

Spin- $\frac{1}{2}$ XX chain in a transverse field with regularly alternating g factors: Static and dynamic properties

Taras Krokhmal'skii,^{1,2} Taras Verkholyak¹,² Ostap Baran¹,³ Vadim Ohanyan¹,^{3,4} and Oleg Derzhko^{1,5}

¹*Institute for Condensed Matter Physics, National Academy of Sciences of Ukraine, Svientsitskii Street 1, 79011 L'viv, Ukraine*

²*Department for Theoretical Physics, Ivan Franko National University of L'viv, Drahomanov Street 12, 79005 L'viv, Ukraine*

³*Laboratory of Theoretical Physics and Joint Laboratory of Theoretical Physics–ICTP Affiliated Centre in Armenia, Yerevan State University, Alex Manoogian Street 1, 0025 Yerevan, Armenia*

⁴*CANDLE Synchrotron Research Institute, Acharyan Street 31, 0040 Yerevan, Armenia*

⁵*Department of Metal Physics, Ivan Franko National University of L'viv, Kyrylo & Mephodiy Street 8, 79005 L'viv, Ukraine*



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We consider the spin- $\frac{1}{2}$ isotropic XY chain in an external magnetic field directed along the z axis with periodically varying g factors. To reveal the effects of regularly alternating g factors, we calculate various static and dynamic equilibrium quantities in the ground state and at finite temperatures. We demonstrate that because of the regularly alternating g factors the saturation field may disappear and the field dependence of the susceptibility in the ground state has additional logarithmic singularity at zero field. Moreover, the zero-field susceptibility has a logarithmic singularity as $T \rightarrow 0$. Furthermore, the dynamic structure factors exhibit much more structure in the “wave vector–frequency” plane that can be traced out to modifications of the two-fermion excitation continua which exclusively determine $S_{zz}(\kappa, \omega)$ and dominate the properties of $S_{xx}(\kappa, \omega)$. We discuss what changes can be observed in dynamic experiments on the corresponding substances.

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I. INTRODUCTION

The magnetic moment of an electron is related to its angular momentum by the g factor. The magnetic moment of a free electron is associated with its spin angular momentum only and the magnitude of the electron g factor (or more precisely the electron spin g factor) is $\approx 2.002\,319$ [1]. In atoms, both orbital angular momentum and spin angular momentum of the electron contribute to the magnetic moment of an atomic electron and the spin g factor has to be replaced by the Landé g factor. Furthermore, in crystalline solids, the Landé g factor (or in what follows simply the g factor) may be, in principle, site dependent.

From the solid-state-physics side, one can mention a number of spin-chain compounds with regularly alternating g -factor values [2–10]. Thus, one-dimensional copper iridium oxide $\text{Sr}_3\text{CuIrO}_6$ which contains both $3d$ (Cu^{2+}) and $5d$ (Ir^{4+}) magnetic ions can be well described by an effective spin- $\frac{1}{2}$ ferromagnetic Heisenberg model with an Ising-like exchange anisotropy ($\Delta \approx 2.5$) [2,3]. Moreover, the Cu sites carry the Cu spin $s = \frac{1}{2}$ with g factor ≈ 2 and the Ir sites carry the Ir isospin $s = \frac{1}{2}$ with g factor ≈ -3 [3,4]. Another instance is a one-dimensional molecular magnet $[\{\text{Co}^{\text{II}}(\Delta)\text{Co}^{\text{II}}(\Delta)\}(\text{ox})_2(\text{phen})_2]_n$ [5]. Magnetic properties of this compound can be explained using a one-dimensional Ising-chain model with two different exchange couplings and two different g factors, 2.5 and 2.1. The next example of a single-chain molecular magnet is a coordination polymer compound $[\{(\text{CuL})_2\text{Dy}\}\{\text{Mo}(\text{CN})_8\}] \cdot 2\text{CH}_3\text{CN} \cdot \text{H}_2\text{O}$, in which L^{2-} is N,N-propylenebis(3-

methoxysalicylideneiminato). The magnetic unit cell in this compound contains four magnetic ions with three different values of the g factors. The presence of the highly anisotropic Dy^{3+} ion makes possible an exact solution for the corresponding spin-chain model [6]. One more example is the spin- $\frac{1}{2}$ chain antiferromagnet $\text{CuCl}_2 \cdot 2[(\text{CD}_3)_2\text{SO}]$ [7]. There are results of very recent studies of another heterotrimetallic coordination-polymer single-chain magnet with large difference between the g factors of the magnetic ions in the magnetic unit cell, $[\text{Cu}^{\text{II}}\text{Mn}^{\text{II}}(\text{L}^1)][\text{Fe}^{\text{III}}(\text{bpb})(\text{CN})_2] \cdot \text{ClO}_4 \cdot \text{H}_2\text{O}$ [8]. In this system, a staggered g tensor and/or Dzyaloshinskii-Moriya interactions lead to a staggered field along the x direction upon application of a uniform field along the z direction. As a result, a spin- $\frac{1}{2}$ antiferromagnetic Heisenberg chain with an alternating g factor emerges (see also Ref. [9] discussing the quasi-one-dimensional spin- $\frac{1}{2}$ antiferromagnet Cu benzoate). Finally, one may also mention a two-sublattice one-dimensional system $\text{Ni}_2(\text{EDTA})(\text{H}_2\text{O})_4 \cdot 2\text{H}_2\text{O}$, the magnetic behavior of which was discussed in terms of a spin-1 g_1 - g_2 antiferromagnetic Heisenberg (or Ising) chain with g_1/g_2 about 1.1 [10].

From the theoretical side, since the g factor enters many standard lattice models of crystalline solids, it is quite natural to address a question about the consequences of a regular nonuniformity of the g factor for the observable magnetic properties. There are several exact calculations for the spin-chain systems aimed at exploring the essential effects of nonuniform g factors. Spin- $\frac{1}{2}$ XY chains provide an excellent playground for such analysis because they correspond to noninteracting fermions [11,12]. Prior work, which

is closely related to our study, concerns the two-sublattice [13,14] and the inhomogeneous periodic (i.e., with several sites in a cell which periodically repeats) [15] spin- $\frac{1}{2}$ XX chain in a z -aligned field with various interaction constant and g -factor values. The reported results refer to the magnetization, susceptibility, and equal-time two-spin zz correlation functions [13,14], as well as to some dynamic quantities related to correlations of the average cell operators [15]. The continued-fraction method was also used to figure out the magnetothermal properties of the general inhomogeneous isotropic XX chain including the case of a random Lorentzian transverse field [16]. The same program has been performed also for the quantum Ising chain [17]. In the most recent papers, the detailed analysis of the ground-state properties for general boundary conditions for the quantum Ising chain with the period-2 modulated transverse field have been done [18]. Free-fermion models in which the period-2 alternation of the nearest-neighbor interactions is accompanied by multiple spin exchange were considered in Refs. [19–21]. XX chains are the extreme limit of the Heisenberg chains with an XY-like exchange anisotropy. The opposite limiting case is the Ising chains. Recently, a spin- $\frac{1}{2}$ Ising chain with period-2 regularly alternating g factors has been studied in the context of unusual properties of $\text{Sr}_3\text{CuIrO}_6$ [3,4]. Moreover, this material, as was mentioned above, features not only alternating g factors of magnetic ions along the chain, but also the negative sign of one of them. Negative g factors (for the pseudospin operators) are interesting by themselves as they are the result of strong interplay between the ligand field and spin-orbit interaction [22–24]. Very recently it has been shown that even in the simplest case of the ferromagnetic Ising model with g factors of different sign on bipartite lattice, the frustration takes place and there are configurations containing ordered and disordered sublattices at the same time [4,25]. Rigorous results for finite quantum spin clusters and an Ising-Heisenberg chain with different g factors have been obtained recently in Ref. [26].

In the present paper we report results of the systematic study of the spin- $\frac{1}{2}$ XX chain in a transverse field with regularly alternating g factors including the case when g factors have different signs. We pay special attention to manifestation of regularly alternating g factors in the transverse magnetization, the static zz susceptibility, as well as in the two dynamic structure factors $S_{zz}(\kappa, \omega)$ and $S_{xx}(\kappa, \omega)$. $S_{yy}(\kappa, \omega)$ behaves identically to $S_{xx}(\kappa, \omega)$ due to the symmetry of the model. Dynamic quantities are accessible experimentally and therefore understanding of the effects generated by nonuniform g factors may be useful for interpreting experimental data. The recent development of the exact and numerical calculations of the spin dynamic structure factors for the integrable one-dimensional quantum spin systems are really impressive [27]. However, the spin-chain model examined in what follows, although corresponding to noninteracting fermions, may be of interest for the full Heisenberg exchange interaction case too: Since the seminal papers by Müller *et al.* [28] we know that many dynamic features of the spin- $\frac{1}{2}$ Heisenberg chain can be analyzed starting from the free-fermion limit.

It might be worthwhile to list here the main findings of the present paper.

(i) We have performed a detailed study of the dynamic properties. We calculated the dynamic structure factors $S_{zz}(\kappa, \omega)$ and $S_{xx}(\kappa, \omega)$ and inspected how they change in the external magnetic field for different period-2 alternations of g factors.

(ii) In the case when both g factors are of the same sign, the correspondence between the boundaries of the zz and xx structure factors is still present.

(iii) On the contrary, if $g_1 g_2 \leq 0$, a large enough magnetic field leads to the highly intense modes in the xx structure factor.

(iv) Analyzing the absorption intensity $I_\alpha(\omega, h)$, we found that in the Voigt configuration ($\alpha = z$), the model with uniform g factors does not have any response. In the case when g_2 differs from g_1 , we obtain the nonzero contribution to the absorption intensity. For sufficiently large frequencies $\omega > 2|J|$ (where J denotes the exchange coupling) the van Hove singularity arises at the magnetic field $h = \sqrt{\omega^2 - 4J^2}/|g_1 - g_2|$.

(v) In the Faraday configuration ($\alpha = x$), the situation is a bit different. The absorption spectra can be observed in the uniform case. It shows a broad maximum at some resonance field. The alternation of g factors leads to the doubling of this resonance line.

(vi) Although in our study we focus on the exactly solvable XX chain, we know that such analysis of dynamics is useful for understanding a more realistic case of the Heisenberg chains. Many qualitative features (e.g., doubling of the resonance line) of the absorption profiles can be found also in case of the Heisenberg XXZ model with alternating g factors.

The rest of the paper is organized as follows. We begin with introducing the model to be studied and the free-fermion representation of the model which emerges after applying the Jordan-Wigner transformation, Sec. II. After that we discuss the magnetization and the susceptibility in the ground state (Sec. III) and some finite-temperature quantities (Sec. IV). In Sec. V we examine the dynamic structure factors of the model. We report the results for $S_{zz}(\kappa, \omega)$ obtained mainly analytically and for $S_{xx}(\kappa, \omega)$ obtained mainly numerically. We conclude the paper with a summary, Sec. VI.

II. THE MODEL AND ITS FREE-FERMION REPRESENTATION

In the present study, we consider the spin- $\frac{1}{2}$ isotropic XY chain in a transverse (i.e., aligned along the z axis) magnetic field. The peculiarity of the model is the regularly alternating g factor which acquires periodically two values, g_1 and g_2 . The Hamiltonian of the model reads

$$H = \sum_{l=1}^{\frac{N}{2}} [J(s_{2l-1}^x s_{2l}^x + s_{2l-1}^y s_{2l}^y + s_{2l}^x s_{2l+1}^x + s_{2l}^y s_{2l+1}^y) - g_1 \mu_B H s_{2l-1}^z - g_2 \mu_B H s_{2l}^z]. \quad (2.1)$$

Here J is the exchange interaction (we may put $|J| = 1$ without loss of generality), μ_B is the Bohr magneton, H is the value of the magnetic field measured, e.g., in teslas (then with $\mu_B \approx 0.67171$ K/T the field $h = \mu_B H$ is measured in kelvins), and $g_1 \mu_B H = g_1 h$, $g_2 \mu_B H = g_2 h$. Furthermore, N is the number of lattice sites which is assumed to be even, and

periodic boundary conditions are imposed for convenience. After introducing

$$g_{\pm} = \frac{g_1 \pm g_2}{2}, \quad (2.2)$$

we can rewrite Eq. (2.1) in a more compact form

$$H = \sum_{l=1}^N [J(s_l^x s_{l+1}^x + s_l^y s_{l+1}^y) - h_l s_l^z],$$

$$h_l = [g_+ - (-1)^l g_-]h. \quad (2.3)$$

This is the Hamiltonian of the spin- $\frac{1}{2}$ isotropic XY chain in a regularly alternating (with period 2) transverse magnetic field.

The defined model is exactly solvable by making use of the famous Jordan-Wigner fermionization [11,12] (see also Refs. [29,30]). In terms of the Jordan-Wigner fermions the spin Hamiltonian (2.3) becomes

$$H = \sum_{l=1}^N \left[\frac{J}{2} (c_l^\dagger c_{l+1} + c_{l+1}^\dagger c_l) - h_l \left(c_l^\dagger c_l - \frac{1}{2} \right) \right]. \quad (2.4)$$

Again periodic boundary conditions are implied in Eq. (2.4) [31]. After the Fourier transformation

$$c_l = \frac{1}{\sqrt{N}} \sum_{\kappa} e^{-ikl} c_{\kappa},$$

$$\kappa = \frac{2\pi j}{N}, \quad j = -\frac{N}{2}, -\frac{N}{2} + 1, \dots, \frac{N}{2} - 1, \quad (2.5)$$

Eq. (2.4) can be cast into

$$H = \sum_{-\pi \leq \kappa < \pi} [(J \cos \kappa - g_+ h) c_{\kappa}^\dagger c_{\kappa} + g_- h c_{\kappa}^\dagger c_{\kappa \pm \pi}]$$

$$+ \frac{g_+ h}{2} N. \quad (2.6)$$

Next, we perform the Bogolyubov transformation,

$$c_{\kappa} = u_{\kappa} \alpha_{\kappa} - v_{\kappa} \alpha_{\kappa + \pi},$$

$$c_{\kappa + \pi} = v_{\kappa} \alpha_{\kappa} + u_{\kappa} \alpha_{\kappa + \pi} \quad (-\pi/2 \leq \kappa < \pi/2),$$

$$u_{\kappa} = \frac{1}{\sqrt{2}} \sqrt{1 + \frac{|J \cos \kappa|}{\sqrt{J^2 \cos^2 \kappa + g_-^2 h^2}}},$$

$$v_{\kappa} = \frac{\text{sgn}(g_- h J \cos \kappa)}{\sqrt{2}} \sqrt{1 - \frac{|J \cos \kappa|}{\sqrt{J^2 \cos^2 \kappa + g_-^2 h^2}}}, \quad (2.7)$$

leading to

$$H = \sum_{-\pi \leq \kappa < \pi} \Lambda_{\kappa} \left(\alpha_{\kappa}^\dagger \alpha_{\kappa} - \frac{1}{2} \right),$$

$$\Lambda_{\kappa} = -g_+ h + \text{sgn}(J \cos \kappa) \sqrt{J^2 \cos^2 \kappa + g_-^2 h^2}. \quad (2.8)$$

Hence, we have arrived at the free-fermion representation (2.8) of the initial spin model (2.1). Within this representation many calculations for the thermodynamically large system can be performed rigorously analytically or with very high accuracy numerically. From Eq. (2.8) it is immediately evident that nonzero magnetic field develops a gap in the excitation spectrum splitting it into two branches. In the limiting case

of large g factors (or field h) the system becomes close to the two-level model with only two possible eigenenergies on each site, $-g_1 h$ and $-g_2 h$. The position of the Fermi level is important for the understanding of the ground state and thermodynamics of the model given in the next section.

Although the isotropic XY interactions may occur in some spin- $\frac{1}{2}$ chain compounds (see, e.g., Ref. [34]), they can be viewed as a limiting case of more common XXZ interactions. Consider the spin- $\frac{1}{2}$ XXZ chain in a z -directed magnetic field. The Hamiltonian of such model contains in addition to the one given in Eqs. (2.1) or (2.2) the interaction of the z components of neighboring spins with the strength $J\Delta$, where Δ is the anisotropy parameter. As a result, in terms of the Jordan-Wigner fermions the spin Hamiltonian becomes

$$H = \sum_{l=1}^N \left[\frac{J}{2} (c_l^\dagger c_{l+1} + c_{l+1}^\dagger c_l) + J\Delta c_l^\dagger c_l c_{l+1}^\dagger c_{l+1} \right.$$

$$\left. - (h_l + J\Delta) c_l^\dagger c_l + \frac{h_l}{2} + \frac{J\Delta}{4} \right]. \quad (2.9)$$

One way to proceed is to apply a mean-field-like approximation for the four-fermion term [35,36]:

$$c_l^\dagger c_l c_{l+1}^\dagger c_{l+1} \rightarrow \left(\frac{1}{2} + m \right) (c_l^\dagger c_l + c_{l+1}^\dagger c_{l+1}) - \left(\frac{1}{2} + m \right)^2$$

$$- t (c_l^\dagger c_{l+1} + c_{l+1}^\dagger c_l) + t^2$$

$$- s c_l^\dagger c_{l+1}^\dagger - s^* c_l c_{l+1} + |s|^2, \quad (2.10)$$

where the parameters $m \equiv \langle c_l^\dagger c_l \rangle - 1/2$, $t \equiv \langle c_l^\dagger c_{l+1} \rangle$, and $s \equiv \langle c_l c_{l+1} \rangle$ have to be determined self-consistently. It should be noted that the Jordan-Wigner fermionization approach was successfully used for examining the static and dynamic properties away from the free-fermion point [37–41].

III. ZERO-TEMPERATURE PROPERTIES

Let us first present the ground-state ($T = 0$) properties of the system. Although some particular results have been already obtained in Refs. [13–15], we provide here the ground-state analysis for consistency. Particularly, we focus on calculating the ground-state energy $e_0 = \langle H \rangle / N$, the transverse magnetization $m = -\partial e_0 / \partial h$, the sublattice average z component of spin, $\langle s_1^z \rangle = -2 \partial e_0 / \partial (g_1 h)$, $\langle s_2^z \rangle = -2 \partial e_0 / \partial (g_2 h)$, and the static zz susceptibility $\chi_{zz} = \partial m / \partial h$. For the model at hand, one has to differ the magnetization and the average of the z component of the spin operator, i.e., the magnetic moment and the angular momentum at site. It is obvious that

$$m = \frac{1}{2} (g_1 \langle s_1^z \rangle + g_2 \langle s_2^z \rangle). \quad (3.1)$$

In what follows we distinguish two cases: $g_1 g_2 > 0$ and $g_1 g_2 < 0$.

The case $g_1 g_2 > 0$. There are two values of the Fermi momenta κ_F defined as the solutions of the equation $\Lambda_{\kappa} = 0$:

$$\kappa_F = \pm \kappa_0, \quad \text{if } 0 < J g_+ h < |J g_+| h_s,$$

$$\kappa_F = \pm (\pi - \kappa_0), \quad \text{if } -|J g_+| h_s < J g_+ h < 0, \quad (3.2)$$

$$\kappa_0 = \arccos |h/h_s| \quad (0 < \kappa_0 < \pi/2),$$

where the saturation field h_s is given by $h_s = |J|/\sqrt{g_1 g_2} > 0$. It is worth noting that the saturation field exists if the fully polarized state $|\uparrow \dots \uparrow\rangle$, which is obviously the eigenstate of the Hamiltonian (2.1), becomes the ground state as the field h exceeds a certain finite value. This is the case for $g_1 g_2 > 0$ but not for $g_1 g_2 < 0$. Here we may consider two separate ranges of the magnetic field h . The first one, when $|h| > h_s$, corresponds to the saturated phase with all spins aligned in the field direction. There is no solution for κ_F and, thus, the ground-state energy as well as the averages of spins have simple expressions:

$$e_0 = -\frac{1}{2}|g_+ h|, \quad m = \text{sgn}(h) \frac{g_+}{2},$$

$$\langle s_1^z \rangle = \langle s_2^z \rangle = \frac{\text{sgn}(h)}{2}, \quad \chi_{zz} = 0. \quad (3.3)$$

More interesting is the second range, $-h_s < h < h_s$, when

$$e_0 = -|g_+ h| \left(\frac{1}{2} - \frac{\kappa_0}{\pi} \right) - \frac{1}{\pi} \sqrt{J^2 + g_-^2 h^2} E(\kappa_0, \varkappa),$$

$$m = g_+ \text{sgn}(h) \left(\frac{1}{2} - \frac{\kappa_0}{\pi} \right) + \frac{g_-^2 h}{\pi \sqrt{J^2 + g_-^2 h^2}} F(\kappa_0, \varkappa),$$

$$\langle s_1^z \rangle = \text{sgn}(h) \left(\frac{1}{2} - \frac{\kappa_0}{\pi} \right) + \frac{g_- h}{\pi \sqrt{J^2 + g_-^2 h^2}} F(\kappa_0, \varkappa),$$

$$\langle s_2^z \rangle = \text{sgn}(h) \left(\frac{1}{2} - \frac{\kappa_0}{\pi} \right) - \frac{g_- h}{\pi \sqrt{J^2 + g_-^2 h^2}} F(\kappa_0, \varkappa),$$

$$\chi_{zz} = \frac{g_+ \varkappa^2}{\pi \sqrt{h_s^2 - h^2}} + \frac{g_-^2}{\pi \sqrt{J^2 + g_-^2 h^2}} [F(\kappa_0, \varkappa) - E(\kappa_0, \varkappa)]. \quad (3.4)$$

Here $\varkappa = |J|/\sqrt{J^2 + g_-^2 h^2}$ and we have also introduced the elliptic integrals of the first and second kind given by the following standard expressions [42]:

$$F(\kappa_0, \varkappa) = \int_0^{\kappa_0} \frac{d\theta}{\sqrt{1 - \varkappa^2 \sin^2 \theta}},$$

$$K(\varkappa) = F\left(\frac{\pi}{2}, \varkappa\right),$$

$$E(\kappa_0, \varkappa) = \int_0^{\kappa_0} d\theta \sqrt{1 - \varkappa^2 \sin^2 \theta},$$

$$E(\varkappa) = E\left(\frac{\pi}{2}, \varkappa\right). \quad (3.5)$$

As can be seen from the reported formulas, the susceptibility diverges at $h = \pm h_s$ showing the square-root singularity

$$\chi_{zz} \approx \frac{g_+^2 - g_-^2}{\pi g_+} \frac{1}{\sqrt{h_s^2 - h^2}}, \quad h \rightarrow |h_s|. \quad (3.6)$$

If $g_1 \neq g_2$ an additional weak divergence of χ_{zz} occurs at $h = 0$:

$$\chi_{zz} \approx \frac{g_+}{\pi h_s} + \frac{g_-^2}{\pi} \left(\ln \frac{2h_s}{h} - 1 \right), \quad |h| \rightarrow 0. \quad (3.7)$$

This was noticed for the first time apparently in Ref. [13].

The case $g_1 g_2 < 0$. In this case the equation for the Fermi momenta $\Lambda_\kappa = 0$ does not have real solutions, which means that the Fermi level lays in the forbidden band between two branches of the spectrum. Since the odd and even spins are directed oppositely in a field, there is also no saturation field; i.e., the magnetization never attains its saturation value corresponding to $\langle s_1^z \rangle = -\langle s_2^z \rangle = \pm 1/2$. The ground-state energy is given by the following formula:

$$e_0 = -\frac{1}{\pi} \sqrt{J^2 + g_-^2 h^2} E(\varkappa). \quad (3.8)$$

After straightforward differentiation we get

$$m = \frac{g_-^2 h}{\pi \sqrt{J^2 + g_-^2 h^2}} K(\varkappa),$$

$$\langle s_1^z \rangle = -\langle s_2^z \rangle = \frac{g_- h}{\pi \sqrt{J^2 + g_-^2 h^2}} K(\varkappa),$$

$$\chi_{zz} = \frac{g_-^2}{\pi \sqrt{J^2 + g_-^2 h^2}} [K(\varkappa) - E(\varkappa)] \quad (3.9)$$

for the magnetization, the sublattice average z component of spin, and the susceptibility, respectively. These formulas can be simplified in the strong-field and weak-field limits. We obtain

$$m \approx \frac{g_-^2 h}{2\sqrt{J^2 + g_-^2 h^2}},$$

$$\chi_{zz} \approx \frac{g_-^2 J^2}{4(J^2 + g_-^2 h^2)^{\frac{3}{2}}}, \quad (3.10)$$

as $|h| \rightarrow \infty$, and

$$m \approx \frac{g_-^2 h}{\pi \sqrt{J^2 + g_-^2 h^2}} \ln \frac{4\sqrt{J^2 + g_-^2 h^2}}{|g_- h|},$$

$$\chi_{zz} \approx \frac{g_-^2}{\pi \sqrt{J^2 + g_-^2 h^2}} \left(\ln \frac{4\sqrt{J^2 + g_-^2 h^2}}{|g_- h|} - 1 \right), \quad (3.11)$$

as $|h| \rightarrow 0$. While Eq. (3.10) demonstrates explicitly that the saturation is never achieved for any finite h , Eq. (3.11) demonstrates a nonanalyticity of the ground-state energy which manifests itself as a logarithmic peculiarity of the magnetization and the susceptibility in vanishing field.

In Fig. 1 we show the ground-state magnetization and susceptibility. In all numerical investigations, without loss of generality, we assume first that $g_2 = g_1 = 1$ and then g_2 starts to decrease. These plots illustrate the analytical results reported above including the asymptotic behavior of the susceptibility. It is worthwhile to stress that the logarithmic singularity of the susceptibility χ_{zz} can be detected not only in the case $g_1 g_2 < 0$, when it is quite natural to expect it, but also in the opposite case $g_1 g_2 > 0$; see Eq. (3.7). This is the consequence of another peculiar property shown in Fig. 2 where the total magnetization and spin moment is confronted with the average spin moments of each sublattices. We can see

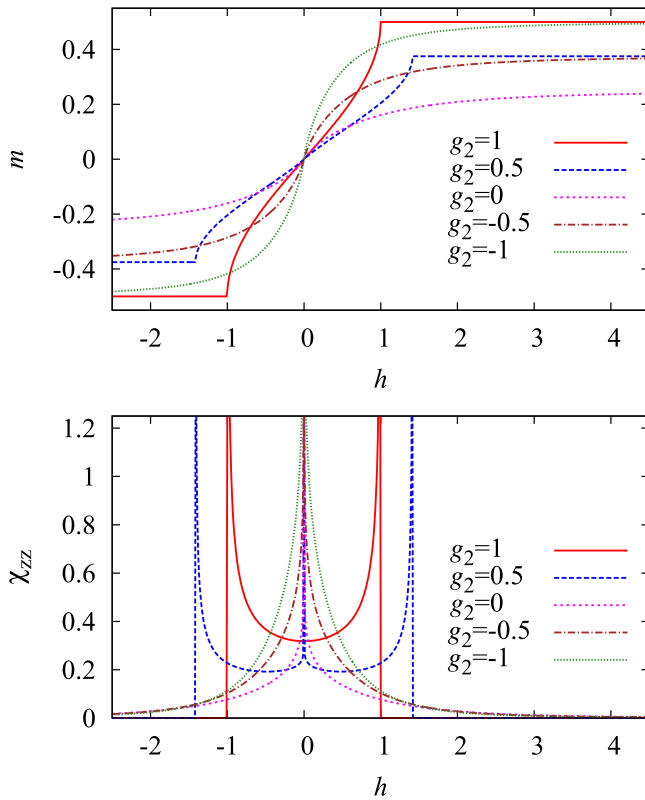


FIG. 1. Ground-state magnetization (upper panel) and susceptibility (lower panel) vs field h . $|J| = 1$, $g_1 = 1$, $g_2 = 1$ (solid), $g_2 = 0.5$ (long-dashed), $g_2 = 0$ (short-dashed), $g_2 = -0.5$ (dashed-dotted), $g_2 = -1$ (dotted).

that even for positive g_2 (see Fig. 2 for $g_2 = 0.1$) the average spin moment at small fields started to evolve in the direction opposite to the field feeling the competition between the applied magnetic field and quantum interaction with stronger magnetized neighboring spins.

Let us denote by h_0 ($h_0 > 0$) the value of the field at which $\langle s_2^z \rangle = 0$ if $|g_2| < |g_1|$ (or $\langle s_1^z \rangle = 0$ if $|g_1| < |g_2|$); h_0 exists in the case $g_1 g_2 > 0$ only. After using approximate formulas for the elliptic integrals one can show that $h_0 \approx 2h_s e^{-2\alpha}$, where

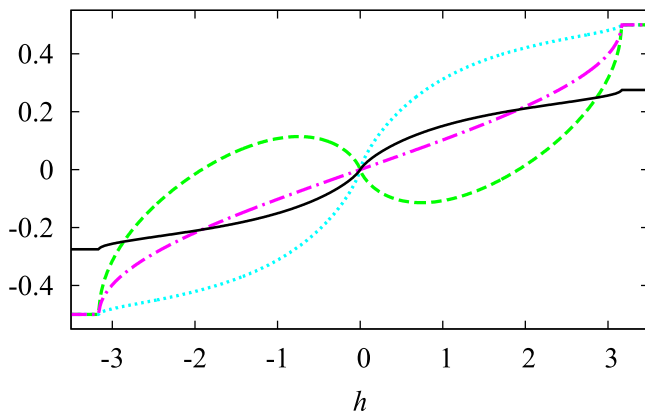


FIG. 2. Ground-state values of $\langle s_1^z \rangle$ (dotted), $\langle s_2^z \rangle$ (dashed), $(\langle s_1^z \rangle + \langle s_2^z \rangle)/2$ (dot-dashed), and m (solid) vs field h . $|J| = 1$, $g_1 = 1$, $g_2 = 0.1$.

$\alpha = \sqrt{g_1 g_2}/|g_1 - g_2|$. If g_2 (or g_1) approaches zero we can again use approximate formulas for the elliptic integrals to conclude that $h_0 \approx h_s/\sqrt{2}$. Both limiting cases can be combined into the following approximate expression,

$$h_0 \approx \frac{2e^{-2\alpha}}{1 + (2\sqrt{2} - 1)e^{-3\alpha}} h_s, \quad (3.12)$$

which yields the correct value of h_0 for the whole region $g_1 g_2 > 0$ with the accuracy of less than 1.5%.

IV. FINITE-TEMPERATURE PROPERTIES

Finite-temperature quantities can be easily calculated from the free energy per site

$$f(T, h) = -\frac{T}{2\pi} \int_{-\pi}^{\pi} d\kappa \ln \left(2 \cosh \frac{\Lambda_\kappa}{2T} \right) \quad (4.1)$$

with Λ_κ given in Eq. (2.8). For example, for the specific heat one finds

$$c(T, h) = \frac{1}{2\pi} \int_{-\pi}^{\pi} d\kappa \left(\frac{\Lambda_\kappa}{2T} \right)^2 \cosh^{-2} \frac{\Lambda_\kappa}{2T}. \quad (4.2)$$

Furthermore, for the finite-temperature magnetization and susceptibility one finds

$$m(T, h) = \frac{1}{4\pi} \int_{-\pi}^{\pi} d\kappa \frac{\partial \Lambda_\kappa}{\partial h} \tanh \frac{\Lambda_\kappa}{2T} \quad (4.3)$$

and

$$\begin{aligned} \chi_{zz}(T, h) &= \frac{1}{4\pi} \int_{-\pi}^{\pi} d\kappa \left[\frac{\partial^2 \Lambda_\kappa}{\partial h^2} \tanh \frac{\Lambda_\kappa}{2T} + \frac{1}{2T} \left(\frac{\partial \Lambda_\kappa}{\partial h} \right)^2 \cosh^{-2} \frac{\Lambda_\kappa}{2T} \right], \end{aligned} \quad (4.4)$$

respectively. Here, the derivatives $\partial \Lambda_\kappa / \partial h$ and $\partial^2 \Lambda_\kappa / \partial h^2$ are given by the following formulas:

$$\begin{aligned} \frac{\partial \Lambda_\kappa}{\partial h} &= -g_+ + \frac{\text{sgn}(J \cos \kappa) g_-^2 h}{\sqrt{J^2 \cos^2 \kappa + g_-^2 h^2}}, \\ \frac{\partial^2 \Lambda_\kappa}{\partial h^2} &= \frac{\text{sgn}(J \cos \kappa) g_-^2 J^2 \cos^2 \kappa}{(J^2 \cos^2 \kappa + g_-^2 h^2)^{3/2}}. \end{aligned} \quad (4.5)$$

In Fig. 3 we demonstrate the temperature behavior of the specific heat (4.2) for several regimes: (1) gapless zero-field and finite-field regimes ($0 < |h| < h_s$) (solid black and dashed brown), (2) two cases when $|h| = h_s$ or $g_2 = 0$ (dashed-dotted blue), and (3) two gapped regimes when $|h| > h_s$, $g_1 g_2 > 0$ or when $g_1 g_2 < 0$ at $h \neq 0$ (dotted green).

The gapless regime features the universal linear-temperature dependence of the specific heat:

$$c(T) \simeq \frac{\pi \mathbf{c}}{3v_F} T, \quad T \rightarrow 0. \quad (4.6)$$

Here, in our case the central charge $\mathbf{c} = 1$ and the Fermi velocity for the case of zero field coincides with those for the XX chain, $v_F = |J|$, whereas for the case of the gapless finite-field regime ($0 < |h| < h_s$, $g_1 g_2 > 0$) it is $v_F = J^2 \sqrt{1 - h^2/h_s^2}/(h_s |g_+|)$. When the magnetic field reaches the saturation value $|h| = h_s$ ($g_1 g_2 > 0$) the Fermi level touches

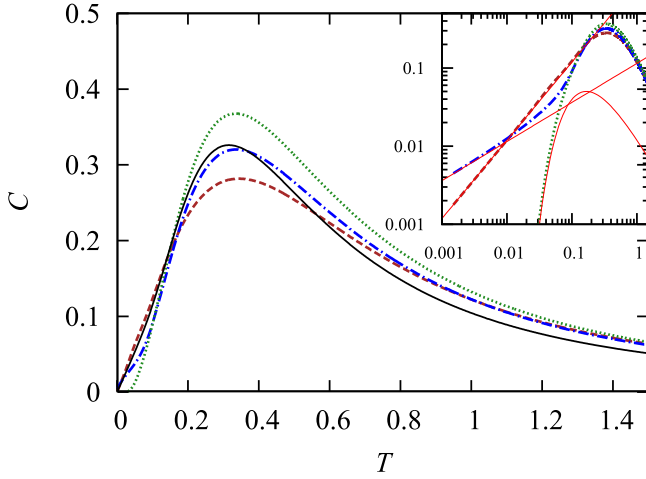


FIG. 3. Temperature dependence of the specific heat for $|J| = 1$ at $h = 0$ (solid black); $h = 0.5$, $g_1 = 1$, $g_2 = 0.5$ (dashed brown); $h = 0.5$, $g_1 = 1$, $g_2 = 0$ (dashed-dotted blue); and $h = 0.5$, $g_1 = 1$, $g_2 = -0.5$ (dotted green). The inset shows the same plots in log-log scale. The linear, square-root, and exponential behavior of the specific heat are clearly visible here. Thin red lines represent the asymptotic forms from Eqs. (4.6), (4.7), and (4.8).

the bottom points of the upper part of the spectrum (van Hove singularity). The low-temperature behavior of the specific heat in this case is given by the square-root temperature dependence,

$$c(T) \simeq \frac{3(\sqrt{2}-1)\zeta(\frac{3}{2})\sqrt{|g_+h|}}{8\sqrt{\pi}|J|}\sqrt{T}, \quad (4.7)$$

where $\zeta(x)$ is the standard zeta function. The same expression is valid for the case $g_2 = 0$ for arbitrary nonzero values of the magnetic field. Finally, two gapped regimes are possible: (i) $|h| > h_s$, $g_1 g_2 > 0$ and (ii) $g_1 g_2 < 0$ at any $h \neq 0$. The specific heat has universal exponential low-temperature behavior, given by

$$c(T) \simeq \frac{\Delta^2}{\sqrt{2\pi r}} \frac{e^{-\frac{\Delta}{T}}}{T^{\frac{3}{2}}}, \quad (4.8)$$

where for the $|h| > h_s$ regime $r = |J|\pi/2$, $\Delta = |g_+h| - \sqrt{J^2 + g_-^2 h^2}$, whereas for the $g_1 g_2 < 0$ regime $r = J^2/(2|g_-h|)$, $\Delta = |g_2 h|$ ($\Delta = |g_1 h|$) if $|g_2| < |g_1|$ ($|g_2| > |g_1|$).

Let us also consider the low-temperature behavior of the magnetic susceptibility at zero field. We have the universal formula with logarithmic singularity given by

$$\chi_{zz}(T) \simeq \frac{1}{\pi|J|} \left[g_+^2 - g_-^2 \left(\ln \frac{\pi T}{4|J|} - C \right) \right], \quad (4.9)$$

where $C \simeq 0.5772156$ is the Euler-Mascheroni constant. As is seen from this expression, the logarithmic divergence at $T \rightarrow 0$ is a consequence of the nonuniformity of the g factors and it disappears when $g_- = 0$. This is illustrated in Fig. 4.

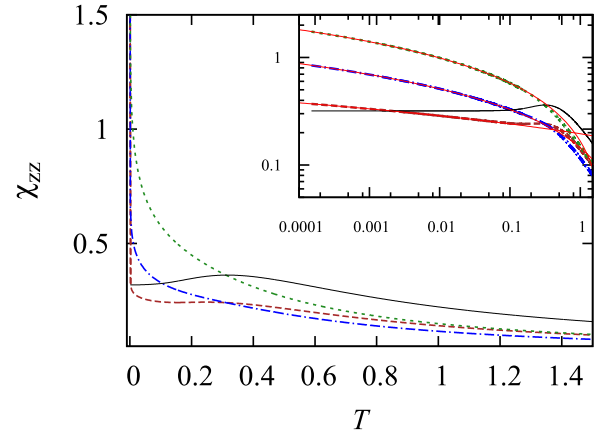


FIG. 4. Low-temperature behavior of the zero-field susceptibility for $|J| = 1$, $g_1 = 1$, and $g_2 = 1$ (solid black), $g_2 = 0.5$ (dashed brown), $g_2 = 0$ (dashed-dotted blue), and $g_2 = -0.5$ (dotted green). The inset shows the same plots in log-log scale. Thin red lines represent the asymptotic form from Eq. (4.9).

V. DYNAMIC PROPERTIES

In this section, we study dynamic quantities of the model. Dynamic properties of quantum spin-chain compounds are observable in the neutron scattering [43] and electron spin resonance (ESR) [44] experiments.

We start with the dynamic structure factor related to the inelastic neutron scattering cross section [43,45]:

$$S_{\alpha\alpha}(\kappa, \omega) = \frac{1}{N} \sum_{j=1}^N \sum_{n=1}^N \exp(ikn) \times \int_{-\infty}^{\infty} dt \exp(i\omega t) g_j g_{j+n} \langle s_j^{\alpha}(t) s_{j+n}^{\alpha} \rangle_c, \quad (5.1)$$

where $\langle s_j^{\alpha}(t) s_{j+n}^{\alpha} \rangle_c = \langle s_j^{\alpha}(t) s_{j+n}^{\alpha} \rangle - \langle s_j^{\alpha} \rangle \langle s_{j+n}^{\alpha} \rangle$ and $s_j^{\alpha}(t) = \exp(iHt) s_j^{\alpha} \exp(-iHt)$. The inclusion of the g factors in Eq. (5.1) here implies that we have the dynamic structure factors of the magnetic moments. In general, g factors may also depend on the probing field direction α . But if we imply that the ratio between g_1 and g_2 is preserved for any direction α , Eq. (5.1) will acquire a scaling factor. In the case of site-independent g factors Eq. (5.1) coincides with the definition of Refs. [46–48]. For the chain with site-dependent g factors with period 2 the dynamic structure factor has the following general structure:

$$S_{\alpha\alpha}(\kappa, \omega) = g_+^2 S_{\alpha\alpha}^0(\kappa, \omega) + g_-^2 S_{\alpha\alpha}^0(\kappa + \pi, \omega) - g_- g_+ [\bar{S}_{\alpha\alpha}^0(\kappa, \omega) + \bar{S}_{\alpha\alpha}^0(\kappa + \pi, \omega)], \quad (5.2)$$

where the uniform spin structure factor $S_{\alpha\alpha}^0(\kappa, \omega)$ and the staggered spin structure factor $\bar{S}_{\alpha\alpha}^0(\kappa, \omega)$ are defined in the standard way:

$$S_{\alpha\alpha}^0(\kappa, \omega) = \frac{1}{N} \sum_{j=1}^N \sum_{n=1}^N \exp(ikn) \times \int_{-\infty}^{\infty} dt \exp(i\omega t) \langle s_j^{\alpha}(t) s_{j+n}^{\alpha} \rangle_c,$$

$$\bar{S}_{\alpha\alpha}^0(\kappa, \omega) = \frac{1}{N} \sum_{j=1}^N \sum_{n=1}^N \exp(ikn) \times \int_{-\infty}^{\infty} dt \exp(i\omega t) (-1)^j \langle s_j^\alpha(t) s_{j+n}^\alpha \rangle_c. \quad (5.3)$$

Furthermore, we consider the $S_{zz}(\kappa, \omega)$ and $S_{xx}(\kappa, \omega)$ structure factors separately. In the former case one faces a problem of two-fermion excitations only and all calculations can be performed analytically. The latter case corresponds to the many-fermion excitation problem and requires, in general, the calculation of Pfaffians. We perform these calculations numerically [30,46–48] carefully controlling the accuracy of computations. As in previous studies on the dynamics of spin- $\frac{1}{2}$ XY chains, both structure factors exhibit some similarities. In what follows, we discuss the changes in these quantities caused by regular alternation of g factors.

The dynamic structure factors allow us to calculate the energy absorption intensities $I_\alpha(\omega, h)$, $\alpha = z, x$ observed in the ESR experiments. Following the procedure given in Appendix A of Ref. [49], we can get for the linearly polarized electromagnetic wave

$$I_\alpha(\omega, h) \propto \omega \chi''_{\alpha\alpha}(0, \omega), \quad (5.4)$$

$$\chi''_{\alpha\alpha}(0, \omega) = \frac{1 - \exp(-\beta\omega)}{2} S_{\alpha\alpha}(0, \omega),$$

where $\chi''_{\alpha\alpha}(0, \omega)$ is the imaginary part of the $\alpha\alpha$ dynamic susceptibility and $S_{\alpha\alpha}(0, \omega)$ is the corresponding dynamic structure factor at $\kappa = 0$ defined in Eq. (5.1). In the ESR experiment two configurations are distinguished [44]: (i) the Voigt configuration, when the magnetic polarization of the electromagnetic wave is collinear with the constant field, and (ii) the Faraday configuration, when the magnetic polarization of the electromagnetic wave is perpendicular to the constant field. In our model, the z [x] polarized electromagnetic wave corresponds to the Voigt [Faraday] configuration; i.e., the absorption intensity is $I_z(\omega, h)$ [$I_x(\omega, h)$]. Again, as discussed in what follows, the regularly alternating g factors change dramatically the ESR absorption intensity.

A. zz dynamics

One can work out the closed-form expression for the dynamic structure factor $S_{zz}(\kappa, \omega)$. It is given by the following expression:

$$S_{zz}(\kappa, \omega) = \int_{-\pi}^{\pi} d\kappa_1 B_+(\kappa; \kappa_1) C(\kappa; \kappa_1) \delta(\omega - D(\kappa; \kappa_1))$$

$$+ \int_{-\pi}^{\pi} d\kappa_1 B_-(\kappa; \kappa_1) C(\kappa + \pi; \kappa_1)$$

$$\times \delta(\omega - D(\kappa + \pi; \kappa_1)),$$

$$B_{\pm}(\kappa; \kappa_1) = [g_{\pm}(u_{\kappa_1} u_{\kappa_1 + \kappa} \pm v_{\kappa_1} v_{\kappa_1 + \kappa})$$

$$\mp g_{\mp}(u_{\kappa_1} v_{\kappa_1 + \kappa} \pm v_{\kappa_1} u_{\kappa_1 + \kappa})]^2,$$

$$C(\kappa; \kappa_1) = n_{\kappa_1}(1 - n_{\kappa_1 + \kappa}),$$

$$D(\kappa; \kappa_1) = \Lambda_{\kappa_1 + \kappa} - \Lambda_{\kappa_1}, \quad (5.5)$$

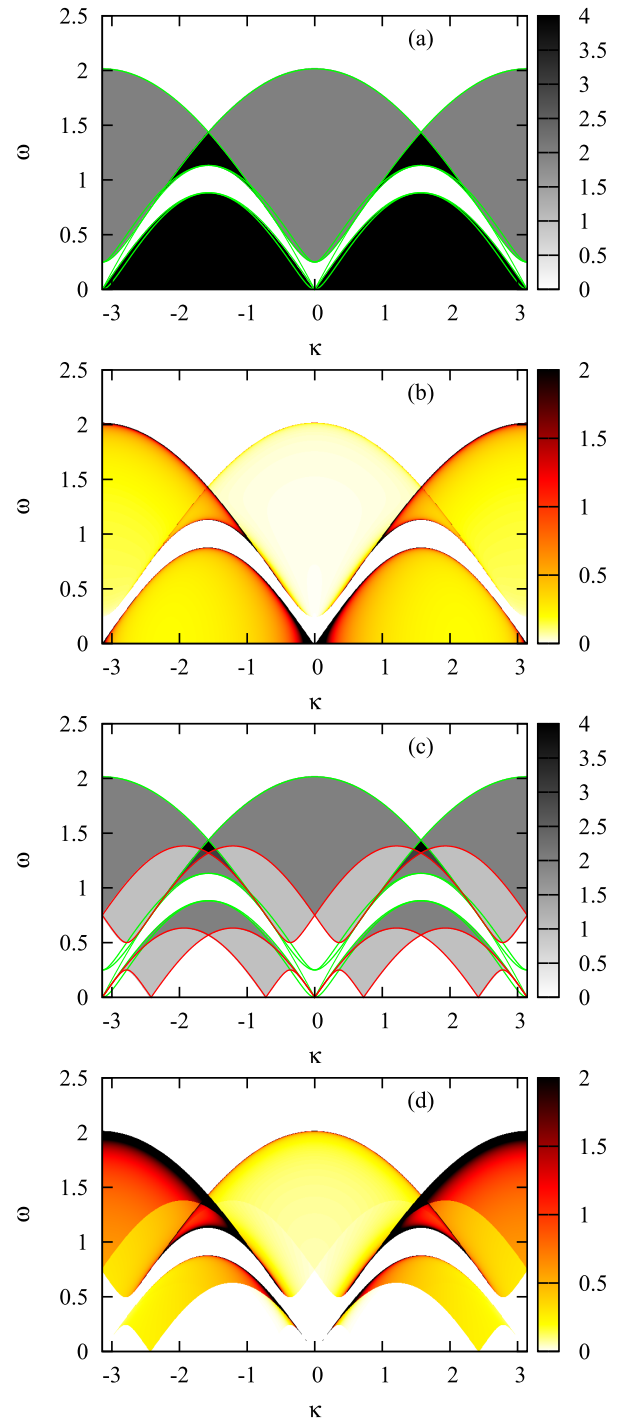


FIG. 5. Toward the dynamic structure factor $S_{zz}(\kappa, \omega)$. $|J| = 1$, $g_1 = 1$, $g_2 = 0.5$, $h = 0.5$. (a) Number of roots of two equations (5.6). (b) $S_{zz}(\kappa, \omega)$ at $T = \infty$. (c) The same as in panel (a) but taking into account the Fermi-Dirac functions at $T = 0$. (d) $S_{zz}(\kappa, \omega)$ at $T = 0$. Green and red lines are the boundaries (A1) and (A2) correspondingly.

where $n_\kappa = 1/(e^{\Lambda_\kappa/T} + 1)$ is the Fermi-Dirac function for the spinless fermions (2.8). Hence, $S_{zz}(\kappa, \omega)$ is governed exclusively by two-fermion excitation continua.

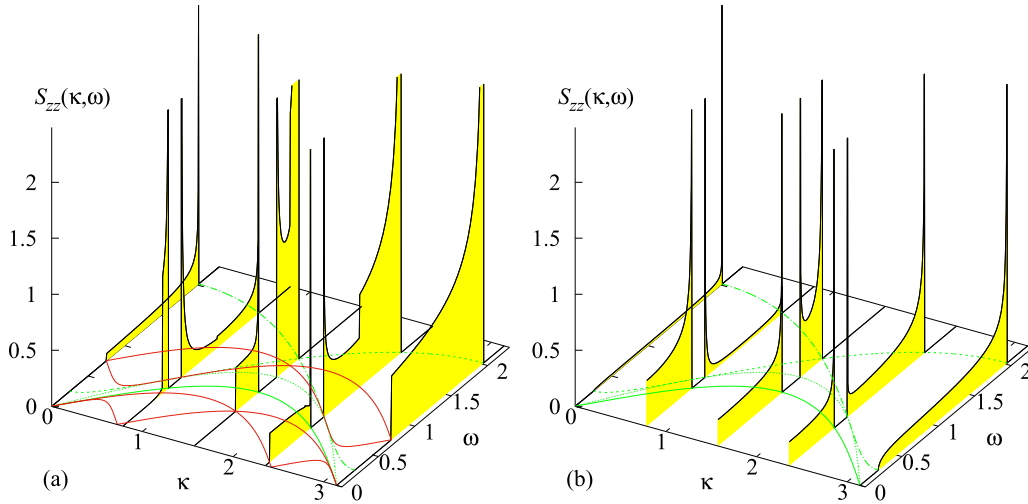


FIG. 6. $S_{zz}(\kappa, \omega)$ vs ω at $\kappa = 0, \kappa = \pi/4, \kappa = \pi/2, \kappa = 3\pi/4$, and $\kappa = \pi$. $|J| = 1, g_1 = 1, g_2 = 0.5, h = 0.5, T = 0$ (left), cf. Fig. 5(d), and $T \rightarrow \infty$ (right), cf. Fig. 5(b). Green and red lines are the boundaries (A1) and (A2) correspondingly.

Let us discuss this two-fermion quantity in more detail. For fixed κ and ω , one has to solve the equations

$$\omega - D(\kappa; \kappa_r) = 0, \quad \omega - D(\kappa + \pi; \kappa'_r) = 0, \quad (5.6)$$

i.e., to find all roots κ_r, κ'_r . Then Eq. (5.5) can be written down as follows:

$$S_{zz}(\kappa, \omega) = \sum_{\kappa_r} \frac{B_+(\kappa; \kappa_r)C(\kappa; \kappa_r)}{A(\kappa; \kappa_r)} + \sum_{\kappa'_r} \frac{B_-(\kappa; \kappa'_r)C(\kappa + \pi; \kappa'_r)}{A(\kappa + \pi; \kappa'_r)}, \quad (5.7)$$

where

$$A(\kappa; \kappa_1) = \left| \frac{\partial D(\kappa; \kappa_1)}{\partial \kappa_1} \right| = J^2 \left| \frac{|\cos(\kappa_1 + \kappa)| \sin(\kappa_1 + \kappa)}{\sqrt{J^2 \cos^2(\kappa_1 + \kappa) + g_-^2 h^2}} - \frac{|\cos \kappa_1| \sin \kappa_1}{\sqrt{J^2 \cos^2 \kappa_1 + g_-^2 h^2}} \right|. \quad (5.8)$$

In Fig. 5(a) we show (for a representative set of parameters) the regions in the κ - ω plane where Eqs. (5.6) have four roots (black), two roots (gray) or no roots (white). In other words, we plot $S_{zz}(\kappa, \omega)$ (5.7) assuming $A(\kappa; \kappa_1) = A(\kappa + \pi; \kappa_1) = 1$ as well as $B_{\pm}(\kappa; \kappa_1) = 1$ and $C(\kappa; \kappa_1) = C(\kappa + \pi; \kappa_1) = 1$. Clearly, the dynamic structure factor $S_{zz}(\kappa, \omega)$ is identically zero within the white regions in the κ - ω plane [Eqs. (5.6) have no roots]. Furthermore, any two-fermion quantity has some structure coming from the factors $1/A(\kappa; \kappa_1)$ and $1/A(\kappa + \pi; \kappa_1)$. This is nicely seen in the infinite-temperature limit when $C(\kappa; \kappa_1) = C(\kappa + \pi; \kappa_1) = 1/4$ shown in Fig. 5(b). Next, deviating from the infinite-temperature limit we have to examine the effect of the Fermi-Dirac functions in Eq. (5.7) which may suppress the dynamic structure factor $S_{zz}(\kappa, \omega)$ even in the gray or black regions, especially at $T = 0$. In Fig. 5(c) we show the effect of the ground-state Fermi-Dirac distributions for the same set of parameters [we plot $S_{zz}(\kappa, \omega)$ (5.7) assuming $A(\kappa; \kappa_1) = A(\kappa + \pi; \kappa_1) = 1$ and

$B_{\pm}(\kappa; \kappa_1) = 1$]. In addition to the two- and four-root regions, the regions with one and three roots, surviving after the thermodynamic averaging, come into play [compare Figs. 5(c) and 5(a)]. Moreover, some previously allowed regions become white at $T = 0$ signaling the action of the Fermi-Dirac functions in the ground state. The final gray-scale plot of the zz dynamic structure factor (5.7) at $T = 0$ is presented in Fig. 5(d). The frequency profiles for the chosen set of parameters are also plotted in Fig. 6 complementing the gray-scale plot in Figs. 5(b) and 5(d). It is clearly seen that the zz dynamic structure factor at $T \rightarrow \infty$ shows the van Hove divergence at the edges of the two-fermion continua which is typical for the XX chains (see Refs. [30,47,48] for a review). $S_{zz}(\kappa, \omega)$ in the ground state [Fig. 5(d)] demonstrates even richer behavior due to the steplike form of the Fermi-Dirac functions [see Figs. 5(c), 5(d) and Fig. 6(a)]. The analytical formulas for the boundaries of the two-fermion continua are given in the Appendix.

We can understand the reported findings taking into account that the dynamic structure factor $S_{zz}(\kappa, \omega)$ is governed by two-fermion continua. The general effect of alternating g factors can be understood from Figs. 7, 8, and 9, where some results for $S_{zz}(\kappa, \omega)$ for different fields h and values of g_2 at $T = 0$ are collected. The decreasing of g_2 from 1 to -1 at fixed value of magnetic field h and $g_1 = 1$ leads to redistribution of the intensity of the zz dynamic structure factor from the boundary to the center of the Brillouin zone. For $g_2 \in (0, 1)$, there are two regions with $S_{zz}(\kappa, \omega) \neq 0$ (top and bottom) which are disconnected; see Figs. 7(b), 8(b) and 9(b). The distances between these top and bottom regions increase with decreasing g_2 and with increasing h . For $g_2 \in [-1, 0]$, the increasing of the magnetic field h leads to redistribution of the intensity of the zz dynamic structure factor to higher frequencies.

Let us consider the effect of changes in the g factors and h in more detail. At zero field, the zz structure factor is extremely simple [see Eqs. (5.2) and (5.3)] and can be presented as a sum of two contributions for the uniform model shifted by π along the wave-vector axis [i.e., Eq. (5.2) in the case of

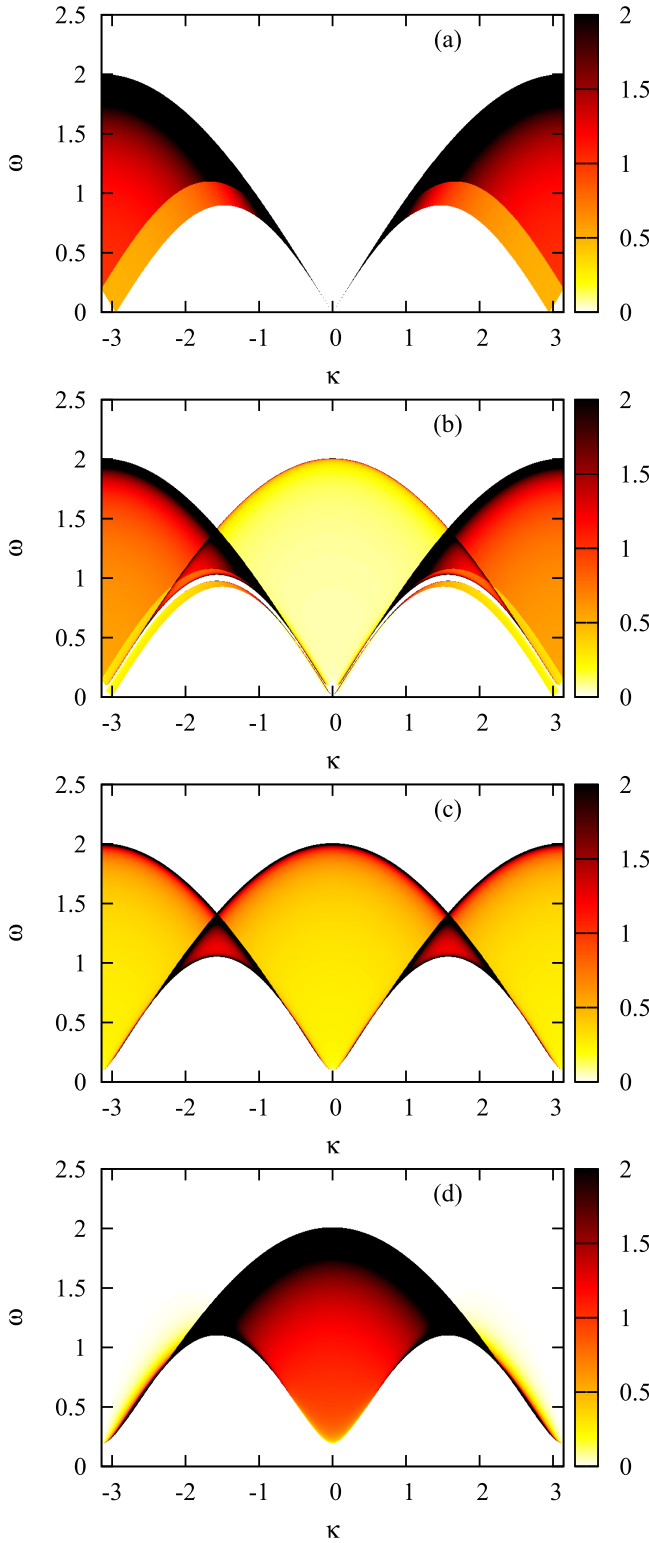


FIG. 7. The density plot of the dynamic structure factor $S_{zz}(\kappa, \omega)$ at $T = 0$: $|J| = 1$, $g_1 = 1$, $g_2 = 1$ (a), $g_2 = 0.5$ (b), $g_2 = 0$ (c), $g_2 = -1$ (d), $h = 0.1$.

zero staggered spin structure factor $\bar{S}_{zz}^0(\kappa, \omega)$]. It is definitely also the case of a small field (see Fig. 7 for $h = 0.1$). It is clearly seen that at small h , the deviation of g_2 from $g_1 = 1$ induces a tiny strip of new two-fermion continuum at lower

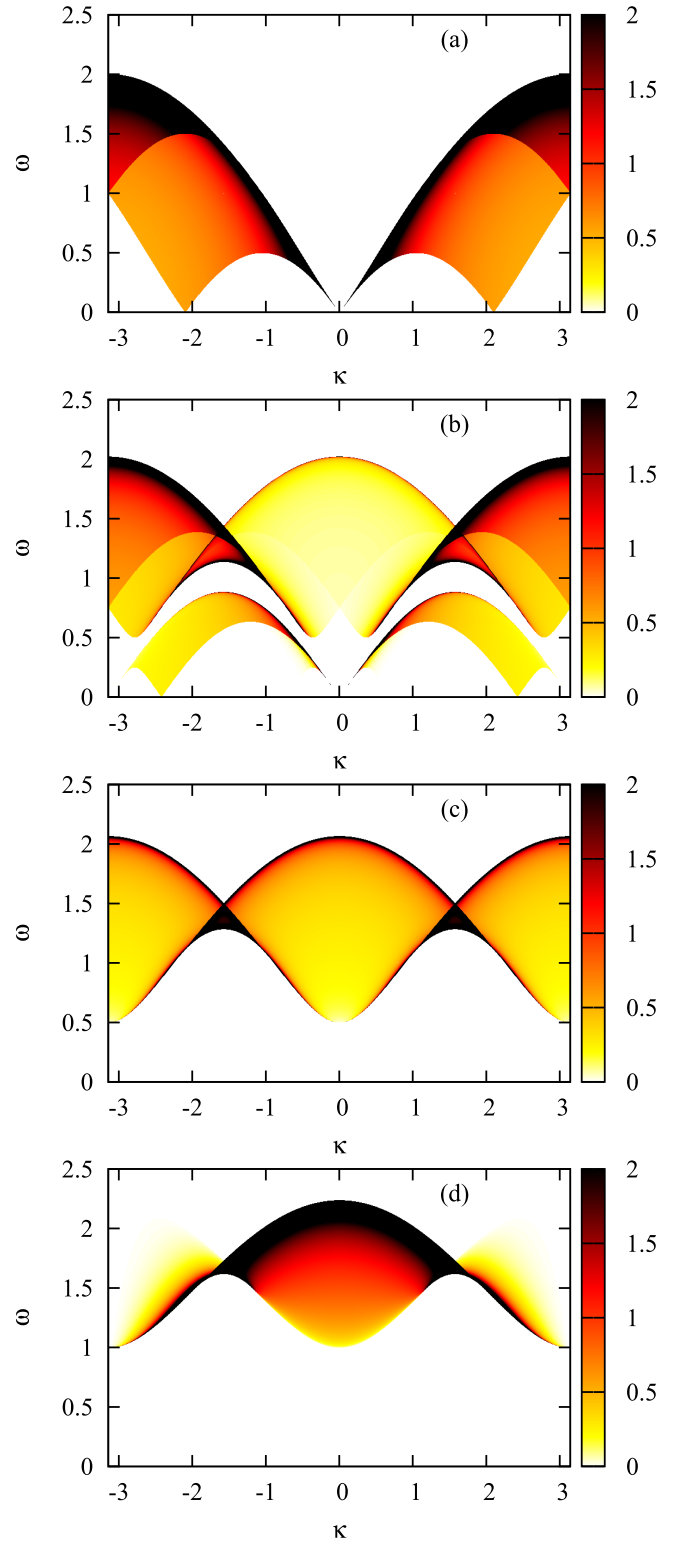


FIG. 8. The density plot of the dynamic structure factor $S_{zz}(\kappa, \omega)$ at $T = 0$: $|J| = 1$, $g_1 = 1$, $g_2 = 1$ (a), $g_2 = 0.5$ (b), $g_2 = 0$ (c), $g_2 = -1$ (d), $h = 0.5$.

frequencies. The intensity of this low-energy two-fermion continuum wanes with decreasing g_2 . Surprisingly, $S_{zz}(\kappa, \omega)$ for $g_2 \leq 0$ does not show any trace of the low-energy continuum anymore [see Figs. 7(c), 7(d)]: The zz structure factor

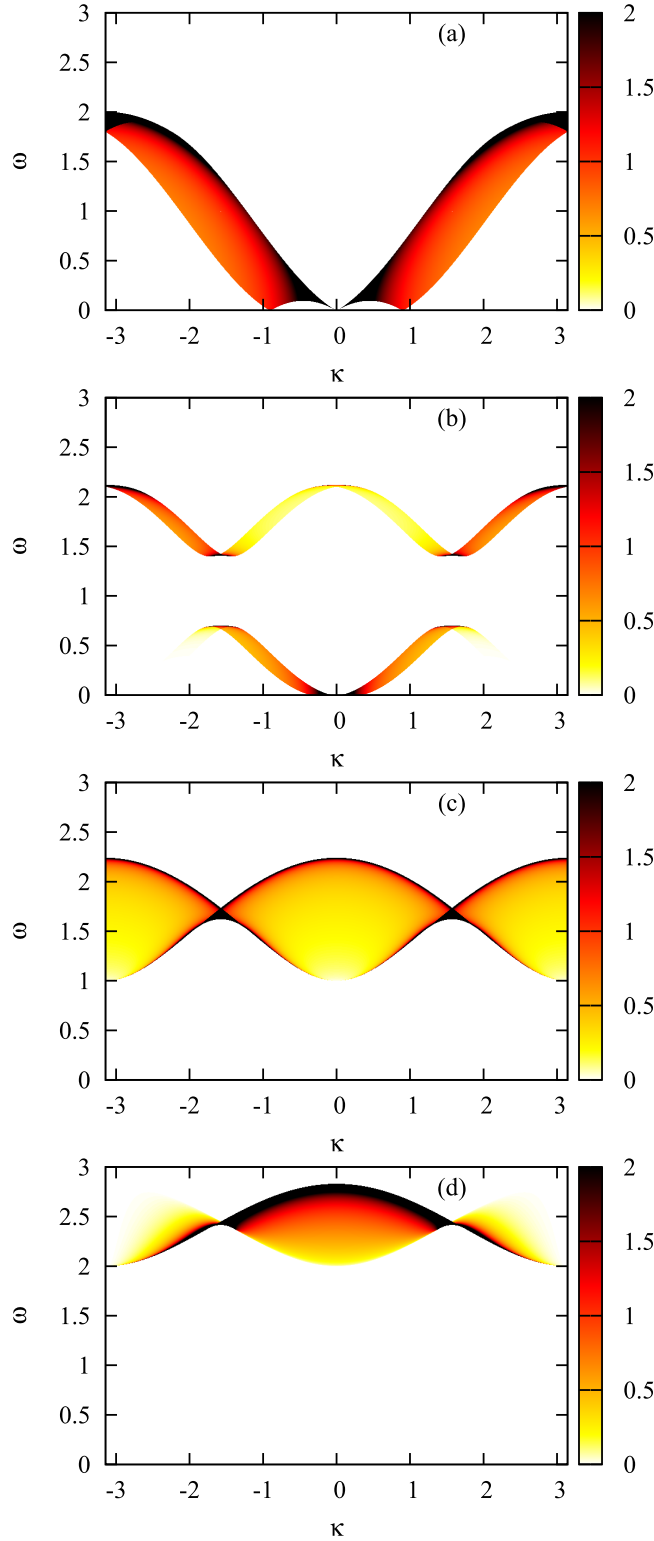


FIG. 9. The density plot of the dynamic structure factor $S_{zz}(\kappa, \omega)$ at $T = 0$: $|J| = 1$, $g_1 = 1$, $g_2 = 1$, $h = 0.9$ (a), $g_2 = 0.5$, $h = 1.4$ (b), $g_2 = 0$, $h = 1$ (c), $g_2 = -1$, $h = 1$ (d).

shows one two-fermion continuum only. In contrast to $h = 0$, at small fields, two opposite cases $g_2 = 1$ and $g_2 = -1$ are not identical [compare Fig. 7(a) and Fig. 7(d)].

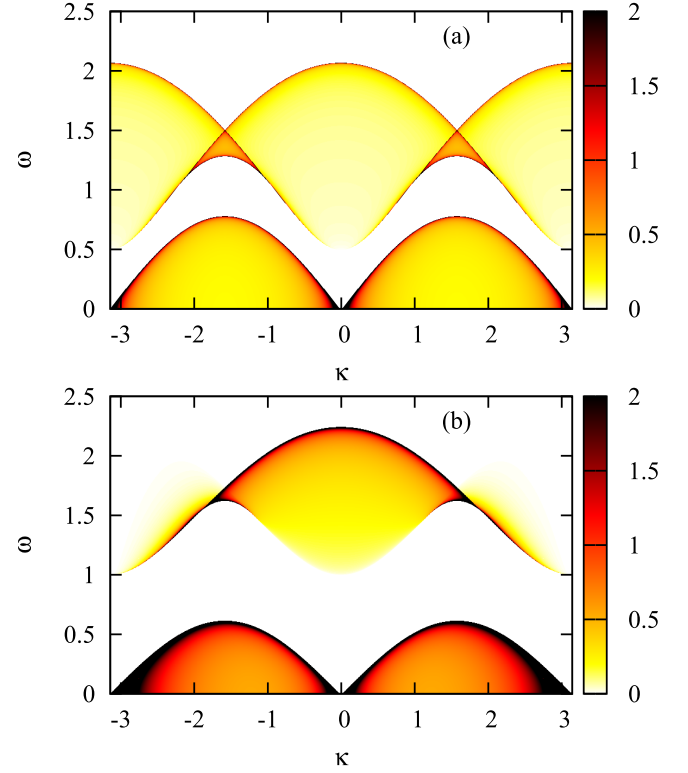


FIG. 10. The density plot of the dynamic structure factor $S_{zz}(\kappa, \omega)$ at $T \rightarrow \infty$: $|J| = 1$, $g_1 = 1$, $h = 0.5$, $g_2 = 0$ (a), $g_2 = -1$ (b).

At higher fields, the magnetic structure factor cannot be approximated by the sum of uniform spin structure factors $S_{zz}^0(\kappa, \omega)$ anymore. Even for a moderate alternation of g factors [$g_1 = 1$, $g_2 = 0.5$ in Fig. 8(b)] we observe the appearance of another two-fermion continuum at lower frequencies. It can be treated as a splitting of the initial continuum inherent in the uniform model [see Fig. 8(a)] into two parts, which is a signal of the two-band structure of the fermion excitation spectrum (2.8). It should be noted that the two-fermion continuum at lower frequencies induced by small deviation of g_2 (from $g_1 = 1$) is not a tiny strip anymore as it was at small fields ($h = 0.1$). At higher fields as well as at small ones, the zz structure factor for $g_2 \leq 0$ shows just one two-fermion continuum only [Figs. 8(c), 8(d)]. This picture keeps the tendency with increasing field as shown in Fig. 9. In the two top panels we present results at magnetic fields close to h_s whereas for $g_1 g_2 \leq 0$ we put $h = 1$ [Figs. 9(c), 9(d)], because at $g_1 g_2 \leq 0$ the saturation field does not exist. The fact that in Fig. 9(b) both the low-energy and high-energy two-fermion continua are tiny strips is caused by the field being very close to h_s .

We also examine the temperature effect on the zz structure factor for nonpositive $g_2 \leq 0$. The results for $T \rightarrow \infty$ in Fig. 10 show an additional two-fermion continuum for low frequencies. In the case of zero temperature this continuum was hidden owing to the Fermi-Dirac functions; compare Fig. 10 to Fig. 8.

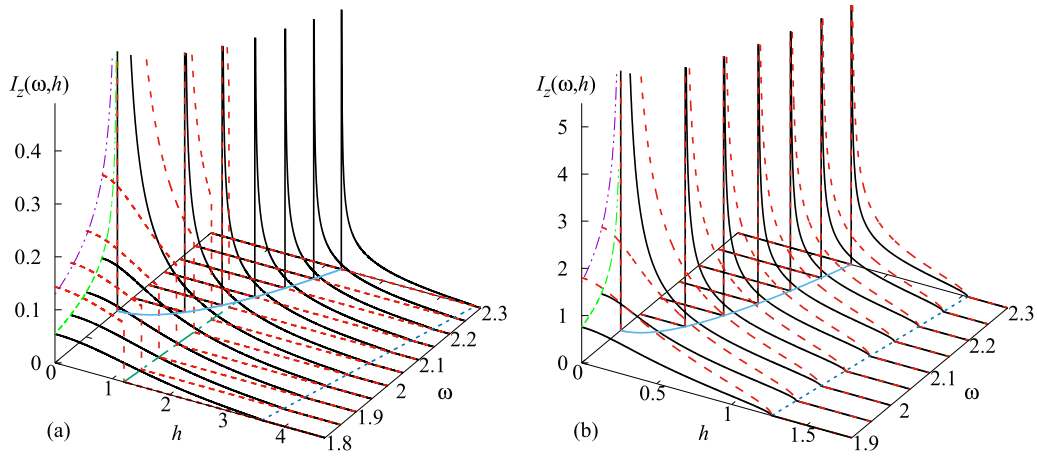


FIG. 11. Field profiles of the absorption intensity $I_z(\omega, h)$ at different frequencies ω for $|J| = 1$, $g_1 = 1$, $g_2 = 0.5$ (a), $g_2 = -0.5$ (b), and temperatures $T = 1$ (solid black curves) and $T = 0$ (dashed red curves). The dashed-dot-dot violet (dashed green) curve indicates the intensity at $h = 0$ and $T = 0$ ($T = 1$). The solid and short-dashed blue curves show the boundaries given in Eq. (5.10) while the dashed-dot green curve in panel (a), given by $h = \omega/(2|g_+|)$, denotes the upper boundary of $I_z(\omega, h)$ at $T = 0$ (see the discussion in the text).

In the case $\kappa = 0$, Eq. (5.5) can be transformed to the following form:

$$S_{zz}(0, \omega) = \delta(\omega) \int_{-\pi}^{\pi} dk_1 (g_+ - 2g_- u_{k_1} v_{k_1})^2 n_{k_1} (1 - n_{k_1}) + \frac{g_-^2 \sqrt{\omega^2 - 4g_-^2 h^2}}{\omega \sqrt{4J^2 + 4g_-^2 h^2 - \omega^2}} \sum_{\kappa_r} n_{\kappa_r} (1 - n_{\kappa_r + \pi}), \quad (5.9)$$

where κ_r are solutions of the equation $\omega = \Lambda_{\kappa_r + \pi} - \Lambda_{\kappa_r}$. The latter equation has solutions only in the restricted region

$$2|g_- h| \leq \omega < 2\sqrt{J^2 + g_-^2 h^2}. \quad (5.10)$$

We can use Eqs. (5.9) and (5.4) to get explicit expressions for the absorption intensity $I_z(\omega, h)$:

$$I_z(\omega, h) \propto \frac{g_-^2 \sqrt{\omega^2 - 4g_-^2 h^2}}{\sqrt{4J^2 + 4g_-^2 h^2 - \omega^2}} \times \frac{1 - \exp(-\beta\omega)}{\{1 + \exp[\beta(g_+ h - \frac{\omega}{2})]\} \{1 + \exp[-\beta(g_+ h + \frac{\omega}{2})]\}}. \quad (5.11)$$

In the ground state we arrive at the following formula:

$$I_z(\omega, h) \propto \frac{g_-^2 \sqrt{\omega^2 - 4g_-^2 h^2}}{\sqrt{4J^2 + 4g_-^2 h^2 - \omega^2}}, \quad (5.12)$$

where in the case of $g_1 g_2 > 0$ the Fermi-Dirac functions shrink further the condition of allowed ω [see Eq. (5.10)] to the following one: $2|g_+ h| < \omega < 2\sqrt{J^2 + g_-^2 h^2}$.

It is evident from Eq. (5.11) that there is no energy absorption in the case of the uniform g factors ($g_1 = g_2 = 1$), since the total magnetization commutes with the Hamiltonian. The alternation of g factors destroys this property and leads immediately to nonzero absorption intensity $I_z(\omega, h)$. From Eqs. (5.12) and (5.11) one can deduce the shape of the absorption line. The field profiles of the absorption intensity for alternating g factors are shown in Fig. 11. The absorption intensity curve $I_z(\omega, h)$ for any frequency ends continuously at $h = \omega/(2|g_-|)$ for both $T = 0$, $g_1 g_2 < 0$ and $T > 0$ cases. This is clearly seen in Figs. 11(a) and 11(b), the short-dashed blue line. If the frequency exceeds $2|J|$, we observe also a van Hove singularity at $h = \sqrt{\omega^2 - 4J^2}/(2|g_-|)$ [see Figs. 11(a) and 11(b), the solid blue line]. In the ground state for $g_1 g_2 > 0$ this singularity disappears at $\omega = 2|J|/\sqrt{1 - (g_-/g_+)^2}$. If $\omega < 2|J|/\sqrt{1 - (g_-/g_+)^2}$ for zero temperature and $g_1 g_2 > 0$, the absorption intensity curve $I_z(\omega, h)$ ends abruptly at $h = \omega/(2|g_+|)$ [see Fig. 11(a), dashed-dot green line], and at $\omega > 2|J|/\sqrt{1 - (g_-/g_+)^2}$ this ground-state absorption intensity vanishes, $I_z(\omega, h) = 0$.

B. xx dynamics

We pass to another dynamic structure factor, namely, the xx structure factor $S_{xx}(\kappa, \omega)$. We perform the computation of the xx time correlation functions numerically using the previously elaborated method [30,46,47]. In what follows, we consider the finite chain of $N = 400$ spins with open boundary conditions. To avoid the boundary effect, we have to adapt Eq. (5.1). Thus, we choose a “central” spin at the site $j = 61, 81$ (depending on the adopted parameters) and then calculate the time correlation functions $\langle s_j^x(t) s_{j+n}^x \rangle$ as well as $\langle s_{j+1}^x(t) s_{j+n+1}^x \rangle$ for $n \geq 0$. Finally, we present the Fourier transform in Eq. (5.1) in the following

symmetrized form:

$$S_{xx}(\kappa, \omega) = \frac{1}{2} \text{Re} \int_0^\infty dt e^{-\epsilon t} e^{i\omega t} \left\{ g_1^2 \left[\langle s_j^x(t) s_j^x \rangle + 2 \sum_{n=1}^{\frac{N}{2}} \cos(2n\kappa) \langle s_j^x(t) s_{j+2n}^x \rangle \right] + 2g_1 g_2 \sum_{n=1}^{\frac{N}{2}} \cos[(2n-1)\kappa] \langle s_j^x(t) s_{j+2n-1}^x \rangle \right. \\ \left. + g_2^2 \left[\langle s_{j+1}^x(t) s_{j+1}^x \rangle + 2 \sum_{n=1}^{\frac{N}{2}} \cos(2n\kappa) \langle s_{j+1}^x(t) s_{j+1+2n}^x \rangle \right] + 2g_1 g_2 \sum_{n=1}^{\frac{N}{2}} \cos[(2n-1)\kappa] \langle s_{j+1}^x(t) s_{j+1+2n-1}^x \rangle \right\}. \quad (5.13)$$

In numerical calculations we restrict the sum over n up to $10 \dots 50$ depending on the correlation length.

The results of the numerical calculation for $S_{xx}(\kappa, \omega)$ at sufficiently low temperature $T = 0.1$ are shown in Figs. 12–15. In contrast to the zz structure factor, $S_{xx}(\kappa, \omega)$ is not governed exclusively by the continuum of two-fermion excitations. However, the deeper inspection of Figs. 12–15 reveals some resemblance between the zz and xx structure factors. Although there are no singular parts visible in $S_{xx}(\kappa, \omega)$ as well as abrupt boundaries for the regions with nonzero values, the dominating contribution in the case of positive g_2 is circumscribed by the boundaries of the two-fermion continua outlined in the Appendix. The same feature was demonstrated earlier for the uniform and dimerized XX chains [47,48]. We can deduce from relation (5.2) and Fig. 12 that the staggered spin structure factor (5.3) is minor at small fields. Thus, one can observe how the intensity of the structure factor $S_{xx}(\kappa, \omega)$ is redistributed between two basic continua of the uniform chain [see Fig. 12(a)] shifted by π with respect to each other when g_2 decreases from 1 up to negative values. One can still recognize the similar feature even at intermediate field $h = 0.5$ in the case of $g_2 > 0$ in Fig. 13(b) where the combination of two continua of $S_{xx}^0(\kappa, \omega)$ and $S_{xx}^0(\kappa + \pi, \omega)$ creates an intricate intensity picture.

Interestingly, the structure factor $S_{xx}(\kappa, \omega)$ for nonpositive $g_2 \leq 0$ is concentrated mainly along the lines

$$\lambda_\kappa^\pm = \sqrt{J^2 \sin^2 \kappa + g_-^2 h^2} \pm g_+ h. \quad (5.14)$$

Although the exact xx correlation functions and the exact xx structure factor are not known for $g_1 g_2 < 0$, one can adapt the procedure of Refs. [48,50] for the case of the uniform and dimerized chains above the saturation field. We need to make the crucial assumption that the action of the Jordan-Wigner phase factors on the ground state is equivalent to its action on the ideal antiferromagnetic state. Then, the problem is reduced to calculation of the pair correlation functions for spinless fermions with the final result

$$S_{xx}(\kappa, \omega) \approx \frac{\pi}{4} \{ [g_+^2 + g_-^2 + 4g_+ g_- \text{sgn}(h) u_{\kappa+\pi/2} |v_{\kappa+\pi/2}|] \delta(\omega - \lambda_\kappa^+) + [g_+^2 + g_-^2 - 4g_+ g_- \text{sgn}(h) u_{\kappa+\pi/2} |v_{\kappa+\pi/2}|] \delta(\omega - \lambda_\kappa^-) \}. \quad (5.15)$$

Equation (5.15) although approximate, agrees with numerics shown in Figs. 13 and 14 for negative g_2 (dashed and dashed-dot lines).

If $g_2 \in (0, 1]$ for magnetic fields close to h_s , the many-fermion continua shrink [see Figs. 14(a) and 14(b)] and above

the saturation fields they reduce to the one-fermion excitation spectrum shifted by π along the κ axis with the reversed sign [i.e., $-\Lambda_{\kappa+\pi}$; dashed line in Figs. 14(a), 14(b)] and if $g_2 \in (0, 1)$, also by the one-fermion excitation spectrum multiplied by -1 [i.e., $-\Lambda_\kappa$; dashed-dot line in Fig. 14(b)],

$$S_{xx}(\kappa, \omega) = \frac{\pi}{2} [(g_+ u_\kappa - g_- v_\kappa)^2 \delta(\omega - \Lambda_\kappa) + (g_+ v_\kappa + g_- u_\kappa)^2 \delta(\omega - \Lambda_{\kappa+\pi})], \quad \text{if } h < -h_s, \\ S_{xx}(\kappa, \omega) = \frac{\pi}{2} [(g_+ v_\kappa - g_- u_\kappa)^2 \delta(\omega + \Lambda_\kappa) + (g_+ u_\kappa + g_- v_\kappa)^2 \delta(\omega + \Lambda_{\kappa+\pi})], \quad \text{if } h > h_s. \quad (5.16)$$

In the case of $g_2 \leq 0$, in Figs. 14(c) and 14(d) we observe for higher field an even more pronounced mode along the lines given in Eq. (5.14).

In Fig. 15 we show the frequency profiles of the structure factor for several values of $\kappa = 0, \pi/4, \pi/2, 3\pi/4, \pi$. It is clearly seen there that the nonuniform g factor leads to a many-peak structure in the frequency dependencies of $S_{xx}(\kappa, \omega)$ at the low temperature $T = 0.1$; see Fig. 15(a). In contrast, the infinite temperature smears out the fine structure of $S_{xx}(\kappa, \omega)$ transforming the frequency profiles into κ -independent Gaussian ridges; see Fig. 15(b). Such a form can be obtained using the exact results for the time correlation functions of dimerized chain [51]. Those correlation functions vanish if the sites are different, which leads to a κ -independent structure factor $S_{xx}(\kappa, \omega)$. Utilizing the result of Ref. [51], we get the following explicit formula for $S_{xx}(\kappa, \omega)$ at $T \rightarrow \infty$:

$$S_{xx}(\kappa, \omega) = \frac{1}{8} \int_{-\infty}^{\infty} dt e^{i\omega t} \text{Re} \{ g_1^2 Z_o(t) + g_2^2 Z_e(t) \}, \\ Z_e(t) = \frac{\theta_3(z, q)}{\theta_3(z_0, q)} \frac{\theta_2(z', q)}{\theta_2(z'_0, q)} \exp \left[ig_+ ht - \left(1 - \frac{E(\tilde{z})}{K(\tilde{z})} \right) J_+^2 t^2 \right], \\ Z_o(t) = \exp(i2g_+ ht) Z_e^*(t), \\ J_\pm = \frac{1}{2} (\sqrt{J^2 + g_-^2 h^2} \pm |g_- h|), \\ \tilde{z} = \frac{J_-}{J_+} = \frac{J^2}{(\sqrt{J^2 + g_-^2 h^2} + |g_- h|)^2}, \\ q = \exp \left(-\frac{\pi K(\sqrt{1 - \tilde{z}^2})}{K(\tilde{z})} \right), \quad (5.17)$$

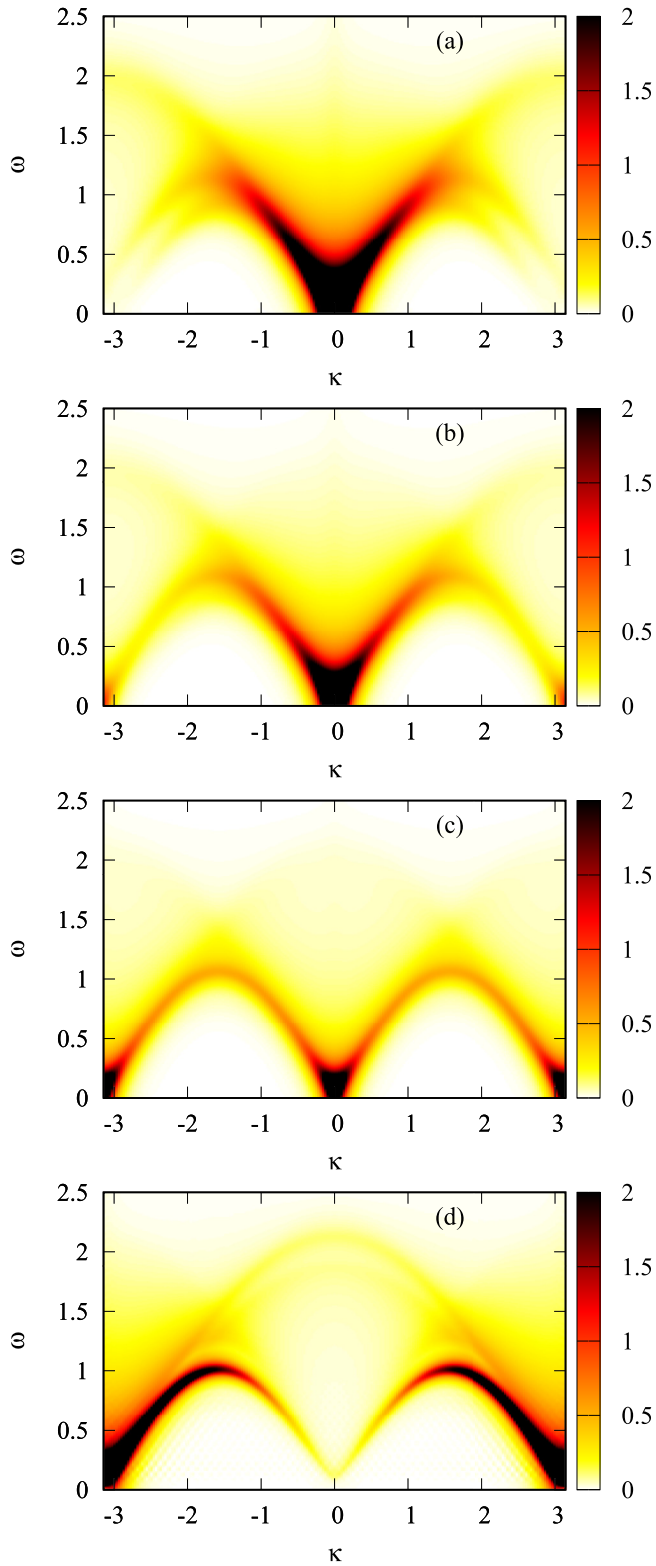


FIG. 12. The density plot of the dynamic structure factor $S_{xx}(\kappa, \omega)$. $J = -1$, $g_1 = 1$, $g_2 = 1$ (a), $g_2 = 0.5$ (b), $g_2 = 0$ (c), $g_2 = -1$ (d), $h = 0.1$ at low temperature $T = 0.1$.

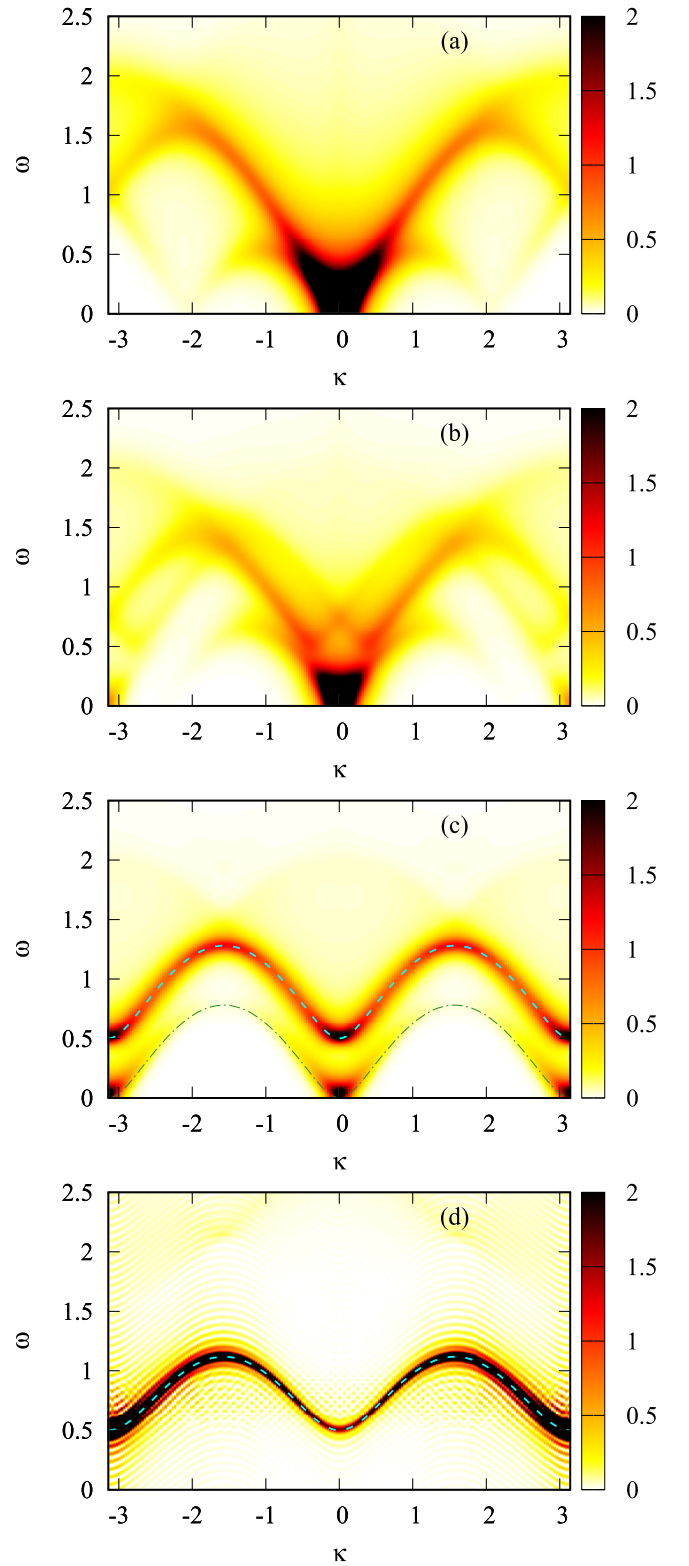


FIG. 13. The density plot of the dynamic structure factor $S_{xx}(\kappa, \omega)$. $J = -1$, $g_1 = 1$, $g_2 = 1$ (a), $g_2 = 0.5$ (b), $g_2 = 0$ (c), $g_2 = -1$ (d), $h = 0.5$ at low temperature $T = 0.1$. Dashed and dashed-dot curves follow Eq. (5.14).

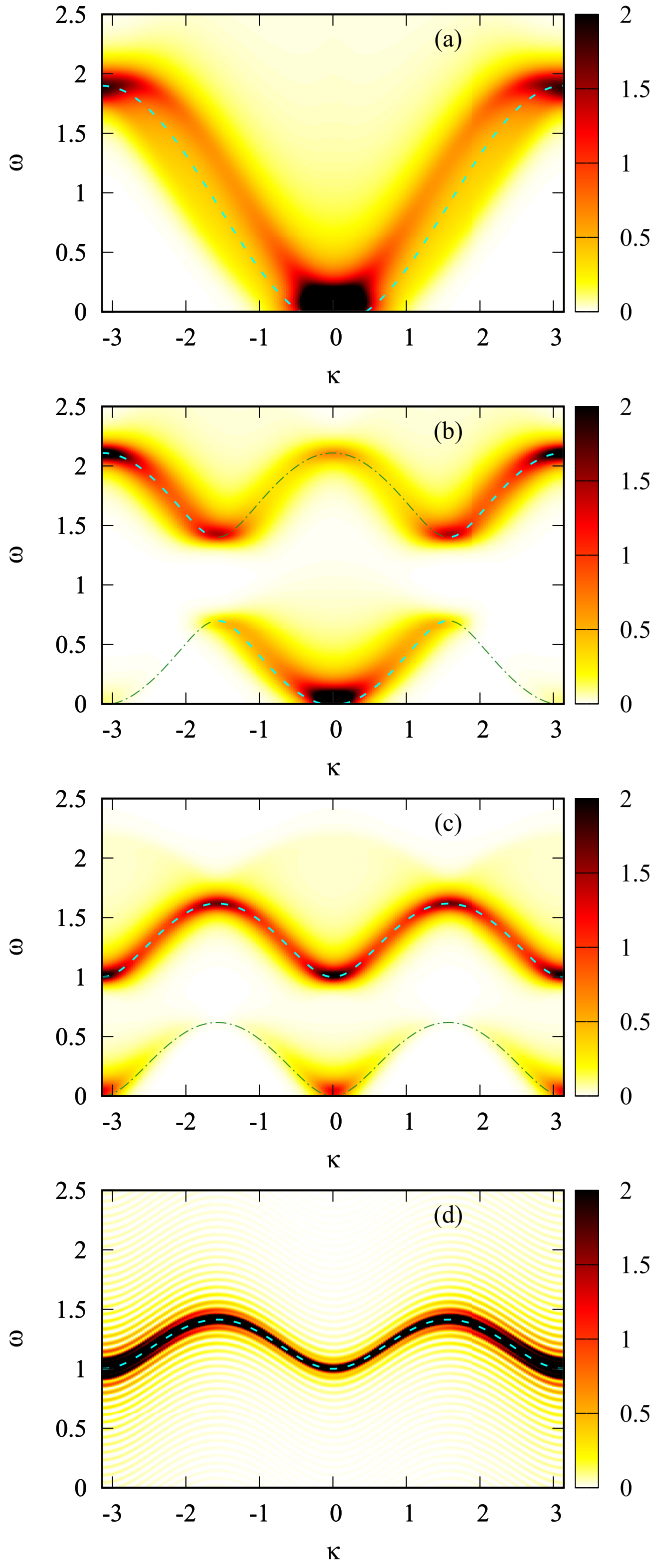


FIG. 14. The density plot of the dynamic structure factor $S_{xx}(\kappa, \omega)$. $J = -1$, $g_1 = 1$, $g_2 = 1$, $h = 0.9$ (a), $g_2 = 0.5$, $h = 1.4$ (b), $g_2 = 0$, $h = 1$ (c), $g_2 = -1$, $h = 1$ (d) at low temperature $T = 0.1$. Dashed and dashed-dot curves in panels (a) and (b) correspond to $-\Lambda_{\kappa+\pi}$ and $-\Lambda_{\kappa}$. Dashed and dashed-dot curves in panels (c), (d) follow Eq. (5.14).

where $\theta_2(z', q)$, $\theta_3(z, q)$ are the Jacobi theta functions (see [51] and references therein) with

$$z = \frac{\pi(J_+ t + i v_0)}{2K(\tilde{\kappa})}, \quad z' = \frac{\pi(J_+ t - i v_0)}{2K(\tilde{\kappa})}, \quad (5.18)$$

$$z_0 = \frac{i\pi v_0}{2K(\tilde{\kappa})}, \quad z'_0 = -\frac{i\pi v_0}{2K(\tilde{\kappa})},$$

and the parameter v_0 is defined by the following relation:

$$\text{dc}(i v_0, \tilde{\kappa}) = \frac{J}{2J_+}, \quad (5.19)$$

where $\text{dc}(i v_0, \tilde{\kappa}) = \text{dn}(v_0, 1 - \tilde{\kappa}^2)$ is the elliptic delta amplitude function for imaginary argument.

In the case of strong magnetic field h and nonuniform g factors $g_- \neq 0$ we have $\tilde{\kappa} \ll 1$. Expanding the correlation functions for small $\tilde{\kappa}$, we get the xx structure factor in the explicit Gaussian form:

$$S_{xx}(\kappa, \omega) \approx \frac{\sqrt{2\pi}}{4|J|} \left[A_- \left(e^{-\frac{(\omega+\omega_-)^2}{2J_-^2}} + e^{-\frac{(\omega-\omega_-)^2}{2J_-^2}} \right) + A_+ \left(e^{-\frac{(\omega+\omega_+)^2}{2J_+^2}} + e^{-\frac{(\omega-\omega_+)^2}{2J_+^2}} \right) \right],$$

$$\omega_{\pm} = J_{\pm} \pm g_{\pm} h,$$

$$A_{\pm} = (g_+^2 + g_-^2) \frac{J_+}{|J|} \pm g_+ g_- \sqrt{\frac{4J_+^2}{J^2} - 1}. \quad (5.20)$$

From Eq. (5.20) it is clear that the intensity of the xx structure factor in the infinite-temperature limit is concentrated near two Gaussian peaks at $\omega = \omega_{\pm}$.

In Fig. 16 we present the absorption intensity $I_x(\omega, h)$ as a function of the magnetic field. In contrast to the $I_z(\omega, h)$ case, here the field profiles do not exhibit any singularities. A prominent feature of the absorption profiles $I_x(\omega, h)$ is a two-peak structure for the case of different nonzero g factors. The cases $g_2 = 0.5$ and $g_2 = -0.5$ demonstrate additional satellite peaks [Figs. 16(b), 16(d)]. For the uniform chain ($g_1 = g_2$) we can see one peak which moves with increasing of frequency to a higher value of magnetic field [Fig. 16(a)]. Qualitatively the same picture is seen for $g_2 = 0$ in Fig. 16(c), where the peak is less steeper in comparison to the case in Fig. 16(a).

VI. SUMMARY

To summarize, we have studied the effect of the alternation of g factors on the static and dynamic properties of the spin- $\frac{1}{2}$ XX chain in a transverse field. The crucial point is that the conservation of the total magnetization is lost in this case. This evokes nontrivial changes in the thermodynamic and dynamic behavior of the model.

While the logarithmic peculiarities of the magnetization and the susceptibility at $T = 0$ were obtained earlier [13], we found peculiarities in the low-temperature thermodynamics. In particular, we have shown that the specific heat can change its behavior from the linear dependence in the spin-liquid phase to the $\sqrt{T}$ dependence at the saturation field, and finally transformed to the exponential law (4.8). The susceptibility at

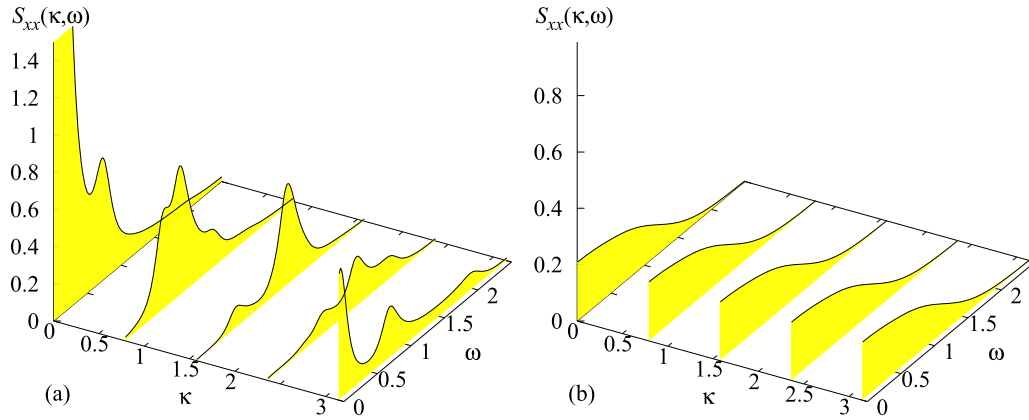


FIG. 15. $S_{xx}(\kappa, \omega)$ vs ω at $\kappa = 0, \kappa = \pi/4, \kappa = \pi/2, \kappa = 3\pi/4$, and $\kappa = \pi$. $J = -1, g_1 = 1, g_2 = 0.5, h = 0.5, T = 0.1$ (a), cf. Fig. 13, and $T \rightarrow \infty$ (b).

zero magnetic field displays the logarithmic divergence with temperature as it follows in Eq. (4.9).

We have performed a detailed study of the dynamic properties. We calculated the dynamic structure factors $S_{zz}(\kappa, \omega)$ and $S_{xx}(\kappa, \omega)$ and inspected how they change in the external magnetic field for different period-2 alternations of g factors. In the case when both g factors are of the same sign, the correspondence between the boundaries of the zz and xx structure factors is still present as was observed previously [47,48]. On the contrary, if $g_1 g_2 \leq 0$, a large enough magnetic field leads to the highly intense modes in the xx structure factor. In addition, we calculated the absorption intensity $I_\alpha(\omega, h)$ for the different configuration of ESR experiments. In the Voigt configuration ($\alpha = z$), the model with uniform g factors does not have any response. In the case when g_2 differs from g_1 , we obtain the nonzero contribution to the absorption intensity. For sufficiently large frequencies $\omega > 2|J|$ the van Hove singularity arises at $h = \sqrt{\omega^2 - 4J^2}/(2|g_-|)$. In the Faraday configuration ($\alpha = x$), the situation is a bit different. The ab-

sorption spectra can be observed in the uniform case. It shows a broad maximum at some resonance field. The alternation of g factors leads to the doubling of this resonance line. Although in our study we focus on the exactly solvable XX chain, from Ref. [28] we know that such analysis of dynamics is useful for understanding a more realistic case of the Heisenberg chains.

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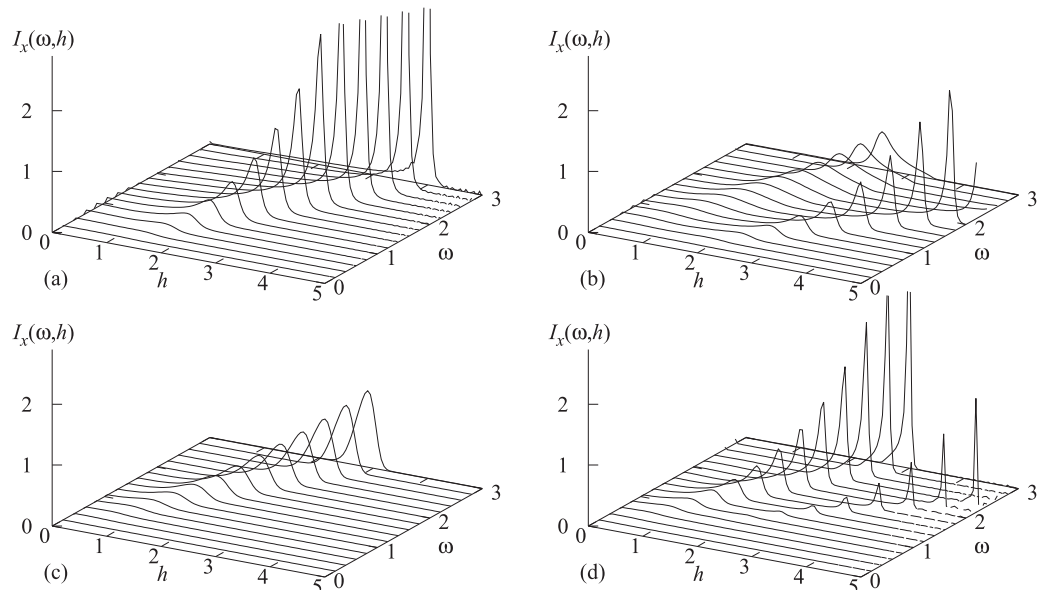


FIG. 16. Field profiles of the absorption intensity $I_x(\omega, h)$ at different frequencies ω for $J = -1, g_1 = 1, g_2 = 1$ (a), $g_2 = 0.5$ (b), $g_2 = 0$ (c), and $g_2 = -0.5$ (d) at $T = 1$.

APPENDIX: BOUNDARIES OF THE TWO-FERMION EXCITATION CONTINUA

Let us present the expressions for the lines in the (κ, ω) plane, which restrict the regions for different numbers of solutions of Eqs. (5.6) as shown in Fig. 5(a), green lines. We have

$$\begin{aligned}\omega_{1,2}(\kappa) &= \sqrt{2(J^2 + 2g_-^2 h^2 \pm J^2 \cos \kappa)}, \\ \omega_{3,4}(\kappa) &= |\sin \kappa| (\sqrt{J^2 + g_-^2 h^2} \pm |g_- h|), \\ \omega_{5,6}(\kappa) &= \sqrt{J^2 \sin^2 \kappa + g_-^2 h^2} \pm |g_- h|. \quad (\text{A1})\end{aligned}$$

Let us also present the expressions in the case $|h| < h_s$, $g_1 g_2 > 0$ for the characteristic lines, which bounded nonzero values of the Fermi-Dirac functions at $T = 0$ [see also Fig. 5(c), red lines]. We have

$$\begin{aligned}\omega_{7,8}(\kappa) &= |g_+ h + \sqrt{J^2 \cos^2(\kappa_0 \pm \kappa) + g_-^2 h^2}|, \\ \omega_{9,10}(\kappa) &= |g_+ h - \sqrt{J^2 \cos^2(\kappa_0 \pm \kappa) + g_-^2 h^2}|. \quad (\text{A2})\end{aligned}$$

Here κ_0 is defined in Eq. (3.2).

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