frac{\omega^{(1)}(\kappa)}{|J|}=2\left|\sin\frac{\kappa}{2}\sin\left(\frac{|\kappa|}{2}-\alpha\right)\right|,$$

$$\frac{\omega^{(2)}(\kappa)}{|J|}=2\left|\sin\frac{\kappa}{2}\sin\left(\frac{|\kappa|}{2}+\alpha\right)\right|,$$

$$\frac{\omega^{(3)}(\kappa)}{|J|}=2\left|\sin\frac{\kappa}{2}\right|, \tag{1.4}$$

where $\alpha=\arccos(|\Omega|/|J|)$ varies from $\pi/2$ (when $\Omega=0$) to 0 (when $|\Omega|=|J|$). The ground-state $S_{zz}(\kappa,\omega)$ is nonzero for $|\Omega|<|J|$ and in a restricted region in the κ-ω plane (we assume $|\kappa|\leqslant\pi$, $\omega\geqslant 0$) with the lower boundary $\omega_l(\kappa)=\omega^{(1)}(\kappa)$ and the upper boundary $\omega_u(\kappa)=\omega^{(2)}(\kappa)$ if $0\leqslant|\kappa|\leqslant\pi-2\alpha$ or $\omega_u(\kappa)=\omega^{(3)}(\kappa)$ if $\pi-2\alpha\leqslant|\kappa|\leqslant\pi$. Moreover, $S_{zz}(\kappa,\omega)$ exhibits a finite jump (increasing its value by 2) along the middle boundary $\omega_m(\kappa)=\omega^{(2)}(\kappa)$, $\pi-2\alpha\leqslant|\kappa|\leqslant\pi$. Finally, $S_{zz}(\kappa,\omega)$ shows a van Hove singularity along the curve $\omega_s(\kappa)=\omega^{(3)}(\kappa)$. As temperature increases, the lower boundary becomes smeared out and finally disappears. The upper boundary is given by $\omega^{(3)}(\kappa)$ and $S_{zz}(\kappa,\omega)$ becomes field independent in the high-temperature limit.

The xx/xy dynamic structure factor is governed by many-fermion excitations and therefore is a much more complicated quantity [the two-fermion contribution to $S_{xx}(\kappa,\omega)$ was discussed in Refs. 23 and 24]. However, the ground-state $S_{xx}(\kappa,\omega)$ and $S_{xy}(\kappa,\omega)$ can be easily calculated for strong fields $|\Omega|>|J|$,[15]

$$S_{xx}(\kappa,\omega)=i\,\mathrm{sgn}(\Omega)S_{xy}(\kappa,\omega)=\frac{\pi}{2}\delta(\omega-|\Omega|-J\cos\kappa). \tag{1.5}$$

Equation (1.5) shows that all the spectral weight in this case is concentrated along the curve

$$\frac{\omega^{\star}(\kappa)}{|J|} = \frac{|\Omega|}{|J|} + \mathrm{sgn}(J)\cos\kappa. \tag{1.6}$$

At sufficiently low temperatures ($k_{\mathrm{B}}T/|J|=0.01,\ldots,0.05$), we know from numerics (see Ref. 16) that although $S_{xx}(\kappa,\omega)$ and $S_{xy}(\kappa,\omega)$ are not *a priori* restricted to a certain region in the κ-ω plane (and indeed these quantities have nonzero values throughout the κ-ω plane), nevertheless, their values are rather small outside the two-fermion excitation continuum discussed above. More precisely, the *xx* and *xy* dynamic structure factors show washed-out excitation branches roughly following the boundaries of the two-fermion excitation continuum [see Eq. (1.4)] for $J<0$ or following these boundaries shifted along the κ axis by π for $J>0$. In the high-temperature limit, we have[13,14]

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

$$iS_{xy}(\kappa,\omega) = \frac{\sqrt{\pi}}{4|J|}\left\{\exp\left[-\frac{(\omega-\Omega)^2}{J^2}\right] - \exp\left[-\frac{(\omega+\Omega)^2}{J^2}\right]\right\}, \tag{1.7}$$

i.e., the *xx* and *xy* dynamic structure factors in this case are κ independent and display Gaussian ridges at $\omega=\pm\Omega$.

Similar results on the dynamic properties of the dimerized spin-1/2 *XX* chain (i.e., with $J_n=J[1-(-1)^n\delta]$, where $0<\delta<1$ is the dimerization parameter, and $D_n=0$ in Eq. (1.1)) can be found in Ref. 25 (and references therein). The dynamic properties of the uniform spin-1/2 *XX* chain with the Dzyaloshinskii-Moriya interaction [i.e., with $J_n=J$, $D_n=D$ in Eq. (1.1)] were discussed in Ref. 26.

In what follows (Secs. II and III), we use the results recalled here to examine the dynamic properties of quantum spin chains with special types of periodically varying or randomly distributed interspin interactions.

II. SPIN-1/2 *XX* CHAIN WITH PERIODICITY AND/ OR RANDOMNESS IN THE SIGN OF EXCHANGE INTERACTION

In this section, we consider the spin model with the Hamiltonian [Eq. (1.1)] assuming $J_n=\lambda_n J$ with $\lambda_n=\pm1$ and $D_n=0$, i.e., the exchange interaction between the sites n and $n+1$ may be either antiferromagnetic if $\lambda_n J>0$ or ferromagnetic if $\lambda_n J<0$ depending on the given sequence $\{\lambda_1,\ldots,\lambda_N\}$. Let us perform a gauge transformation,

$$s_n^x \to \tilde{s}_n^x = \lambda_1\lambda_2\ldots\lambda_{n-1}s_n^x,$$

$$s_n^y \to \tilde{s}_n^y = \lambda_1\lambda_2\ldots\lambda_{n-1}s_n^y,$$

$$s_n^z \to \tilde{s}_n^z = s_n^z, \tag{2.1}$$

after which the Hamiltonian H transforms into the Hamiltonian $\tilde{H}$ of the homogeneous model with exchange constant $J_n\equiv J$ (up to an inessential boundary term). [We denote the quantities related to the transformed (homogeneous) model by a tilde.] Obviously, according to Eq. (2.1), the *zz* dynamic structure factor (as well as all thermodynamic quantities) does not feel an inhomogeneous sequence of signs $\{\lambda_1,\ldots,\lambda_N\}$. In contrast, the *xx* and *xy* dynamic structure factors do depend on $\{\lambda_1,\ldots,\lambda_N\}$. Below, we consider separately the cases of periodic sequences and of random sequences of signs.

A. Periodic case

We begin with the case of period $p=2$, i.e., $\{\lambda_n\}=\{1,-1,1,-1,\ldots\}$. After performing the transformation [Eq. (2.1)], we have $\tilde{s}_{2j-1}^{\alpha}=(-1)^{j+1}s_{2j-1}^{\alpha}$, $\tilde{s}_{2j}^{\alpha}=(-1)^{j+1}s_{2j}^{\alpha}$, $j=1,2,\ldots$ (here and to the end of the paper, $\alpha,\beta=x,y$) and therefore according to Eq. (1.2), we can write

$$S_{\alpha\beta}(\kappa,\omega) = \frac{1}{2}\sum_{m=1}^{N}\exp(-i\kappa m)\int_{-\infty}^{\infty}dt\,\exp(i\omega t)a_m\langle\tilde{s}_1^{\alpha}(t)\tilde{s}_{1+m}^{\beta}\rangle + \frac{1}{2}\sum_{m=1}^{N}\exp(-i\kappa m)\int_{-\infty}^{\infty}dt\,\exp(i\omega t)b_m\langle\tilde{s}_2^{\alpha}(t)\tilde{s}_{2+m}^{\beta}\rangle, \tag{2.2}$$

where $\{a_1,a_2,a_3,\ldots\}=\{1,-1,-1,1,1,-1,-1,\ldots\}$, $\{b_1,b_2,b_3,\ldots\}=\{-1,-1,1,1,-1,-1,1,\ldots\}$. Noting that $a_m=[(1-i)/2]\exp(i\pi m/2)+[(1+i)/2]\exp(3i\pi m/2)$ and $b_m=a_{m+1}$, we immediately find from Eq. (2.2) that

$$S_{\alpha\beta}(\kappa,\omega) = \frac{1}{2}\tilde{S}_{\alpha\beta}\left(\kappa+\frac{\pi}{2},\omega\right) + \frac{1}{2}\tilde{S}_{\alpha\beta}\left(\kappa+\frac{3\pi}{2},\omega\right). \tag{2.3}$$

On the left-hand side in Eq. (2.3), we have the dynamic structure factors for the periodic chain $S_{\alpha\beta}(\kappa,\omega)$, whereas on the right-hand side (rhs) in Eq. (2.3), the dynamic structure factors $\tilde{S}_{\alpha\beta}(\kappa,\omega)$ refer to the uniform chain with the exchange constant J; the latter quantities were discussed in Sec. I. These calculations can be easily extended for periodic chains of larger periods. For example, for $p=3$ with $\{\lambda_n\}=\{1,1,-1,1,1,-1,\ldots\}$ after performing similar calculations, we arrive instead of Eq. (2.3) at

$$S_{\alpha\beta}(\kappa,\omega) = \frac{4}{9}\tilde{S}_{\alpha\beta}\left(\kappa+\frac{\pi}{3},\omega\right) + \frac{1}{9}\tilde{S}_{\alpha\beta}(\kappa+\pi,\omega) + \frac{4}{9}\tilde{S}_{\alpha\beta}\left(\kappa+\frac{5\pi}{3},\omega\right). \tag{2.4}$$

To illustrate the effect of a regularly alternating sign of exchange interaction on $S_{xx}(\kappa,\omega)$, we display this quantity calculated according to Eqs. (2.3) and (2.4) in Fig. 1. Evidently, in the high-temperature limit owing to the κ independence of $S_{xx}(\kappa,\omega)$ [see Eq. (1.7)], regular alternation of the exchange interaction signs does not manifest itself in the *xx* dynamic structure factor. However, at low temperatures, it may lead to rather intricate frequency and/or wave-vector patterns (see Fig. 1). Interestingly, we may reproduce the sequence $\{\lambda_n\}$ knowing the number of soft modes κ_0 and their position. In the limit $T=0$ and $|\Omega|>|J|$, we may insert

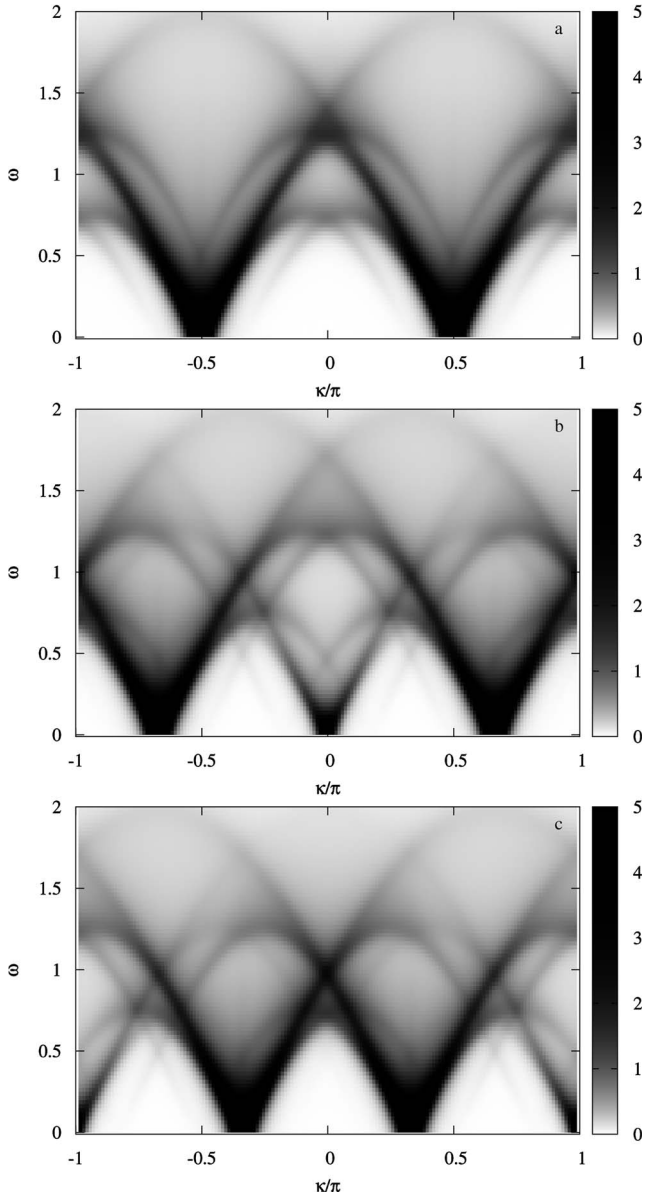

FIG. 1. $S_{xx}(\kappa,\omega)$ for the spin-1/2 *XX* chain with periodic sequences of exchange interactions (a) $\{J,-J,J,-J,\ldots\}$, $J=1$, and $\{J,J,-J,J,J,-J,\ldots\}$ with (b) $J=1$ and with (c) $J=-1$ for $\Omega=0.25$ at low temperature, $\beta=20$.

Eq. (1.5) into the rhs of Eqs. (2.3) and (2.4) to find that the spectral weight is concentrated along the curves which follow from Eq. (1.6) after corresponding shifts along the κ axis.

The results of this subsection are complementary to the earlier results on thermodynamic and dynamic properties of periodic spin-1/2 *XX* chains (see Refs. [27–29] and references therein).

B. Random case

We now proceed with the case of randomly distributed signs of exchange interactions assuming $\{\lambda_n\}$ to be a sequence of independent random variables each with the following bimodal probability distribution:

$$p(\lambda_n) = p\,\delta(\lambda_n+1) + (1-p)\,\delta(\lambda_n-1), \tag{2.5}$$

where $0\leqslant p\leqslant 1$. We are interested in random-averaged quantities and denote the average over all realizations of randomness as $\overline{(\cdots)}=\Pi_n\int_{-\infty}^{\infty}d\lambda_n p(\lambda_n)(\cdots)$. Random chains of that type (in fact, for more general *XXZ* coupling) were studied in Refs. 30 and 31.

Exploiting the gauge transformation [Eq. (2.1)] and Eq. (2.5), we find

$$\overline{\langle s_j^\alpha(t)s_{j+m}^\beta\rangle} = (1-2p)^{|m|}\langle\tilde{s}_j^\alpha(t)\tilde{s}_{j+m}^\beta\rangle. \tag{2.6}$$

Introducing the correlation length $\xi=-1/\ln|1-2p|$, the last expression [Eq. (2.6)] can be rewritten as

$$\overline{\langle s_j^\alpha(t)s_{j+m}^\beta\rangle} = \begin{cases} \exp\left(-\dfrac{|m|}{\xi}\right)\langle\tilde{s}_j^\alpha(t)\tilde{s}_{j+m}^\beta\rangle, & 0\leqslant p\leqslant\frac{1}{2} \\ (-1)^m\exp\left(-\dfrac{|m|}{\xi}\right)\langle\tilde{s}_j^\alpha(t)\tilde{s}_{j+m}^\beta\rangle, & \frac{1}{2}\leqslant p\leqslant 1. \end{cases} \tag{2.7}$$

As a result, the random-averaged dynamic structure factors [Eq. (1.2)] can be written as follows:

$$\overline{S_{\alpha\beta}(\kappa,\omega)} = \sum_{m=0,\pm1,\pm2,\ldots}\exp\left(-i\kappa m-\frac{|m|}{\xi}\right)\int_{-\infty}^{\infty}dt\exp(i\omega t) \times\langle\tilde{s}_j^\alpha(t)\tilde{s}_{j+m}^\beta\rangle. \tag{2.8}$$

Here, $0\leqslant p\leqslant 1/2$. If $1/2\leqslant p\leqslant 1$, a factor $(-1)^m$ [see Eq. (2.7)] should be taken into account in Eq. (2.8) and the resulting expression $\overline{S_{\alpha\beta}(\kappa,\omega)}$ for $1/2\leqslant p\leqslant 1$ corresponds to $\overline{S_{\alpha\beta}(\kappa\mp\pi,\omega)}$ in formula (2.8). We use Eq. (2.8) to compute $\overline{S_{\alpha\beta}(\kappa,\omega)}$ through the known results for $\langle\tilde{s}_j^\alpha(t)\tilde{s}_{j+m}^\beta\rangle$ for the uniform chain with exchange constant J obtained analytically or numerically[16,32] (see Fig. 2).

Let us consider the case $T=0$, $|\Omega|>|J|$ when the *xx* dynamic structure factor $\tilde{S}_{xx}(\kappa,\omega)$ is given by Eq. (1.5). In the site representation, we have

$$\begin{aligned}\tilde{S}_{xx}(m,\omega) &= \int_{-\infty}^{\infty}dt\exp(i\omega t)\langle\tilde{s}_j^x(t)\tilde{s}_{j+m}^x\rangle \\ &= \frac{1}{N}\sum_\kappa\exp(i\kappa m)\tilde{S}_{xx}(\kappa,\omega) \\ &= \frac{1}{4}\int_{-\pi}^{\pi}d\kappa\exp(i\kappa m)\,\delta(\omega-|\Omega|-J\cos\kappa) \\ &= \frac{\cos(m\kappa_0)}{2|J\sin\kappa_0|}\,\theta(\omega-|\Omega|+|J|)\,\theta(|\Omega|+|J|-\omega),\end{aligned} \tag{2.9}$$

where $\kappa_0=\arccos[(\omega-|\Omega|)/J]$. [In Eqs. (2.9)–(2.11), the θ functions simply indicate the frequency range within which the equation $\omega-|\Omega|-J\cos\kappa=0$ has the solutions $\kappa=\pm\kappa_0$.] Consider first the case $0\leqslant p\leqslant 1/2$. After substitution of Eq. (2.9) into Eq. (2.8) and some simple calculations, one finds

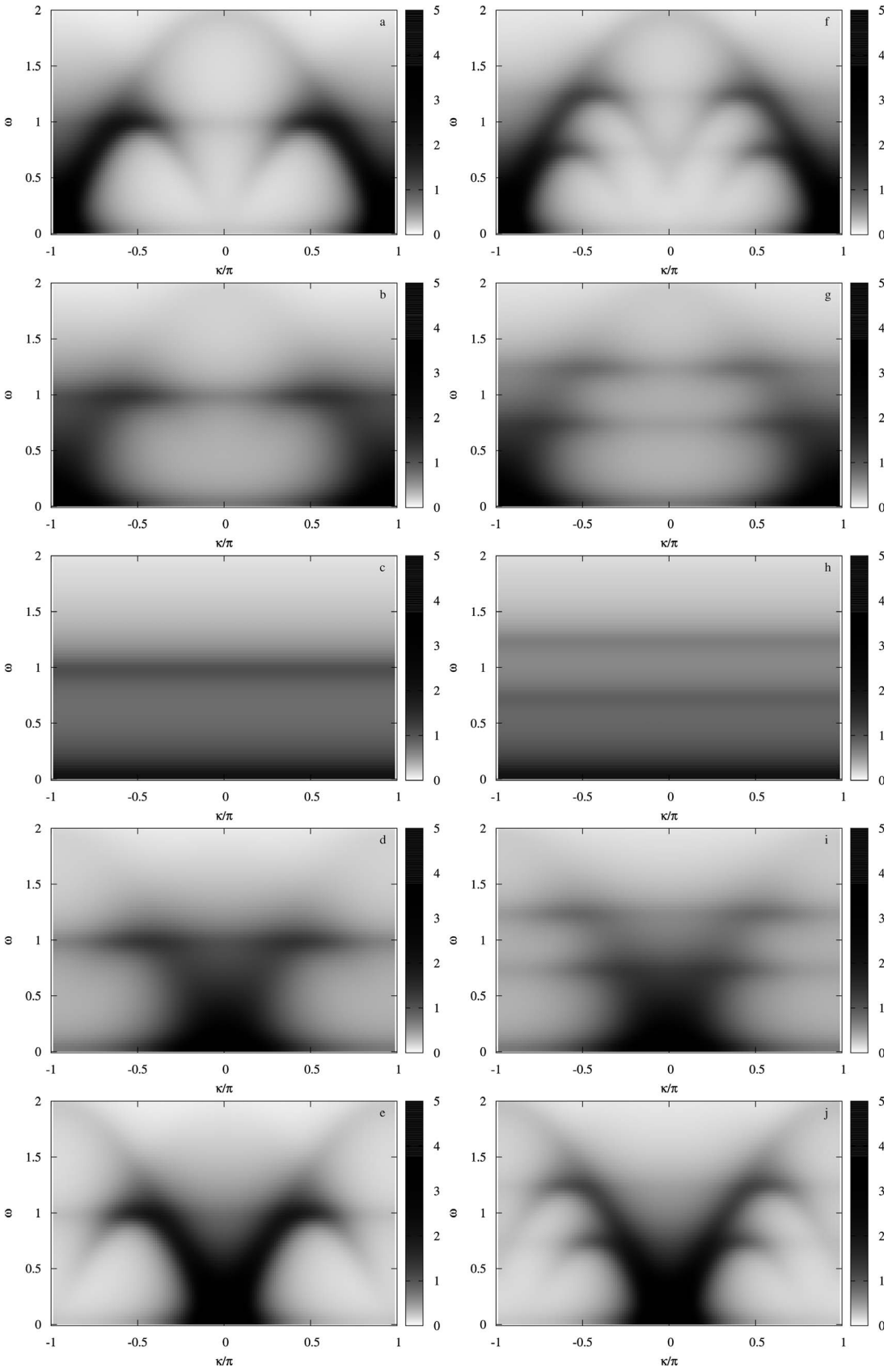

FIG. 2. $\overline{S_{xx}(\kappa,\omega)}$ for the spin-1/2 XX chain with random-sign exchange interaction $J=1$, [(a)–(e)] $\Omega=0.01$, and [(f)–(j)] $\Omega=0.25$, $\beta=20$. The values of p in Eq. (2.5) are as follows: from top to bottom $p=0.1$ ($\xi\approx 4.48$), $p=0.25$ ($\xi\approx 1.44$), $p=0.5$ ($\xi=0$), $p=0.75$ ($\xi\approx 1.44$), and $p=0.9$ ($\xi\approx 4.48$).

$$\overline{S_{xx}(\kappa,\omega)} = \sum_{m=0,\pm1,\pm2,\ldots} \exp\left(-i\kappa m - \frac{|m|}{\xi}\right)\tilde{S}_{xx}(m,\omega)$$

$$= \frac{1}{2|J\sin\kappa_0|}\sum_{m=0,\pm1,\pm2,\ldots} \exp\left(-i\kappa m - \frac{|m|}{\xi}\right)\cos(m\kappa_0)\,\theta(\omega-|\Omega|+|J|)\,\theta(|\Omega|+|J|-\omega)$$

$$= \frac{1}{2\sqrt{J^2-(\omega-|\Omega|)^2}} \frac{J\sinh\frac{1}{\xi}\left(J\cosh\frac{1}{\xi}-(\omega-|\Omega|)\cos\kappa\right)}{\left(\omega-|\Omega|-J\cosh\frac{1}{\xi}\cos\kappa\right)^2+J^2\sinh^2\frac{1}{\xi}\sin^2\kappa}\,\theta(\omega-|\Omega|+|J|)\,\theta(|\Omega|+|J|-\omega). \quad (2.10)$$

If $1/2 \leqslant p \leqslant 1$, $\overline{S_{xx}(\kappa,\omega)}$ follows from Eq. (2.10) after the change $\kappa \to \kappa \mp \pi$. One can easily note that Eq. (2.10) transforms into Eq. (1.5) in the nonrandom limit $1/\xi \to 0$ (i.e., $p \to 0$ or $p \to 1$) (to show this, one has to exploit the relation $\lim_{\Gamma\to+0}\{\Gamma/[(\omega-\omega_0)^2+\Gamma^2]\}=\pi\delta(\omega-\omega_0)$). In the opposite limit of a completely random system $1/\xi \to \infty$ (i.e., $p \to 1/2$), Eq. (2.10) becomes

$$\overline{S_{xx}(\kappa,\omega)} = \frac{1}{2\sqrt{J^2-(\omega-|\Omega|)^2}}\,\theta(\omega-|\Omega|+|J|)\,\theta(|\Omega|+|J|-\omega). \quad (2.11)$$

One immediately recognizes that Eq. (2.11) contains the contribution of only the autocorrelation function (as it should be since the correlation length ξ tends to zero) and since in the limit considered $4\langle s_j^x(t)s_j^x\rangle=(1/N)\Sigma_\kappa \exp(-i\Lambda_\kappa t)$,[15] the xx dynamic structure factor is proportional to the density of states of elementary excitations $\rho(E)=(1/N)\Sigma_\kappa\delta(E-\Lambda_\kappa)$, i.e., $\overline{S_{xx}(\kappa,\omega)}=(\pi/2)\rho(\omega)$ independent of κ. For other values of $p\overline{S_{xx}(\kappa,\omega)}$ [Eq. (2.10)] is restricted to the frequency region $|\Omega|-|J|<\omega<|\Omega|+|J|$ and shows square-root singularities as $\omega \to |\Omega|\pm|J|$. The frequency profiles at fixed κ resemble (although are not identical to) Lorentzian shapes centered at $\omega=|\Omega|+J\cosh(1/\xi)\cos\kappa$ with the linewidth $\Gamma=|J\sinh(1/\xi)\sin\kappa|$.

For nonzero temperature, $T\neq 0$, and for subcritical field values, $|\Omega|<|J|$, Eq. (2.8) must be evaluated numerically (see Fig. 2). In the case $p=1/2$, the correlation length $\xi \to 0$ and one expects only the autocorrelation function to contribute to the κ-independent $\overline{S_{xx}(\kappa,\omega)}$ and the frequency shape for any κ is determined by the ω dependence of $\tilde{S}_{xx}(0,\omega)=\int_{-\infty}^{\infty}dt\,\exp(i\omega t)\langle\tilde{s}_j^x(t)\tilde{s}_j^x\rangle$ (κ-independent stripes near frequencies which dominate the autocorrelation function).

We note some similarities to recent numerical results on the spin-1/2 Ising chain in a random transverse field.[33] In particular, the horizontal (κ-independent) stripelike patterns in Fig. 2 resemble the results of Ref. 33 for strong disorder. This is to be expected since for strong enough disorder, only local correlations survive and lead to a κ-independent dynamic structure factor.

The scheme presented here can be also easily adapted to more complex models where alternation and randomness are mixed. For example, the ferromagnetic-antiferromagnetic random alternating quantum spin chain compound $(CH_3)_2CHNH_3Cu(Cl_xBr_{1-x})_3$ can be viewed as a spin-1/2 random alternating quantum Heisenberg chain,[21]

$$H=\sum_n (J_{2n-1}\vec{s}_{2n-1}\cdot\vec{s}_{2n}+J_{2n}\vec{s}_{2n}\cdot\vec{s}_{2n+1}), \quad (2.12)$$

where $J_{2n-1}=J$ is the weak uniform exchange bond, $J_{2n}=2\lambda_{2n}J$ is the strong random-sign exchange bond, and $\{\lambda_{2n}\}$ is the sequence of independent random variables each with the bimodal probability distribution [Eq. (2.5)]. If we restrict ourselves to isotropic XY interactions between spins in Eq. (2.12), the randomness can be excluded from the Hamiltonian by a slightly modified gauge transformation $\tilde{s}_{2n-1}^\alpha=s_{2n-1}^\alpha\Pi_{m=1}^{n-1}\lambda_{2m}$, $\tilde{s}_{2n}^\alpha=s_{2n}^\alpha\Pi_{m=1}^{n-1}\lambda_{2m}$, $n=2,3,\ldots$, obtaining finally the Hamiltonian of a dimerized XX chain with the periodically varying exchange couplings $J,2J,J,2J,\ldots$. The random-averaged dynamic structure factors can be calculated analogously to Eqs. (2.6)–(2.10).

III. SPIN-1/2 *XX* CHAIN WITH PERIODICITY AND/OR RANDOMNESS IN THE SIGN OF DZYALOSHINSKII-MORIYA INTERACTION

We now consider the spin model with the Hamiltonian [Eq. (1.1)] assuming $J_n=J$ and $D_n=\lambda_n D$ with $\lambda_n=\pm1$. (We note that the case $J_n=\lambda_n J$, $D_n=D$ may be analyzed on the basis of the results reported below after exploiting the unitary transformation discussed in Ref. 34.) It is generally known[26,35–38] that the Dzyaloshinskii-Moriya interaction D_n can be eliminated from the Hamiltonian H [Eq. (1.1)] (up to an inessential boundary term) by the spin coordinate transformation

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

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

$$s_n^z \to \tilde{s}_n^z = s_n^z, \quad (3.1)$$

where $\phi_n=\Sigma_{m=0}^{n-1}\varphi_m$, φ_0 is an arbitrary angle which is usually assumed to be zero, and $\tan\varphi_m=D_m/J$, $m=1,2,\ldots$. As a result, one faces the Hamiltonian $\tilde{H}$ [Eq. (1.1)] without the Dzyaloshinskii-Moriya interaction, however, with a renor-

malized XX exchange interaction $\tilde{J}_n=\mathrm{sgn}(J)\sqrt{J^2+D_n^2}$. In the uniform case, when $D_n=D$, the unitary transformation [Eq. (3.1)] was used in the recent studies of dynamics of quantum spin chains.[26,37,38] In this section, we consider separately the two cases of periodically varying Dzyaloshinskii-Moriya interaction and of random-sign Dzyaloshinskii-Moriya interaction focusing on the xx dynamic structure factor $S_{xx}(\kappa,\omega)$.

A. Periodic case

We begin with the case $p=2$ with $\{\lambda_n\}=\{1,-1,1,-1,\ldots\}$, i.e., $D_n=(-1)^{n+1}D$. Then, we have to put in Eq. (3.1) $\varphi_m=(-1)^{m+1}\varphi$, $\varphi=\arctan(D/J)$. Moreover, it is convenient to assume that $\varphi_0=-\varphi/2$. Then, $\phi_n=(-1)^n\varphi/2$ and the inverse transformation to the one given by Eq. (3.1) reads

$$s_n^x=\cos\frac{\varphi}{2}\tilde{s}_n^x-(-1)^n\sin\frac{\varphi}{2}\tilde{s}_n^y,$$

$$s_n^y=(-1)^n\sin\frac{\varphi}{2}\tilde{s}_n^x+\cos\frac{\varphi}{2}\tilde{s}_n^y,$$

$$s_n^z=\tilde{s}_n^z. \tag{3.2}$$

By substituting Eq. (3.2) into Eq. (1.2), one immediately finds that the xx dynamic structure factor $S_{xx}(\kappa,\omega)$ of the XX chain with the alternating Dzyaloshinskii-Moriya interaction $D,-D,D,-D,\ldots$ can be expressed through the xx dynamic structure factor $\tilde{S}_{xx}(\kappa,\omega)$ of the uniform chain with only XX exchange interaction $\tilde{J}=\mathrm{sgn}(J)\sqrt{J^2+D^2}$ as follows:

$$S_{xx}(\kappa,\omega)=\cos^2\frac{\varphi}{2}\tilde{S}_{xx}(\kappa,\omega)+\sin^2\frac{\varphi}{2}\tilde{S}_{xx}(\kappa\mp\pi,\omega). \tag{3.3}$$

We notice here that in the case when in Eq. (1.1) $J_n=J$, $D_n=D_0$, that is, for uniform XX and Dzyaloshinskii-Moriya couplings, the relation for $S_{xx}(\kappa,\omega)$ is quite different: $S_{xx}(\kappa,\omega)=[\tilde{S}_{xx}(\kappa-\varphi,\omega)+\tilde{S}_{xx}(\kappa+\varphi,\omega)+i\tilde{S}_{xy}(\kappa-\varphi,\omega)-i\tilde{S}_{xy}(\kappa+\varphi,\omega)]/2$; here, $\tilde{S}_{\alpha\beta}(\kappa,\omega)$ is related to the uniform chain with only XX exchange interaction $\tilde{J}=\mathrm{sgn}(J)\sqrt{J^2+D_0^2}$ (see Ref. 26). It is worth therefore to consider also the more complicated case of the chain [Eq. (1.1)] with $J_n=J$ and $D_n=D_0-(-1)^nD$. This choice of a dimerized Dzyaloshinskii-Moriya interaction covers both limiting cases (i) of the alternating-sign Dzyaloshinskii-Moriya interaction when $D_0=0$ and (ii) of the constant Dzyaloshinskii-Moriya interaction when $D=0$. Exploiting the transformation [Eq. (3.1)] with $\varphi_m=\arctan\{[D_0-(-1)^mD]/J\}$, we arrive at a chain without the Dzyaloshinskii-Moriya interaction but only with the dimerized XX exchange interaction $\tilde{J}_n=\mathrm{sgn}(J)\sqrt{J^2+[D_0-(-1)^nD]^2}$. To find the relation between the xx dynamic structure factor $S_{xx}(\kappa,\omega)$ of the XX chain with the dimerized Dzyaloshinskii-Moriya interaction and the dynamic structure factors $\tilde{S}_{\alpha\beta}(\kappa,\omega)$ of the dimerized XX chain without the Dzyaloshinskii-Moriya interaction, we proceed as follows. First, we note that exploiting Eq. (3.1) in Eq. (1.2) yields

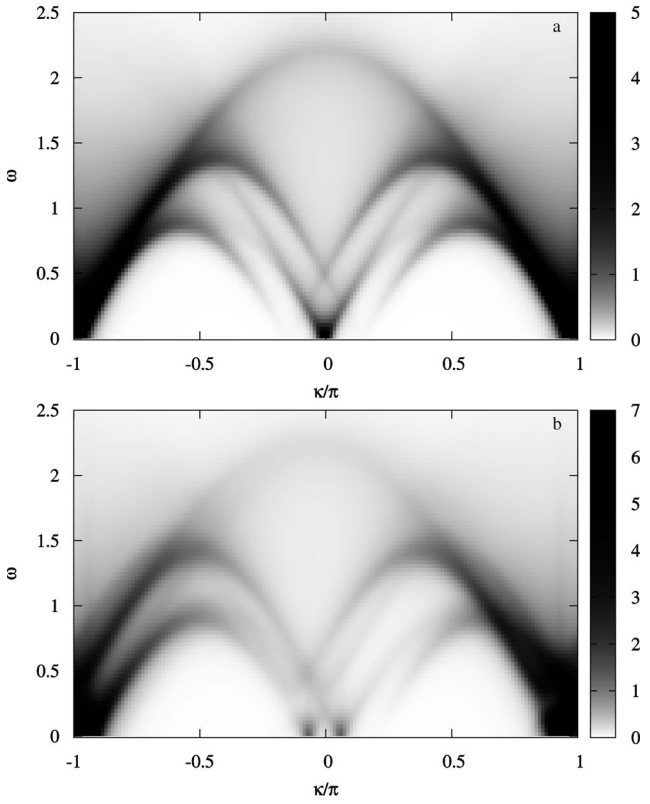

FIG. 3. $S_{xx}(\kappa,\omega)$ for the chain [Eq. (1.1)] with $J_n=1$, $D_n=D_0-(-1)^nD$, (a) $D_0=0$, (b) $D_0=0.25$, and $D=0.5$, $\Omega=0.25$ at low temperature, $\beta=20$.

$$S_{xx}(\kappa,\omega)=\frac{1}{N}\sum_{j=1}^{N}\sum_{m=1}^{N}\exp(-i\kappa m)\int_{-\infty}^{\infty}dt\exp(i\omega t)[\cos(\phi_{j+m}-\phi_j)\langle\tilde{s}_j^x(t)\tilde{s}_{j+m}^x\rangle-\sin(\phi_{j+m}-\phi_j)\langle\tilde{s}_j^x(t)\tilde{s}_{j+m}^y\rangle]. \tag{3.4}$$

After introducing the notations $\varphi_o=\arctan[(D_0+D)/J]$, $\varphi_e=\arctan[(D_0-D)/J]$, and $\varphi^{\pm}=(\varphi_o\pm\varphi_e)/2$, we can write $\phi_{j+m}-\phi_j=m\varphi^+ +(-1)^j\{[(-1)^m-1]/2\}\varphi^-$. Then, after inserting this result into Eq. (3.4) and some manipulations, Eq. (3.4) becomes

$$\begin{aligned}S_{xx}(\kappa,\omega)=&\frac{1}{2}\cos^2\frac{\varphi^-}{2}[\tilde{S}_{xx}(\kappa-\varphi^+,\omega)+\tilde{S}_{xx}(\kappa+\varphi^+,\omega)+i\tilde{S}_{xy}(\kappa-\varphi^+,\omega)-i\tilde{S}_{xy}(\kappa+\varphi^+,\omega)]+\frac{1}{2}\sin^2\frac{\varphi^-}{2}[\tilde{S}_{xx}(\kappa\mp\pi-\varphi^+,\omega)\\&+\tilde{S}_{xx}(\kappa\mp\pi+\varphi^+,\omega)+i\tilde{S}_{xy}(\kappa\mp\pi-\varphi^+,\omega)-i\tilde{S}_{xy}(\kappa\mp\pi+\varphi^+,\omega)].\end{aligned} \tag{3.5}$$

Equation (3.5) in the limit $D_0=0$ transforms into Eq. (3.3) since $\varphi^+=0$, $\varphi^-=\varphi=\arctan(D/J)$. Equation (3.5) also contains the result of Ref. 26 in the limit $D=0$ since $\varphi^+=\arctan(D_0/J)$, $\varphi^-=0$.

In Fig. 3, we illustrate the effect of the dimerized Dzyaloshinskii-Moriya interaction on the xx dynamic structure factor at low temperatures. Panel (a) corresponds to the

case $D_0=0$ [$S_{xx}(\kappa,\omega)$ is obtained using Eq. (3.3)], whereas panel (b) corresponds to the case $D_0\neq 0$ [$S_{xx}(\kappa,\omega)$ is obtained using the more general Eq. (3.5)].

B. Random case

Finally, we pass to the case when the Dzyaloshinskii-Moriya interaction $D_n=\lambda_n D$ is given by a sequence of independent random variables $\{\lambda_n\}$, each with the bimodal probability distribution [Eq. (2.5)]. For a specific realization of the signs of the Dzyaloshinskii-Moriya interaction, we can eliminate D_n from the Hamiltonian H [Eq. (1.1)] by the transformation [Eq. (3.1)] with $\varphi_m=\lambda_m\varphi$, $\varphi=\arctan(D/J)$ arriving at the model $\tilde{H}$ with only XX exchange interaction $\tilde{J}=\mathrm{sgn}(J)\sqrt{J^2+D^2}$. To calculate the random-averaged xx dynamic structure factor, we need

$$\overline{\langle s_j^x(t)s_{j+m}^x\rangle}=\overline{\cos(\phi_{j+m}-\phi_j)}\langle\tilde{s}_j^x(t)\tilde{s}_{j+m}^x\rangle-\overline{\sin(\phi_{j+m}-\phi_j)}\times\langle\tilde{s}_j^x(t)\tilde{s}_{j+m}^y\rangle. \tag{3.6}$$

Noting that

$$\begin{aligned}\overline{\cos[(\lambda_1+\cdots+\lambda_m)\varphi]}&=\frac{1}{2}[p\exp(-i\varphi)+(1-p)\exp(i\varphi)]^m\\&\quad+\frac{1}{2}[p\exp(i\varphi)+(1-p)\exp(-i\varphi)]^m\\&=[\cos^2\varphi+(1-2p)^2\sin^2\varphi]^{m/2}\\&\quad\times\cos\{m\arctan[(1-2p)\tan\varphi]\},\\ \overline{\sin[(\lambda_1+\cdots+\lambda_m)\varphi]}&=[\cos^2\varphi+(1-2p)^2\sin^2\varphi]^{m/2}\\&\quad\times\sin\{m\arctan[(1-2p)\tan\varphi]\}\end{aligned} \tag{3.7}$$

and introducing the notations $\xi_D=-1/\ln\sqrt{\cos^2\varphi+(1-2p)^2\sin^2\varphi}$, $\varphi_D=\arctan[(1-2p)\tan\varphi]$, one finds that

$$\overline{\langle s_j^x(t)s_{j+m}^x\rangle}=\exp\left(-\frac{|m|}{\xi_D}\right)[\cos(m\varphi_D)\langle\tilde{s}_j^x(t)\tilde{s}_{j+m}^x\rangle-\sin(m\varphi_D)\times\langle\tilde{s}_j^x(t)\tilde{s}_{j+m}^y\rangle]. \tag{3.8}$$

Using Eq. (3.8), the random-averaged xx dynamic structure factor can be written as follows:

$$\overline{S_{xx}(\kappa,\omega)}=\sum_{m=0,\pm1,\pm2,\ldots}\exp\left(-i\kappa m-\frac{|m|}{\xi_D}\right)\int_{-\infty}^{\infty}dt\exp(i\omega t)\times[\cos(m\varphi_D)\langle\tilde{s}_j^x(t)\tilde{s}_{j+m}^x\rangle-\sin(m\varphi_D)\langle\tilde{s}_j^x(t)\tilde{s}_{j+m}^y\rangle]. \tag{3.9}$$

On the rhs in Eq. (3.9), we have the correlation functions of the uniform XX chain with the exchange constant $\mathrm{sgn}(J)\sqrt{J^2+D^2}$. We use Eq. (3.9) to calculate $\overline{S_{xx}(\kappa,\omega)}$ for the model with the random-sign Dzyaloshinskii-Moriya interaction through the known results for $\langle\tilde{s}_j^\alpha\tilde{s}_{j+m}^\beta\rangle$.[16,32] The results are shown in Fig. 4. The correlation length ξ_D attains its minimal (nonzero) value $-1/\ln|\cos\varphi|$ at $p=1/2$. A comparison of Figs. 4(c) and 4(h) to Figs. 2(a) and 2(f) shows that $\overline{S_{xx}(\kappa,\omega)}$ looks very similar for weak disorder ($p=0.1$) in the sign of the exchange interaction, on one hand, and for maximum disorder ($p=1/2$) in the sign of the Dzyaloshinskii-Moriya interaction, on the other hand. It looks as if the random-sign Dzyaloshinskii-Moriya interaction at $p=1/2$ does not manifest itself in $\overline{S_{xx}(\kappa,\omega)}$. This similarity becomes evident if we notice that the correlation lengths ξ and ξ_D are of the same order for the considered conditions (see the captions to Figs. 2 and 4) and φ_D tends to zero, which cancels any signals of the Dzyaloshinskii-Moriya interaction due to formula (3.9).

We can proceed with analytical calculations for the case $T=0$, $|\Omega|>\sqrt{J^2+D^2}$. Comparing Eqs. (3.9) and (2.10), we see that the result we are interested in follows from Eq. (2.10) after the changes $J\to\tilde{J}=\mathrm{sgn}(J)\sqrt{J^2+D^2}$, $\kappa\to\kappa-\mathrm{sgn}(\Omega)\varphi_D$. In particular, for the nonrandom case when $p=0$ or $p=1$, we recover the result reported in Ref. 26, $\overline{S_{xx}(\kappa,\omega)}=(\pi/2)\delta\{\omega-|\Omega|-\tilde{J}\cos[\kappa-\mathrm{sgn}(\Omega)\varphi]\}$.

Interestingly, we can extend the scheme explained above to more complicated random chains assuming $J_n=\mathcal{J}\cos[f(\lambda_n)]$, $D_n=\mathcal{J}\sin[f(\lambda_n)]$, where $f(x)$ is an arbitrary function, for example, $f(x)=A+Bx$, and λ_n is a random variable with an arbitrary probability distribution $p(\lambda_n)$ (not necessarily with the bimodal probability distribution [Eq. (2.5)]). After exploiting the transformation [Eq. (3.1)] with $\varphi_m=A+B\lambda_m$, we arrive at the Hamiltonian $\tilde{H}$ given by Eq. (1.1) with $J_n=\mathcal{J}$, $D_n=0$. $\langle s_j^x(t)s_{j+m}^x\rangle$ is again given by Eq. (3.6); however, Eq. (3.7) now reads

$$\begin{aligned}\overline{\cos[mA+B(\lambda_1+\cdots+\lambda_m)]}&=|F(B)|^m\cos(m\{A+\arg[F(B)]\}),\\ \overline{\sin[mA+B(\lambda_1+\cdots+\lambda_m)]}&=|F(B)|^m\sin(m\{A+\arg[F(B)]\}),\end{aligned} \tag{3.10}$$

where

$$F(B)=\int d\lambda_n p(\lambda_n)\exp(iB\lambda_n)=|F(B)|\exp\{i\arg[F(B)]\} \tag{3.11}$$

is the characteristic function of the random variable λ_n. Now, we introduce the notations $\xi_D=-1/\ln|F(B)|$, $\varphi_D=A+\arg[F(B)]$ and arrive at Eqs. (3.8) and (3.9). For the model with the bimodal distribution considered earlier, we have to put $\mathcal{J}=\mathrm{sgn}(J)\sqrt{J^2+D^2}$, $A=0$, $B=\arctan(D/J)=\varphi$, and therefore $F(B)=p\exp(-i\varphi)+(1-p)\exp(i\varphi)$, $|F(B)|=\sqrt{\cos^2\varphi+(1-2p)^2\sin^2\varphi}$, $\arg[F(B)]=\arctan[(1-2p)\tan\varphi]$, and we reproduce Eqs. (3.8) and (3.9) with the expressions for ξ_D and φ_D given just before Eq. (3.8).

IV. CONCLUSIONS

To summarize, we have considered a number of inhomogeneous (periodic or random) spin-1/2 XX chains, to examine their dynamic properties. The models considered are dis-

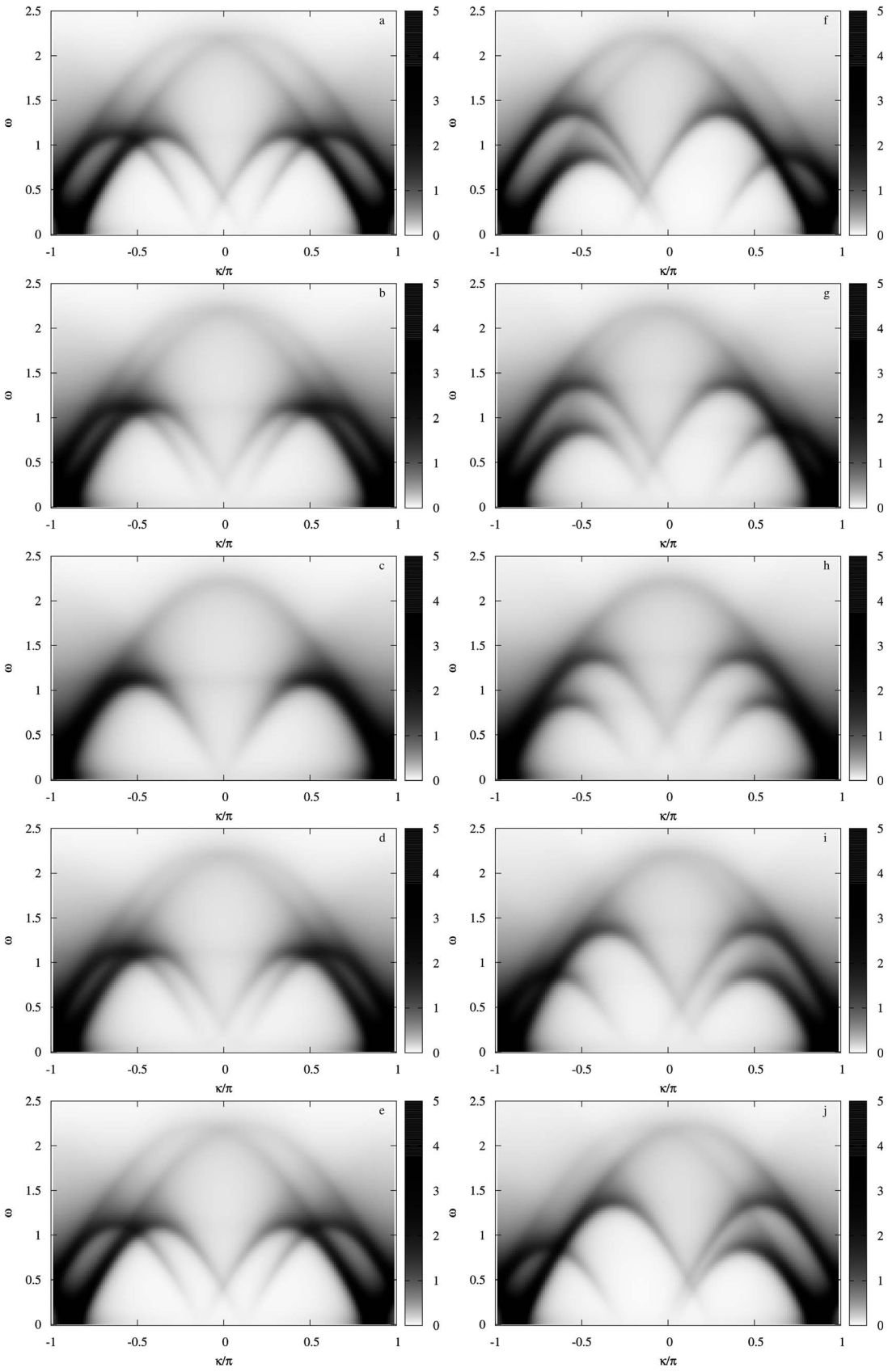

FIG. 4. $\overline{S_{xx}(\kappa,\omega)}$ for the chain [Eq. (1.1)] with $J_n=1$, $D_n=\lambda_n D$, where λ_n is a random variable with the probability distribution [Eq. (2.5)]. $D=0.5$, [(a)–(e)] $\Omega=0.01$, and [(f)–(j)] $\Omega=0.25$, $\beta=20$. The values of p in Eq. (2.5) are as follows: from top to bottom $p=0.1$ ($\xi_D \approx 26.77$), $p=0.25$ ($\xi_D \approx 12.31$), $p=0.5$ ($\xi_D \approx 8.96$), $p=0.75$ ($\xi_D \approx 12.31$), and $p=0.9$ ($\xi_D \approx 26.77$).

tinguished by the possibility to eliminate the inhomogeneity from the spin Hamiltonian by a suitable unitary transformation [see Eqs. (2.1) and (3.1)] and therefore to reduce the problem to the well known one for the uniform model. We use exact analytical and precise numerical data to analyze the dynamic structure factors of the periodic and/or random spin-1/2 *XX* chains. The models considered show rather complex behavior which, however, can be explained by the corresponding properties of the basic uniform model. Thus, for the periodic chains, only the correspondingly modified characteristic curves [Eqs. (1.4) and (1.6)] are seen in the complex pattern displayed by the dynamic structure factor at low temperatures. In the high-temperature limit, only Eq. (1.7) is relevant. In the cases considered, the observed complexity has a simple origin. We also stress here that we have reported rigorous analytical results for dynamic structure factors of some periodic and/or random quantum spin chains. In comparison, direct numerical treatment of random quantum spin chains would imply many calculations of dynamic quantities for different realizations of the random couplings and a subsequent average over these realizations, which altogether would require an enormous amount of computer time.

It is interesting to note that the effects of temperature and of random couplings on the xx/xy dynamic structure factors are different [compare Eqs. (1.7), (2.8), and (2.11)]. Although in both cases only the autocorrelation function determines the dynamic structure factor (for sufficiently high temperature or sufficiently strong randomness), at high temperatures, the dynamic structure factor is κ independent and shows Gaussian ridges [see Eq. (1.7)]. This is due to the Gaussian time decay of the autocorrelation function,[13,14] which should be contrasted to the slow long-time decay of the autocorrelation function at low temperatures.

The spin chain models discussed in our study are obviously of a rather special kind, and it would be highly desirable to obtain reliable results also for more general types of inhomogeneity in the interspin couplings, where not only the signs but also the absolute values of the couplings vary. For those more general models, however, the present methods are not applicable, and different methods or approximations have to be employed, such as in Refs. 33 and 39, for example. The special models treated in our present study will then be useful in providing a testing ground for the more general (but possibly less reliable) methods capable of dealing with a broader class of systems.

Finally, the dynamic structure factors provide benchmarks for determining interspin interactions. In our paper, we have demonstrated by some examples how periodic modulations or random variations in the signs of nearest-neighbor interactions manifest themselves in the dynamic structure factor. We note that the techniques used here for *XX* chains may also be applied to study dynamic structure factors of more general *XXZ* chains with periodic or random-sign changes in the *XY* part of the interactions, provided that sufficiently precise data for the corresponding uniform systems become available.

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