Dynamical correlations of the spin-$\frac{1}{2}$ Heisenberg XXZ chain in a staggered field

Igor Kuzmenko[1,2] and Fabian H. L. Essler[1]
[1]*The Rudolf Peierls Centre for Theoretical Physics, University of Oxford, 1 Keble Road, Oxford OX1 3NP, United Kingdom*
[2]*Department of Physics, Lancaster University, Lancaster LA1 4YB, United Kingdom*
(Received 2 September 2008; revised manuscript received 25 November 2008; published 5 January 2009)

We consider the easy-plane anisotropic spin-$\frac{1}{2}$ Heisenberg chain in combined uniform longitudinal and transverse staggered magnetic fields. The low-energy limit of his model is described by the sine-Gordon quantum field theory. Using methods of integrable quantum field theory we determine the various components of the dynamical structure factor. To do so, we derive explicit expressions for all matrix elements of the low-energy projections of the spin operators involving at most two particles. We discuss applications of our results to experiments on one-dimensional quantum magnets.

DOI: 10.1103/PhysRevB.79.024402 PACS number(s): 75.10.Jm

I. INTRODUCTION

The field-induced gap problem in anisotropic quasi-one-dimensional spin-$\frac{1}{2}$ Heisenberg antiferromagnets has attracted much experimental[1–15] and theoretical[9,16–28] attention in recent years. Two scenarios have been studied in particular. For isotropic exchange interaction a gap can be induced by the application of a uniform magnetic field in presence of a staggered g-tensor and/or a Dzyaloshinskii-Moriya interaction.[16] This is the case for materials such as copper benzoate,[1–6] $CuCl_{2\cdot 2}$ (dimethylsulfoxide) (CDC),[7] copper-pyrimidine,[8–12] and Yb_4As_3.[13,14] Theoretical studies have analyzed the excitation spectrum,[16–18] the dynamical structure factor,[17,19] the specific heat,[20] the magnetic susceptibility,[9,21] and the electron-spin resonance lineshape.[22] In the materials mentioned above application of a uniform magnetic field $\boldsymbol{H}$ induces a staggered field perpendicular to $\boldsymbol{H}$. It is the induced staggered field that leads to a spectral gap. The staggered field is generated both by a staggered g-tensor[29,30] and a Dzyaloshinskii-Moriya (DM) interaction. The simplest Hamiltonian describing such field-induced gap systems is given by[16]

$$\mathcal{H} = J\sum_J \boldsymbol{S}_j \cdot \boldsymbol{S}_{j+1} - H\sum_J S_j^z + h\sum_J (-1)^j S_j^x, \tag{1}$$

where $h=\gamma H$. The constant γ is given in terms of the staggered g tensor[29,30] and the DM interaction. In critical systems with exchange anisotropy such as the spin-1/2 Heisenberg XXZ chain a second mechanism for inducing a gap by application of a uniform magnetic field exists. While application of a field perpendicular to the easy plane leaves the system critical, applying a field in the easy plane leads to the formation of a spectral gap.[23–26,31,32]

The purpose of the present work is to extend the theoretical analysis of the staggered field mechanism for generating a spectral gap to the case of the anisotropic Heisenberg chain,

$$\mathcal{H} = J\sum_J [S_j^x S_{j+1}^x + S_j^y S_{j+1}^y + \delta S_j^z S_{j+1}^z] - H\sum_J S_j^z + h\sum_J (-1)^j S_j^x. \tag{2}$$

In what follows we will consider the region $-1<\delta\le 1$ which corresponds to an "XY"-like exchange anisotropy. It is important for our analysis that the staggered field is transverse to the anisotropy whereas the magnetic field is along the anisotropy axis. Only in this case does the low-energy limit map onto an integrable model, the sine-Gordon quantum field theory.

The outline of this paper is as follows: in Sec. II we construct the continuum limit of model (2). In Sec. III we derive a spectral representation of the dynamical structure factor at low energies. In Sec. IV we present the calculations for retarded two-point correlation functions. In Sec. V we present our results for the components of the dynamical structure factors. Section VI summarizes our results. The technical aspects of our analysis are summarized in several appendixes: in Appendix A we discuss how the parameters of the low-energy field theory can be determined from the Bethe ansatz solution of the Heisenberg chain in a magnetic field. Appendixes B and C present results for the form factors of the operators entering the calculation of the dynamical structure factor.

II. CONTINUUM LIMIT

In the limit $|h|\ll H,J$ the staggered field can be taken into account as a perturbation to the low-energy limit of the XXZ chain in a magnetic field. It is well known that the low-energy limit of the spin-$\frac{1}{2}$ Heisenberg XXZ chain with XY-like anisotropy $|\delta|<1$ is given by a free bosonic theory[33–36]

$$\mathcal{H}_{h=0} = \frac{v}{16\pi}\int dx[(\partial_x\Phi)^2 + (\partial_x\Theta)^2], \tag{3}$$

where the field $\Phi(x)$ and its dual field $\Theta(x)$ are compactified

$$\Theta(x) \equiv \Theta(x) + \frac{2\pi}{\beta}, \quad \Phi \equiv \Phi + 8\pi\beta. \tag{4}$$

The commutation relation between Φ and Θ reads

$$[\Theta(x),\Phi(x')] = 8\pi i\,\vartheta_H(x-x'), \tag{5}$$

where $\vartheta_H(x)$ is the Heaviside step function, equal to 0 for $x<0$, 1 for $x>0$, and 1/2 for $x=0$. The parameters v, β, and

k_F (see below) in the low-energy theory can be calculated directly from the Bethe ansatz solution on the XXZ chain.[37] How this is done is briefly reviewed in Appendix A. The result as well as the other parameters used are listed in Table I for the anisotropic parameter $\delta=0.3$. In the continuum limit the lattice spin operators have the following expansions:

$$S_j^\alpha = \sum_{a=1}^{3} e^{iQ_a^\alpha x}\mathcal{S}_a^\alpha(x) + \cdots, \tag{6}$$

where $x=ja_0$ and a_0 is the lattice spacing. The wave numbers Q_a^α are

$$Q_1^x = -Q_3^x = Q = \frac{\pi}{a_0} - 2k_F, \quad Q_2^x = \frac{\pi}{a_0}, \tag{7}$$

$$Q_a^y = Q_a^x, \tag{8}$$

$$Q_1^z = 0, \quad Q_2^z = -Q_3^z = 2k_F, \tag{9}$$

where the Fermi momentum is given by

$$k_F = \frac{\pi}{2a_0}(1 - 2\langle S_j^z\rangle). \tag{10}$$

Here $\langle S_j^z\rangle$ is the magnetization per site. The continuum fields $\mathcal{S}_a^\alpha$ are given in terms of the canonical boson Φ and its dual field Θ as

$$\mathcal{S}_1^x(x) = \frac{1}{2}\mathcal{A}(H)[\mathcal{O}_\beta^1(x) + \mathcal{O}_{-\beta}^1(x)], \tag{11}$$

$$\mathcal{S}_2^x(x) = c(H)\cos[\beta\Theta(x)], \tag{12}$$

$$\mathcal{S}_3^x(x) = [\mathcal{S}_1^x(x)]^\dagger, \tag{13}$$

$$\mathcal{S}_1^y(x) = \frac{1}{2i}\mathcal{A}(H)[\mathcal{O}_\beta^1(x) - \mathcal{O}_{-\beta}^1(x)], \tag{14}$$

$$\mathcal{S}_2^y(x) = c(H)\sin[\beta\Theta(x)], \tag{15}$$

$$\mathcal{S}_3^y(x) = [\mathcal{S}_1^y(x)]^\dagger, \tag{16}$$

$$\mathcal{S}_1^z(x) = \frac{a_0}{8\pi\beta}\partial_x\Phi(x), \tag{17}$$

$$\mathcal{S}_2^z(x) = [\mathcal{S}_3^z(x)]^\dagger = -\frac{1}{2i}a(H)\mathcal{O}_0^1(x), \tag{18}$$

where

$$\mathcal{O}_a^1 = \exp\left\{\frac{i\Phi}{4\beta} + ia\Theta\right\}. \tag{19}$$

We are using normalizations such that

$$\langle\mathcal{O}_a^1(\tau,x)\mathcal{O}_{-a}^{-1}(0,0)\rangle = \left[\frac{v\tau+ix}{v\tau-ix}\right]^{a/\beta}\left[\frac{a_0^2}{v^2\tau^2+x^2}\right]^{2a^2+1/8\beta^2}. \tag{20}$$

The coefficients $a(H)$, $c(H)$, and $\mathcal{A}(H)$ have been determined numerically in Ref. 38. The staggered magnetic field perturbation can be bosonized using Eqs. (11)–(18), which leads to a sine-Gordon model,

$$\mathcal{H} = \int dx\left\{\frac{v}{16\pi}\{[\partial_x\Phi(x)]^2 + [\partial_x\Theta(x)]^2\} + \mu(h,H)\cos[\beta\Theta(x)]\right\}, \tag{21}$$

where $\mu(h,H)=hc(H)$. We note that as we have chosen to bosonize in a finite magnetic field, the cutoff of the theory is H rather than J. However, it is straightforward to recover the zero field limit (where one bosonizes at $H=0$ and the cutoff is J) in the expressions for the structure factor we give below.

A. Elementary excitations

The sine-Gordon model is integrable and its spectrum and scattering matrices are known exactly.[39–44] In the relevant range of the parameter β $(0<\beta<1)$ the spectrum of elementary excitations consists of a soliton-antisoliton doublet and several soliton-antisoliton bound states called "breathers." There are altogether $[1/\xi]$ breathers, where $[x]$ denotes the integer part of x and $\xi=\frac{\beta^2}{1-\beta^2}$. In order to distinguish the various single-particle states we introduce labels s and $\bar{s}$ for solitons and antisolitons, respectively, and $b_1,\ldots,b_{[1/\xi]}$ for breathers. Energy and momentum carried by the elementary excitations are expressed in terms of the rapidity θ as

$$vP_\epsilon = \Delta_\epsilon\sinh(\theta), \quad E_\epsilon = \Delta_\epsilon\cosh(\theta), \tag{22}$$

where $\Delta_s=\Delta_{\bar{s}}=\Delta$, $\Delta_{b_k}\equiv\Delta_k=2\Delta\sin(\frac{\pi\xi k}{2})$. The soliton gap as a function of parameters H and h is[20,45]

$$\frac{\Delta}{J} = \frac{2v}{Ja_0\sqrt{\pi}}\frac{\Gamma\left(\frac{\xi}{2}\right)}{\Gamma\left(\frac{1+\xi}{2}\right)}\left[\frac{Ja_0c(H)\pi}{2v}\frac{\Gamma\left(\frac{1}{1+\xi}\right)}{\Gamma\left(\frac{\xi}{1+\xi}\right)}\frac{h}{J}\right]^{(1+\xi)/2}. \tag{23}$$

When $\delta\approx1$ and the magnetization is small the leading irrelevant perturbation to the Gaussian model needs to be taken into account, leading to[21]

$$\frac{\Delta}{J} = \left(\frac{h}{J}\right)^{(1+\xi)/2}\left[B\left(\frac{J}{H}\right)^{1/2-2\beta^2}(2-8\beta^2)^{1/4}\right]^{-(1+\xi)/2}, \tag{24}$$

where $B=0.422\,169$.

B. Scattering states

It is useful to introduce creation and annihilation operators $A_\epsilon^\dagger(\theta)$ and $A_\epsilon(\theta)$ for the elementary excitations. Here ϵ

TABLE I. Amplitudes $\mathcal{A}$, a, and c, the dimensionless spin velocity v/Ja_0, the coupling β, and the field H as functions of the magnetization m for the anisotropic parameter δ=0.3. The amplitudes are determined in Ref. 38.

m	$\mathcal{A}$	a	c	v/Ja_0	β	H/J
0.02	0.3044	0.3953	0.5275	1.1804	0.386192	0.09093
0.04	0.3065	0.3913	0.5268	1.17114	0.385821	0.18186
0.06	0.3096	0.3867	0.5256	1.15828	0.385332	0.2598
0.08	0.3130	0.3817	0.5240	1.13738	0.384573	0.35073
0.10	0.3173	0.3769	0.5219	1.11423	0.383768	0.42867
0.12	0.3226	0.3713	0.5194	1.08072	0.38265	0.5196
0.14	0.3284	0.3661	0.5164	1.04600	0.381535	0.59754
0.16	0.3354	0.3610	0.5129	1.01244	0.380489	0.66249
0.18	0.3433	0.3559	0.5088	0.966005	0.379084	0.74043
0.20	0.3527	0.3508	0.5041	0.921509	0.377775	0.80538
0.22	0.3642	0.3460	0.4988	0.870927	0.376322	0.87033
0.24	0.3773	0.3415	0.4929	0.813165	0.374702	0.93528
0.26	0.3923	0.3371	0.4861	0.760734	0.37326	0.98724
0.28	0.4102	0.3329	0.4785	0.701482	0.371658	1.0392
0.30	0.4321	0.3286	0.4699	0.651491	0.370326	1.07817
0.32	0.4596	0.3253	0.4602	0.575147	0.368318	1.13013
0.34	0.493	0.3222	0.4492	0.507976	0.366572	1.16910
0.36	0.5342	0.3193	0.4367	0.456492	0.365244	1.19508
0.38	0.588	0.3166	0.4222	0.389204	0.363518	1.22431
0.40	0.664	0.3141	0.4053	0.326360	0.361913	1.24704
0.42	0.769	0.3131	0.3851	0.259866	0.360218	1.26652
0.44	0.934	0.3125	0.3602	0.186561	0.358349	1.28276
0.46	1.214	0.3127	0.3279	0.122936	0.356722	1.29251
0.48	1.89	0.3142	0.2796	0.0448071	0.354713	1.299

$=s,\bar{s},b_1,\ldots,b_{[1/\xi]}$. The creation or annihilation operators fulfill the so-called Faddeev-Zamolodchikov (FZ) algebra,

$$A_a(\theta_1)A_b(\theta_2) = S_{ab}^{a'b'}(\theta_1-\theta_2)A_{b'}(\theta_2)A_{a'}(\theta_1),$$

$$A_a^\dagger(\theta_1)A_b^\dagger(\theta_2) = S_{ab}^{a'b'}(\theta_1-\theta_2)A_{b'}^\dagger(\theta_2)A_{a'}^\dagger(\theta_1),$$

$$A_a^\dagger(\theta_1)A_b(\theta_2) = S_{ba'}^{b'a}(\theta_1-\theta_2)A_{b'}(\theta_1)A_{a'}^\dagger(\theta_1) + 2\pi\delta_{ab}\delta(\theta_1-\theta_2). \quad (25)$$

Here $S(\theta)$ is the scattering matrix of the sine-Gordon model.[41–43] Multiparticle scattering states of (anti)solitons and breathers are given in terms of the FZ creation operators as

$$|\{\epsilon_n,\theta_n\}\rangle = A_{\epsilon_n}^\dagger(\theta_n)\cdots A_{\epsilon_1}^\dagger(\theta_1)|0\rangle. \quad (26)$$

Energy and momentum of these states are,

$$E_{\{n\}} = \sum_{i=1}^{n} E_{\epsilon_i}, \quad P_{\{n\}} = \sum_{i=1}^{n} P_{\epsilon_i}. \quad (27)$$

The resolution of the identity in the normalization implied by Eq. (25) reads,

$$I = \sum_{n=0}^{\infty}\sum_{\{\epsilon_j\}}\int \frac{d\theta_1\ldots d\theta_n}{n!\,(2\pi)^n}|\{\epsilon_n,\theta_n\}\rangle\langle\{\epsilon_n,\theta_n\}|. \quad (28)$$

C. Discrete symmetries

The Hamiltonian is invariant with respect to charge conjugation,

$$C\Theta C^{-1} = -\Theta, \quad C\Phi C^{-1} = -\Phi. \quad (29)$$

The action of the charge conjugation operator C on physical states follows from

$$C|0\rangle = |0\rangle,$$

$$CA_s^\dagger(\theta)C^{-1} = A_{\bar{s}}^\dagger(\theta),$$

TABLE II. Topological charge $\mathcal{Q}$ and eigenvalue (where applicable) under charge conjugation C of the continuum spin operators.

	$\mathcal{S}_1^x$	$\mathcal{S}_2^x$	$\mathcal{S}_3^x$	$\mathcal{S}_1^y$	$\mathcal{S}_2^y$	$\mathcal{S}_3^y$	$\mathcal{S}_1^z$	$\mathcal{S}_2^z$	$\mathcal{S}_3^z$
$\mathcal{Q}$	−1	0	1	−1	0	1	0	−1	1
C		+			−		−		

$$CB_k^\dagger(\theta)C^{-1}=(-1)^k B_k^\dagger(\theta). \tag{30}$$

We see that even breathers are invariant under charge conjugation, while odd breathers change sign. The topological charge,

$$\mathcal{Q}=\frac{\beta}{2\pi}\int_{-\infty}^{\infty}dx\partial_x\Theta(x),$$

is a conserved quantity. We will use the conventions in which soliton or antisoliton and breathers have topological charge ∓1 and zero, respectively.

III. DYNAMICAL STRUCTURE FACTOR

The central object of our study is the inelastic neutron scattering intensity, which is proportional to[46]

$$I(\omega,\mathbf{k})\propto\sum_{\alpha,\alpha'}\left(\delta^{\alpha\alpha'}-\frac{k^\alpha k^{\alpha'}}{\mathbf{k}^2}\right)S^{\alpha\alpha'}(\omega,k). \tag{31}$$

Here $\alpha,\alpha'=x,y,z$, k denotes the component of $\mathbf{k}$ along the chain direction, and the dynamical structure factor on a chain with L sites is defined as

$$S^{\alpha\alpha'}(\omega,k)=\frac{1}{L}\sum_{l,l'}\int_{-\infty}^{\infty}\frac{dt}{2\pi}e^{i\omega t-ik(l-l')}\langle 0|S_l^\alpha(t)S_{l'}^{\alpha'}|0\rangle. \tag{32}$$

Substituting the low-energy expressions [Eq. (6)] into Eq. (32) we obtain

$$S^{\alpha\alpha'}(\omega,k)=\sum_{a,b=1}^{3}\frac{1}{L}\sum_{l,l'}\int_{-\infty}^{\infty}\frac{dt}{2\pi}e^{i\omega t-i(k-Q_a^\alpha)l+i(k+Q_b^{\alpha'})l'}\times\langle 0|\mathcal{S}_a^\alpha(t,x)\mathcal{S}_b^{\alpha'}(0,y)|0\rangle, \tag{33}$$

where $x=la_0$, $y=l'a_0$, and $\mathcal{S}_a^\alpha(x)$ are the leading terms in the low-energy limits [Eq. (6)] of the lattice spin operators. Using that the expectation value is a slowly varying function of $x-y$ we see that only terms with

$$k\approx Q_a\approx-Q_b \tag{34}$$

contribute to Eq. (33).[47] The dynamical structure factor can be expressed by means of a Lehmann representation in terms of scattering states of solitons, antisolitons and breathers. Inserting a complete set of states [Eq. (28)] between the operators in Eq. (33) and using

$$\langle 0|\mathcal{S}_a^\alpha(t,x)|\{\epsilon_n,\theta_n\}\rangle=e^{-iE_{\{n\}}t+iP_{\{n\}}x}\langle 0|\mathcal{S}_a^\alpha(0,0)|\{\epsilon_n,\theta_n\}\rangle,$$

we arrive at

$$S^{\alpha\alpha'}(\omega,Q_a^\alpha+q)\simeq\frac{2\pi}{a_0}\sum_{n=1}^{\infty}\sum_{\{\epsilon_n\}}\sum_{b=1}^{3}\delta_{Q_a^\alpha,-Q_b^{\alpha'}}\int\frac{d\theta_1\cdots d\theta_n}{n!\,(2\pi)^n}\langle 0|\mathcal{S}_a^\alpha|\{\epsilon_n,\theta_n\}\rangle\times\langle\{\epsilon_n,\theta_n\}|\mathcal{S}_b^{\alpha'}|0\rangle\delta(q-P_{\{n\}})\delta(\omega-E_{\{n\}}). \tag{35}$$

Here q is assumed to be sufficiently small ($q\sim\frac{\Delta}{v}\ll k_F,\frac{\pi}{a_0}$). Due to energy-momentum conservation only a finite number of intermediate states contributes to the correlator [Eq. (35)]. Moreover, at low energies contributions of intermediate states with large numbers of particles to the correlator [Eq. (35)] are generally small.[48,49] We therefore restrict our following analysis to one and two particle contributions. Many matrix elements in Eq. (35) are in fact zero as can be established by using charge conjugation symmetry and topological charge conservation. The relevant properties of the continuum spin operators $\mathcal{S}_s^\alpha$ are summarized in Table II. Using these properties we furthermore conclude that at low energies the nonvanishing components of the dynamical structure factor are,

(1) S^{xx}, S^{yy} in the vicinity of the points $k=\pm Q$;
(2) S^{xx}, S^{yy} near the point $k=\frac{\pi}{a_0}$;
(3) S^{zz} in the vicinity of the point $k=0$;
(4) S^{zz} near $k=\pm 2k_F$.

In the following we determine these in the "two-particle approximation," i.e., keeping only terms with $n\le 2$ in the spectral representation [Eq. (35)]. In order to do so we make use of the exact form of the matrix elements entering the Lehmann representation, which follow from the form-factor bootstrap approach.[50,51] We note that as a consequence of charge conjugation symmetry the components of the structure factor in the vicinities of $k=Q_a$ and $k=-Q_a$ are the same.

IV. CALCULATION OF CORRELATION FUNCTIONS: KINEMATICS

The formalism we employ to calculate the dynamical structure factor can be used quite generally to determine (real and imaginary parts of) two-point correlation functions. The retarded two-point function of two bosonic operators A and B has a spectral representations of the form,

$$G^{AB}(\omega,q)=\frac{2\pi v}{a_0}\sum_{n=1}^{\infty}\sum_{\{\epsilon_n\}}\int\frac{d\theta_1\cdots d\theta_n}{n!\,(2\pi)^n}\Bigg\{\langle 0|A|\{\epsilon_n,\theta_n\}\rangle\times\langle\{\epsilon_n,\theta_n\}|B|0\rangle\frac{\delta(vq-P_{\{n\}})}{\omega-E_{\{n\}}+i\eta}-\langle 0|B|\{\epsilon_n,\theta_n\}\rangle\times\langle\{\epsilon_n,\theta_n\}|A|0\rangle\frac{\delta(vq+P_{\{n\}})}{\omega+E_{\{n\}}+i\eta}\Bigg\}. \tag{36}$$

Here η is a positive infinitesimal, $|\{\epsilon_n,\theta_n\}\rangle$ are n-particle scattering states of solitons, antisolitons and breathers [Eq. (26)] with energies and momenta are given by Eqs. (27) and (22), respectively. The leading contribution to the spectral sum in Eq. (36) is due to intermediate states with one and two particles. Using momentum conservation it is possible to simplify the expressions for these contributions as we discuss next.

A. One-particle kinematics

Resolving the momentum conservation delta function leads to the following result for the one-particle contributions to G^{AB}:

$$G_{1p}^{AB}(\omega,q) = \frac{v}{a_0}\sum_a \int d\theta\Bigg[\langle 0|A|\theta\rangle_{aa}\langle\theta|B|0\rangle\frac{\delta(vq-\Delta_a\sinh\theta)}{\omega-\Delta_a\cosh\theta+i\eta} - \langle 0|B|\theta\rangle_{aa}\langle\theta|A|0\rangle\frac{\delta(vq+\Delta_a\sinh\theta)}{\omega+\Delta_a\cosh\theta+i\eta}\Bigg]$$
$$= \sum_a \frac{v}{a_0\varepsilon_a(q)}\Bigg[\frac{\langle 0|A|\theta_0^a\rangle_{aa}\langle\theta_0^a|B|0\rangle}{\omega-\varepsilon_a(q)+i\eta} - \frac{\langle 0|B|\theta_0^a\rangle_{aa}\langle\theta_0^a|A|0\rangle}{\omega+\varepsilon_a(q)+i\eta}\Bigg], \tag{37}$$

where a runs over all single-particle labels (i.e., soliton, antisoliton, and breathers) and

$$\varepsilon_a(q) = \sqrt{\Delta_a^2+v^2q^2}, \tag{38}$$

$$\theta_0^a = \text{arcsinh}\left(\frac{vq}{\Delta_a}\right). \tag{39}$$

B. Two-particle kinematics

As two-particle form factors of scalar operators depend only on the rapidity difference, it is useful to change variables to $\theta_\pm=(\theta_1\pm\theta_2)/2$. Resolving the momentum conservation delta function then gives

$$G_{2p}^{AB}(\omega,q) = \frac{v}{a_0}\sum_{a_1,a_2}\int\frac{d\theta_1 d\theta_2}{2(2\pi)^2}\Bigg[\langle 0|A|\theta_2,\theta_1\rangle_{a_2a_1a_1a_2}\langle\theta_1,\theta_2|B|0\rangle\frac{\delta\left(vq-\sum_{j=1}^2\Delta_{a_j}\sinh\theta_j\right)}{\omega-\sum_{j=1}^2\Delta_{a_j}\cosh\theta_j+i\eta} - \langle 0|B|\theta_2,\theta_1\rangle_{a_2a_1a_1a_2}\langle\theta_1,\theta_2|A|0\rangle\frac{\delta\left(vq+\sum_{j=1}^2\Delta_{a_j}\sinh\theta_j\right)}{\omega+\sum_{j=1}^2\Delta_{a_j}\cosh\theta_j+i\eta}\Bigg]$$
$$= \frac{v}{a_0}\sum_{a,b}\int\frac{d\theta_-}{2\pi}\Bigg[\frac{\langle 0|A|\theta_0^{ab}-\theta_-,\theta_0^{ab}+\theta_-\rangle_{baab}\langle\theta_0^{ab}+\theta_-,\theta_0^{ab}-\theta_-|B|0\rangle}{\varepsilon_{ab}(q,\theta_-)(\omega-\varepsilon_{ab}(q,\theta_-)+i\eta)} - \frac{\langle 0|B|\theta_0^{ab}-\theta_-,\theta_0^{ab}+\theta_-\rangle_{baab}\langle\theta_0^{ab}+\theta_-,\theta_0^{ab}-\theta_-|A|0\rangle}{\varepsilon_{ab}(q,\theta_-)(\omega+\varepsilon_{ab}(q,\theta_-)+i\eta)}\Bigg], \tag{40}$$

where

$$\varepsilon_{ab}(q,\theta) = [v^2q^2+\Delta_a^2+\Delta_b^2+2\Delta_a\Delta_b\cosh(2\theta)]^{1/2},$$

$$\theta_0^{ab} = \ln\left[\frac{vq+\varepsilon_{ab}(q,\theta_-)}{\Delta_a\exp(\theta_-)+\Delta_b\exp(-\theta_-)}\right].$$

The imaginary part of $G_{2p}^{AB}(\omega,q)$ can be simplified using

$$-\frac{1}{\pi}\text{Im}\frac{1}{\varepsilon_{ab}(q,\theta_-)[\omega-\varepsilon_{ab}(q,\theta_-)+i\eta]} = \frac{\delta\left(\theta_- - \frac{\theta_{ab}(s)}{2}\right)+\delta\left(\theta_- + \frac{\theta_{ab}(s)}{2}\right)}{\sqrt{s^2-(\Delta_a+\Delta_b)^2}\sqrt{s^2-(\Delta_a-\Delta_b)^2}}, \tag{41}$$

where

$$s^2 = \omega^2 - v^2q^2, \tag{42}$$

$$\theta_{ab}(s) = \text{arccosh}\left[\frac{s^2-\Delta_a^2-\Delta_b^2}{2\Delta_a\Delta_b}\right]. \tag{43}$$

Carrying out the θ_- integral using the delta functions we obtain

$$-\frac{1}{\pi}\text{Im}\,G_{2p}^{AB}(\omega>0,q) = \frac{v}{2\pi a_0}\sum_{a,b}\sum_{\sigma=\pm}\frac{\langle 0|A|\theta_{ba}^{\sigma}(\omega,q),\theta_{ab}^{-\sigma}(\omega,q\ \rangle_{baab}\langle\theta_{ab}^{-\sigma}(\omega,q),\theta_{ba}^{\sigma}(\omega,q)|B|0\rangle}{\sqrt{s^2-(\Delta_a+\Delta_b)^2}\sqrt{s^2-(\Delta_a-\Delta_b)^2}}\vartheta_H(s-\Delta_a-\Delta_b), \tag{44}$$

where $\vartheta_H(x)$ is the Heaviside function and

$$\theta^{\pm}_{ab}(\omega,q) = \text{arcsinh}\left[\frac{1}{2\Delta_a s^2}\{vq(s^2+\Delta_a^2-\Delta_b^2) \pm \omega\sqrt{[s^2-(\Delta_a-\Delta_b)^2][s^2-(\Delta_a+\Delta_b)^2]}\}\right],$$

$$\theta^{\sigma}_{ab}(\omega,q) - \theta^{-\sigma}_{ba}(\omega,q) = \sigma\theta_{ab}(s). \quad (45)$$

The two terms in Eq. (44) arise from the two delta functions in Eq. (41). Using the results summarized in this section we can determine the one and two particle contributions to both real and imaginary parts of two-point functions. The two particle contributions to the real part involve one (principal part) integration, which is readily performed numerically. In order to determine the dynamical structure factor we only require the imaginary part of several two-point functions.

V. RESULTS FOR THE DYNAMICAL STRUCTURE FACTOR

Below we present results for the dynamical structure factor $S^{\alpha\beta}(\omega,Q_a^{\alpha}+q)$ [Eq. (35)] in the regime $-1<\delta\leq 1$ and for magnetic fields $H<H_c=J(1+\delta)$. We note that if $H\approx H_c$ or $\delta\approx -1$ the cutoff in the field theory is very small, which limits the utility of our approach. For the sake of clarity we use a particular set of parameters in all plots

$$\gamma = \frac{h}{H} = 0.011\,91, \quad \delta = 0.3, \quad H = 0.2598J. \quad (46)$$

These correspond to a magnetization per site of $\langle S^z\rangle=0.06$ (see Table I) and $\xi=0.174\,371$. The spectrum consists of soliton and antisoliton with gap $\Delta\approx 0.048\,97J$ and five breathers with gaps

$$\Delta_1 = 0.540\,98\Delta, \quad \Delta_2 = 1.041\,62\Delta, \quad \Delta_3 = 1.464\,61\Delta,$$

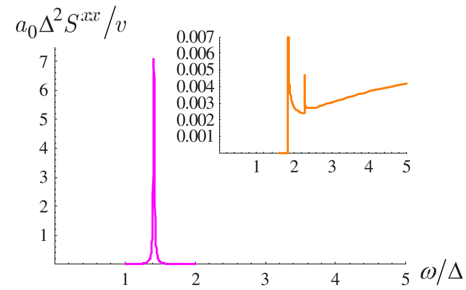

FIG. 1. (Color online) One and two-particle contributions to $S^{xx}(\omega,-Q+\Delta/v)$ as a function of ω for $\delta=0.3$ and $H=0.2598J$. The delta-function peak (pink) has been broadened to make it visible.

$$\Delta_4 = 1.778\,41\Delta, \quad \Delta_5 = 1.959\,62\Delta. \quad (47)$$

In order to broaden delta functions appearing in one-particle contributions, we introduce a small imaginary part in ω, equal to $\eta=0.01\Delta$.

A. $S^{xx}(\omega,k)$

In the continuum limit $S^{xx}(\omega,k)$ is nonvanishing in the vicinity of the points $k=\pm Q$ and $\frac{\pi}{a_0}$. We will consider both cases in turn. As we have noted before, the response at $k=\pm Q$ is identical as a result of charge conjugation symmetry, so that it is sufficient to consider $k\approx -Q$.

1. Momenta $k\approx -Q=-\frac{2\pi}{a_0}\langle S_j^z\rangle$

In the continuum limit $S^{xx}(\omega,-Q+q)$ with $q\ll Q$ is given by the two-point function of $\mathcal{S}_3^x$ with $\mathcal{S}_1^x$ [Eq. (11)]. This is because vQ is a large energy scale proportional to the cutoff in the theory. Using Table II we find that the following intermediate states with at most two particles contribute:

(1) Single-soliton states.

(2) Two particle states containing one soliton and one breather.

The corresponding matrix elements are calculated in Appendix B. Using the results of Sec. IV to carry out the rapidity integrals we arrive at the following expression for $S^{xx}(\omega,-Q+q)$ within the two-particle approximation:

$$S^{xx}(\omega>0,-Q+q) \approx \frac{2v\tilde{\mathcal{A}}^2}{a_0}\frac{v^2q^2}{\Delta^2}\delta(s^2-\Delta^2) + \frac{v\tilde{\mathcal{A}}^2}{4\pi a_0}\sum_{k=1}^{(1/\xi)}(N^{\beta}_{sb_k})^2\frac{|F^{\min}_{sb_k}[\theta_{sb_k}(s)]|^2\vartheta_H(s-\Delta-\Delta_k)}{\sqrt{[s^2-(\Delta-\Delta_k)^2][s^2-(\Delta+\Delta_k)^2]}} \times \sum_{\sigma=\pm}\{K^{\beta}_{sb_k}[\sigma\theta_{sb_k}(s)]e^{\theta^{\sigma}_{sb_k}(\omega,q)} + K^{-\beta}_{sb_k}[\sigma\theta_{sb_k}(s)]e^{-\theta^{\sigma}_{sb_k}(\omega,q)}\}^2. \quad (48)$$

Here s is the Mandelstam variable [Eq. (42)], the overall normalization is

$$\tilde{\mathcal{A}} = \mathcal{A}(H)[Z_1(\beta)]^{1/2}, \quad (49)$$

where $Z_1(\beta)$ is given by Eq. (B2), the minimal form factors $F^{\min}_{sb_k}(\theta)$ by Eq. (B6), the pole functions $K^{\pm}_{sb_k}(\theta)$ by Eq. (B22) for k even and Eq. (B23) for k odd, the normalization factor $N^{\beta}_{sb_k}$ by Eq. (B20) and the functions $\theta_{sb_k}(s)$ and $\theta^{\sigma}_{sb_k}(\omega,q)$ are presented in Eqs. (43) and (45), respectively.

We note that $S^{xx}(\omega,-Q+q)$ vanishes when $q\to 0$. In Fig. 1 we therefore plot $S^{xx}(\omega,-Q+\Delta/v)$ as a function of ω. In order to broaden delta-function contributions we introduce a small imaginary part in ω. Two features are clearly visible: there is a coherent peak corresponding to the contribution of single-soliton excitations at energy at $\Delta\sqrt{2}$. At higher energies breather-soliton continua appear. Their contributions grow with increasing ω because $\mathcal{S}_3^x$ is an irrelevant operator. It is instructive to compare our result to the gapless spin-1/2 Heisenberg XXZ chain (see e.g., Ref. 52). There one has

$$S^{xx}(\omega>0,-Q+q)\propto\frac{\omega^2+v^2q^2}{(\omega^2-v^2q^2)^{1-\nu}}, \tag{50}$$

where $\nu=2(\beta+\frac{1}{4\beta})^2>1$. For large ω this increases as $\omega^{2\nu}$, while is goes to zero in a power-law fashion for $\omega\to vq$. In presence of a staggered field, the dynamical structure factor [Eq. (48)] has divergence for $\omega\to\sqrt{(\Delta+\Delta_k)^2+v^2q^2}$ ($k=1,2,\ldots,[1/\xi]$), while the large frequency behavior is the same as without the staggered field.

2. Vicinity of antiferromagnetic wave number: $k\approx\pi/a_0$

In the continuum limit $S^{xx}(\omega,\frac{\pi}{a_0}+q)$ with $qa_0\ll\pi$ is given by the two-point function of the charge neutral operator $\mathcal{S}_2^x$ [Eq. (13)]. Using Table II and Eq. (30) we find that the following intermediate states with at most two particles contribute to the two-point function of $\mathcal{S}_2^x$:

(1) Single breather states even under charge conjugation, i.e., $B_{2n}^\dagger(\theta)|0\rangle$.

(2) Two particle states containing one soliton and one antisoliton.

(3) Two particle states containing two even or two odd breathers.

Using the results of Sec. IV, we obtain the following expression in the two-particle approximation:

$$S^{xx}\left(\omega>0,\frac{\pi}{a_0}+q\right)\approx\frac{vc^2(H)}{\pi a_0}\Bigg\{2\pi\sum_{k=1}^{(1/2\xi)}|F^{\beta}_{b_{2k}}|^2\delta(s^2-\Delta_{2k}^2)+\frac{|F_{s\bar{s}}^{\cos(\beta\Theta)}[\theta_{s\bar{s}}(s)]|^2\vartheta_H(s-2\Delta)}{s\sqrt{s^2-4\Delta^2}}$$
$$+\sum_{k,k'=1}^{[1/\xi]}\delta^{\rm even}_{k+k'}|F^{\beta}_{b_kb_{k'}}[\theta_{b_kb_{k'}}(s)]|^2\frac{\vartheta_H(s-\Delta_k-\Delta_{k'})}{\sqrt{[s^2-(\Delta_k-\Delta_{k'})^2][s^2-(\Delta_k+\Delta_{k'})^2]}}\Bigg\}. \tag{51}$$

Here the single-breather form factors $F^{\beta}_{b_k}$ are given by Eq. (C14), the soliton-antisoliton form factor $F_{s\bar{s}}^{\cos(\beta\Theta)}(\theta)$ by Eq. (C10) and the breather-breather form factors $F^{\beta}_{b_kb_{k'}}(\theta)$ by Eq. (C24), respectively. The function $\theta_{\epsilon\epsilon'}(s)$ is given by Eq. (43) and

$$\delta_k^{\rm even}=\begin{cases}1 & \text{if } k \text{ is even}\\ 0 & \text{overwise}.\end{cases} \tag{52}$$

In Fig. 2 we plot the dynamical structure factor [Eq. (51)] as a function of frequency. We note that because $\mathcal{S}_2^x$ is a scalar operator $S^{xx}(\omega,\frac{\pi}{a_0}+q)$ depends only on the Mandelstam variable s [Eq. (42)] rather than on ω and q separately. The first peak in $S^{xx}(\omega,\frac{\pi}{a_0})$ is due to the b_2 single-breather excitation (blue line). At $\omega=\Delta_4$ there is a second single-breather contribution, due to b_4. Above $\omega=2\Delta_1$ a strong b_1b_1 two-breather continuum occurs (pink line). Around $\omega=2\Delta$ contributions from soliton antisoliton and b_1b_3 and b_2b_2 two-breather continua are visible. We note that the thresholds of b_1b_3, $s\bar{s}$ and b_2b_2 continua all occur around 2Δ is a peculiarity of the parameters we have chosen in the plots.

B. $S^{yy}(\omega,k)$

Next we turn to the yy component of the dynamical structure factor. In the continuum limit $S^{yy}(\omega,k)$ is nonvanishing in the vicinity of the points $k=\pm Q$ and $\frac{\pi}{a_0}$. We will consider both cases in turn.

1. Momenta $k\approx-Q=-\frac{2\pi}{a_0}\langle S_j^z\rangle$

In the continuum limit $S^{yy}(\omega,-Q+q)$ with $q\ll Q$ is given by the two-point function of $\mathcal{S}_3^y$ with $\mathcal{S}_1^y$ [Eq. (14)]. Using Table II we find that the following intermediate states with at most two particles contribute to the two-point function:

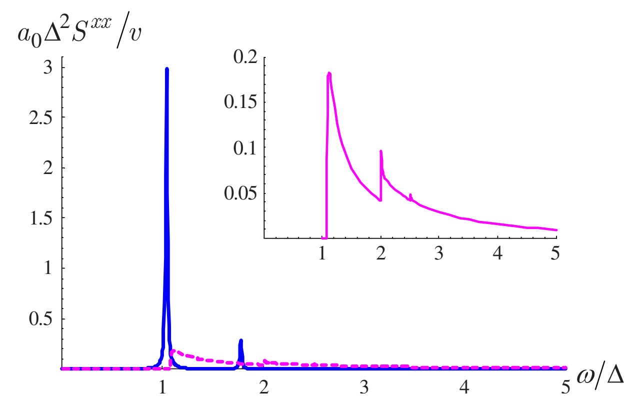

FIG. 2. (Color online) One and two-particle contributions to $S^{xx}(\omega,\frac{\pi}{a_0})$ as a function of ω for $\delta=0.3$ and $H=0.2598J$. Delta-function peaks (blue) have been broadened to make them visible.

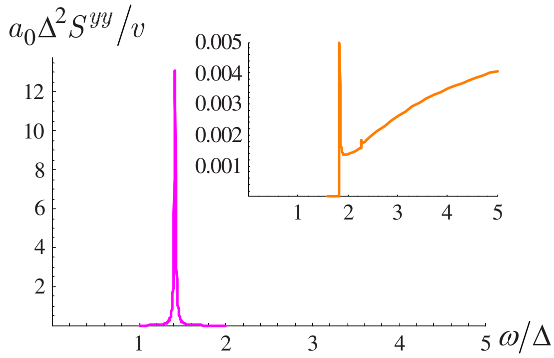

FIG. 3. (Color online) One and two-particle contributions to $S^{yy}(\omega,-Q+\Delta/v)$ as a function of ω for δ=0.3 and H=0.2598J. The delta-function peak (pink) has been broadened to make it visible. Inset: the soliton-breather two-particle contributions.

(1) Single-soliton states.

(2) Two particle states containing one soliton and one breather.

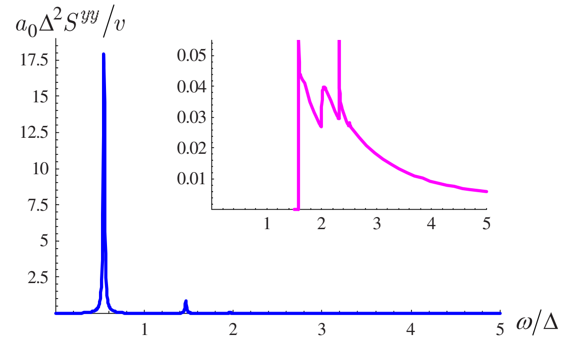

FIG. 4. (Color online) One and two-particle contributions to $S^{yy}(\omega,\frac{\pi}{a_0})$ as a function of ω for δ=0.3 and H=0.2598J. Delta-function peaks (blue) have been broadened to make them visible. Inset: the soliton-antisoliton and breather-breather two-particle contributions.

The corresponding matrix elements are calculated in Appendix B. Carrying out the rapidity integrals (see Sec. IV) we arrive at the following expression for $S^{yy}(\omega,-Q+q)$ within the two-particle approximation:

$$S^{yy}(\omega>0,-Q+q)\approx\frac{2v\tilde{\mathcal{A}}^2}{a_0}\frac{v^2q^2+\Delta^2}{\Delta^2}\delta(s^2-\Delta^2)+\frac{v\tilde{\mathcal{A}}^2}{4\pi a_0}\sum_{k=1}^{(1/\xi)}(N^{\beta}_{sb_k})^2\frac{|F^{\min}_{sb_k}[\theta_{sb_k}(s)]|^2\vartheta_H(s-\Delta-\Delta_k)}{\sqrt{[s^2-(\Delta-\Delta_k)^2][s^2-(\Delta+\Delta_k)^2]}}$$
$$\times\sum_{\sigma=\pm}\{K^{\beta}_{sb_k}[\sigma\theta_{sb_k}(s)]e^{\theta^{\sigma}_{sb_k}(\omega,q)}-K^{\beta}_{sb_k}[-\sigma\theta_{sb_k}(s)]e^{-\theta^{\sigma}_{sb_k}(\omega,q)}\}^2. \tag{53}$$

Here the overall normalization $\tilde{\mathcal{A}}$ is given by Eq. (49), the minimal form factor $F^{\min}_{sb_k}(\theta)$ by Eq. (B6), the pole function $K^{\beta}_{sb_k}(\theta)$ by Eq. (B22) for k even and Eq. (B23) for k odd, the functions $\theta_{sb_k}(s)$ and $\theta^{\sigma}_{sb_k}(\omega,q)$ by Eqs. (43) and (45), respectively.

We plot $S^{yy}(\omega,-Q+\Delta/v)$ as a function of ω in Fig. 3. Delta-function contributions have been broadened to make them visible. We see that there is a coherent peak corresponding to the contribution of single-soliton excitations atenergy at $\Delta\sqrt{2}$. At higher energies breather-soliton continua appear. Their contributions grow with increasing ω because $\mathcal{S}^y_3$ is an irrelevant operator.

2. Vicinity of antiferromagnetic wave number: $k\approx\pi/a_0$

In the continuum limit $S^{yy}(\omega,\frac{\pi}{a_0}+q)$ with $qa_0\ll\pi$ is given by the two-point function of the charge neutral operator $\mathcal{S}^y_2$ [Eq. (15)]. Using Table II and Eq. (30) we find that the following intermediate states with at most two particles contribute to the two-point function of $\mathcal{S}^y_2$:

(1) Single breather states odd under charge conjugation, i.e., $B^{\dagger}_{2n+1}(\theta)|0\rangle$.

(2) Two particle states containing one soliton and one antisoliton.

(3) Two particle states containing one even and one odd breather.

Using the results of Sec. IV, we obtain the following expression in the two-particle approximation:

$$S^{yy}\left(\omega>0,\frac{\pi}{a_0}+q\right)\approx\frac{vc^2(H)}{\pi a_0}\left\{2\pi\sum_{k=1}^{(1/\xi)}\delta^{\rm odd}_k|F^{\beta}_{b_k}|^2\delta(s^2-\Delta_k^2)+\frac{|F^{\sin(\beta\Theta)}_{s\bar{s}}[\theta_{s\bar{s}}(s)]|^2\vartheta_H(s-2\Delta)}{s\sqrt{s^2-4\Delta^2}}\right.$$
$$\left.+\sum_{k,k'=1}^{[1/\xi]}\delta^{\rm odd}_{k+k'}|F^{\beta}_{b_kb_{k'}}[\theta_{b_kb_{k'}}(s)]|^2\frac{\vartheta_H(s-\Delta_k-\Delta_{k'})}{\sqrt{[s^2-(\Delta_k-\Delta_{k'})^2][s^2-(\Delta_k+\Delta_{k'})^2]}}\right\}. \tag{54}$$

Here the single-breather form factors $F^{\beta}_{b_k}$ are given by Eq. (C14), the soliton-antisoliton form factor $F^{\sin(\beta\Theta)}_{s\bar{s}}(\theta)$ by Eq. (C11), the two-breather form factors $F^{\beta}_{b_kb_{k'}}(\theta)$ by Eq. (C24), the function $\theta_{ab}(s)$ by Eq. (43) and

$$\delta^{\rm odd}_k=\begin{cases}1 & \text{if } k \text{ is odd}\\ 0 & \text{overwise.}\end{cases} \tag{55}$$

We plot $S^{yy}(\omega,\frac{\pi}{a_0})$ as a function of ω in Fig. 4. We see that it is dominated by the contribution of the first breather b_1 (the corresponding delta function has been broadened). The contributions from b_3 and b_5 single-breather states are small in comparison. Similarly, the two-particle $b_1 b_2$, $s\bar{s}$, and $b_1 b_4$ continua shown in the inset of Fig. 4 are negligible.

C. Longitudinal structure factor $S^{zz}(\omega,k)$

We now consider the zz component of dynamical structure factor. In the continual limit $S^{zz}(\omega,k)$ is nonvanishing in the vicinity of the points $k=0$ and $\pm 2k_F$. We will consider both cases in turn.

1. Vicinity of ferromagnetic wave number: $k\approx 0$

In the continuum limit $S^{zz}(\omega,q)$ with $qa_0 \ll \pi$ is given by the two-point function of the charge neutral operator $\mathcal{S}_1^z$ [Eq. (17)]. Using Table II and Eq. (30) we find that the following intermediate states with at most two particles contribute to the two-point function of $\mathcal{S}_1^z$:

(1) Single breather states odd under charge conjugation, i.e., $B^\dagger_{2n+1}(\theta)|0\rangle$.

(2) Two particle states containing one soliton and one antisoliton.

(3) Two particle states containing one even and one odd breather.

Using the results of Sec. IV, we obtain the following expression in the two-particle approximation:

$$S^{zz}(\omega>0,q) \approx \frac{2a_0\tilde{b}^2\omega^2}{v}\sum_{k=1}^{(1/\xi)} \delta_k^{\mathrm{odd}} |F^{\Theta}_{b_k}|^2 \delta(s^2-\Delta_k^2) + \frac{a_0\tilde{b}^2\omega^2}{v}\frac{|F^{\Theta}_{s\bar{s}}[\theta_{s\bar{s}}(s)]|^2 \vartheta_H(s-2\Delta)}{s\sqrt{s^2-4\Delta^2}}$$
$$+ \frac{a_0\tilde{b}^2\omega^2}{v}\sum_{k,k'=1}^{[1/\xi]} \delta^{\mathrm{odd}}_{k+k'} |F^{\Theta}_{b_k b_{k'}}[\theta_{b_k b_{k'}}(s)]|^2 \frac{\vartheta_H(s-\Delta_k-\Delta_{k'})}{\sqrt{[s^2-(\Delta_k-\Delta_{k'})^2][s^2-(\Delta_k+\Delta_{k'})^2]}}, \quad (56)$$

where the single-breather form factor $F^{\Theta}_{b_k}$ is given by Eq. (C15), the soliton-antisoliton form factor $F^{\Theta}_{s\bar{s}}(\theta)$ by Eq. (C12), the breather-breather form factor $F^{\Theta}_{b_k b_{k'}}(\theta)$ by Eq. (C26), $\theta_{ab}(s)$ is given by Eq. (43), s is the Mandelstam variable [Eq. (42)], δ_k^{odd} is given in Eq. (55) and the overall normalization is

$$\tilde{b} = \frac{1}{4\pi\beta}. \quad (57)$$

The dynamical structure factor [Eq. (56)] is shown in Fig. 5. Note that since $\mathcal{S}_1^z$ is a scalar operator, $S^{zz}(\omega,q)$ depends on the Mandelstam variable s [Eq. (42)] rather than on ω and q separately. In order to broaden the delta-function contributions we introduce a small imaginary part in ω. The dominant peak in $S^{zz}(\omega,q)$ is due to a b_1 breather contribution. The contributions due to b_3 and b_5 breather states are much smaller. The soliton-antisoliton and breather-breather contributions to $S^{zz}(\omega,q)$ are barely visible in the figure.

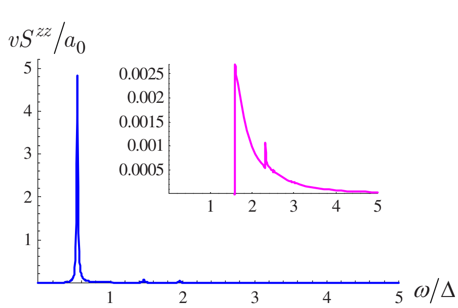

FIG. 5. (Color online) One and two particle contribution to $S^{zz}(\omega,0)$ [Eq. (56)] as a function of ω for δ=0.3 and H=0.2598J. Delta-function peaks (blue) have been broadened to make them visible. Inset: the soliton-antisoliton and breather-breather two-particle contributions.

2. Momenta $k\approx -2k_F$

In the continuum limit $S^{zz}(\omega,-2k_F+q)$ with $qa_0 \ll \pi$ is given by the two-point function of $\mathcal{S}_3^z$ with $\mathcal{S}_2^z$ [Eq. (18)]. Using Table II and Eq. (30) we find that the following intermediate states with at most two particles contribute to the two-point function of

(1) Single-soliton state.

(2) Two particle states containing one soliton and one breather.

Using the results of Sec. IV, we obtain the following expression in the two-particle approximation:

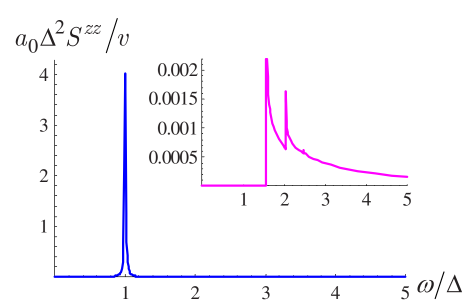

FIG. 6. (Color online) One and two particle contribution to $S^{zz}(\omega,-2k_F)$ [Eq. (58)] as a function of ω for δ=0.3 and H =0.2598J. Delta-function peak (blue) has been broadened to make it visible. Inset: the soliton-breather two particle contributions.

$$S^{zz}(\omega>0,-2k_F+q)\approx\frac{v\tilde{a}^2}{a_0}\delta(s^2-\Delta^2)+\frac{v\tilde{a}^2}{2\pi a_0}\sum_{k=1}^{(1/\xi)}(N^0_{sb_k})^2\{K^0_{sb_k}[\theta_{sb_k}(s)]\}^2\frac{|F^{\min}_{sb_k}[\theta_{sb_k}(s)]|^2\vartheta_H(s-\Delta-\Delta_k)}{\sqrt{[s^2-(\Delta-\Delta_k)^2][s^2-(\Delta+\Delta_k)^2]}}. \quad (58)$$

Here the minimal form factor $F^{\min}_{sb_k}(\theta)$ is given by Eq. (B6), the pole function $K^0_{sb_k}(\theta)$ by Eq. (B22) for k even and Eq. (B23) for k odd, the function $\theta_{sb_k}(s)$ by Eq. (43), the overall normalization is

$$\tilde{a}=a(H)\sqrt{\frac{Z(0)}{2}}. \quad (59)$$

The dynamical structure factor [Eq. (58)] is shown in Fig. 6. Here we chose $q=0$. The strong low-energy peak in $S^{zz}(\omega,-2k_F)$ is due to a one-soliton state. Soliton-breather continua appear at higher energies.

VI. SUMMARY AND CONCLUSIONS

In this work we have determined the low-energy dynamical spin response of the anisotropic spin-1/2 Heisenberg XXZ chain in the presence of both uniform and staggered magnetic fields. The uniform field was taken to be along the anisotropy axis and the staggered field perpendicular to it. The qualitative features of the model such as a field induced gap and the formation of bound states are similar to the case of isotropic exchange, which has been previously studied in detail.[9,16–18,20–22,27,28] The main effect of a strong exchange anisotropy is to generate further bound states and increase the binding energy. We have analyzed these effects on the dynamic response and determined for the first time all two-particle contributions, in particular those containing one soliton and one breather. The results obtained here can be used to study a quasi-one-dimensional array of anisotropic Heisenberg chains in a uniform magnetic field by combining a mean-field approach with an RPA-like approximation.[53–55] This is of interest in view of neutron scattering experiments on the quasi-1D anisotropic Heisenberg magnet Cs_2CoCl_4.[32]

ACKNOWLEDGMENT

This work was supported by the EPSRC under Grant No. EP/D0500952/1.

APPENDIX A: SPIN VELOCITY, FERMI MOMENTUM, AND COMPACTIFICATION RADIUS

In this appendix we summarize how to determine the parameters of the Gaussian model (3), Eq. (4) that describes the continuum limit of the Heisenberg XXZ chain in a magnetic field from the Bethe ansatz solution.[37] The velocity, Fermi momentum, and compactification radius are expressed in terms of the solutions of the following set of linear integral equations for the dressed energy $\varepsilon(\lambda)$, dressed momentum $p(\lambda)$, dressed density $\rho(\lambda)$, and dressed charge $Z(\lambda)$

$$\varepsilon(\lambda)-\int_{-A}^{A}\frac{d\mu}{2\pi}K(\lambda-\mu)\varepsilon(\mu)=H-\frac{J\sin^2\gamma}{\cosh 2\lambda-\cos\gamma},$$

$$p(\lambda)=\frac{2\pi}{a_0}\int_0^{\lambda}d\mu\rho(\mu),$$

$$\rho(\lambda)-\int_{-A}^{A}\frac{d\mu}{2\pi}K(\lambda-\mu)\rho(\mu)=\frac{2\sin\gamma}{2\pi[\cosh 2\lambda-\cos\gamma]},$$

$$Z(\lambda)-\int_{-A}^{A}\frac{d\mu}{2\pi}K(\lambda-\mu)Z(\mu)=1. \quad (A1)$$

Here the exchange anisotropy is parametrized as $\delta=\cos(\gamma)$ and the integral kernel is given by

$$K(\lambda)=-2\sin 2\gamma/(\cosh 2\lambda-\cos 2\gamma). \quad (A2)$$

The integration boundary A is fixed by the condition

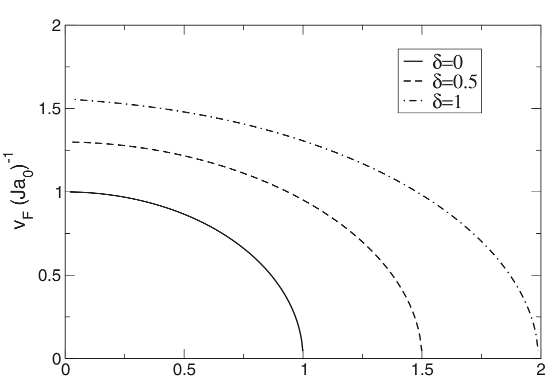

FIG. 7. Spin velocity as a function of magnetic field for different values of δ.

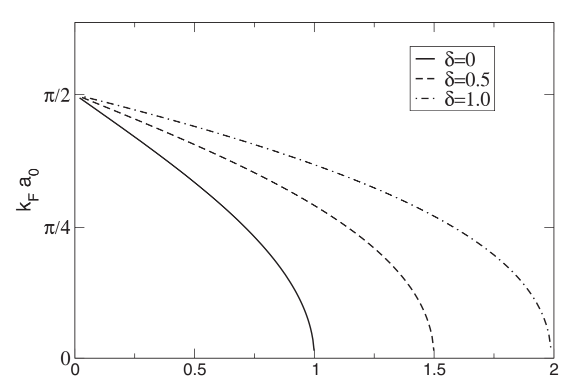

FIG. 8. "Fermi momentum" k_F as a function of magnetic field for different values of δ.

$$\varepsilon(\pm A) = 0. \quad \text{(A3)}$$

The physical meaning of the various quantities is as follows: $\varepsilon(\lambda)$ and $p(\lambda)$ are the energy and momentum of an elementary "spinon" excitation carrying spin $S^z = \pm\frac{1}{2}$. We note that spinons can only be excited in pairs. The magnetization per site in the ground state is given in terms of the ground state root density $\rho(\lambda)$ as

$$\langle S_j^z \rangle = \frac{1}{2} - \int_{-A}^{A} d\lambda \rho(\lambda). \quad \text{(A4)}$$

The Fermi momentum is equal to

$$k_F = p(A) = \frac{2\pi}{a_0}\int_0^A d\lambda \rho(\lambda) = \frac{\pi}{a_0}\left[\frac{1}{2} - \langle S_j^z \rangle\right], \quad \text{(A5)}$$

where we have used that $\rho(-\lambda) = \rho(\lambda)$. The spin velocity is equal to the derivative of the spinon energy with respect to the momentum at the Fermi points

$$v = \left.\frac{\partial \epsilon(\lambda)}{\partial p(\lambda)}\right|_{\lambda=A} = \left.\frac{\partial \epsilon(\lambda)/\partial\lambda}{2\pi\rho(\lambda)}\right|_{\lambda=A} a_0. \quad \text{(A6)}$$

Finally, the dressed charge is related to β by

$$\beta = \frac{1}{\sqrt{8}Z(A)}. \quad \text{(A7)}$$

In order to determine v and β we solve Eq. (A1) numerically, which is easily done to very high precision as the equations are linear. The results are shown in Fig. 7–9.

For zero magnetic field we have $k_F = \pi/2a_0$, $\beta^2 = \frac{1}{4\pi}\arccos(-\delta)$, and

$$v = \frac{Ja_0}{2}\frac{\sin 4\pi\beta^2}{1-4\beta^2}. \quad \text{(A8)}$$

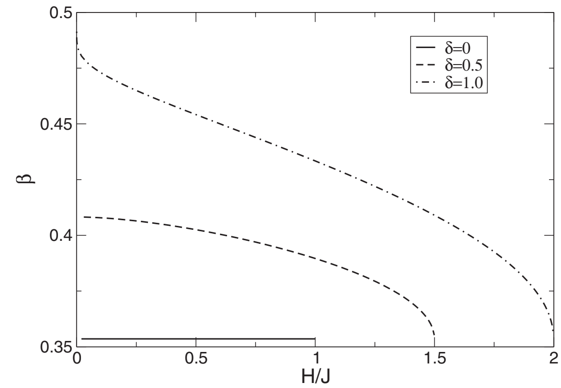

FIG. 9. Parameter β as a function of magnetic field for different values of δ.

APPENDIX B: FORM FACTORS OF THE EXPONENTIAL FIELD $\mathcal{O}_a^{-1}$

The exponential field $\mathcal{O}_a^{-1}$ [Eq. (19)] has topological charge +1. Hence it has nonvanishing matrix elements between the ground state $|0\rangle$ and one-soliton states, two-particle soliton-breather sb_n states, etc. In this appendix we determine all one and two-particle form factors. Our results hold generally for the sine-Gordon model in the attractive regime.

1. One soliton form factors

The one-soliton form factor is[56]

$$F_s^{1a}(\theta) = \sqrt{Z_1(a)}e^{i\pi a/2\beta}e^{a\theta/\beta}, \quad \text{(B1)}$$

where

$$\sqrt{Z_1(a)} = \left(\frac{\mathcal{C}_2}{2\mathcal{C}_1^2}\right)^{1/4}\left(\frac{\xi\mathcal{C}_2}{16}\right)^{-1/8}\left\{\frac{\sqrt{\pi}\Delta a_0\Gamma[(3+\xi)/2]}{v\Gamma(\xi/2)}\right\}^{2a^2+1/8\beta^2} \times\exp\left\{\int_0^\infty \frac{dt}{t}\left\{\frac{\cosh(4\xi at/\beta)e^{-(1+\xi)t}-1}{4\sinh(t\xi)\sinh[t(\xi+1)]\cosh(t)} + \frac{1}{1\sinh(t\xi)} - \left(2a^2+\frac{1}{8\beta^2}\right)e^{-2t}\right\}\right\}. \quad \text{(B2)}$$

2. *S* matrices, their analytical properties and minimal form factors

The soliton-breather S matrix is given by[57]

$$S_{sb_n}(\theta) = (-1)^n \exp\left[2\int_0^\infty \frac{dt}{t}\frac{\cosh(\xi t)\sinh(n\xi t)}{\cosh(t)\sinh(\xi t)}\sinh\left(\frac{2\theta t}{i\pi}\right)\right] = \prod_{j=1}^{n}\frac{\sinh\left[\theta + i\frac{\pi\xi(n+1-2j)}{2}\right] + i\cos\left(\frac{\pi\xi}{2}\right)}{\sinh\left[\theta - i\frac{\pi\xi(n+1-2j)}{2}\right] - i\cos\left(\frac{\pi\xi}{2}\right)}. \quad \text{(B3)}$$

The corresponding soliton-breather three-particle coupling is

$$g^{s}_{sb_n} = \left| 2\cot\left(\frac{n\pi\xi}{2}\right)\prod_{l=1}^{n-1}\cot^2\left(\frac{l\pi\xi}{2}\right)\right|^{1/2}. \tag{B4}$$

Note that by crossing symmetry we must have

$$g^{s}_{sb_n} = g^{b_n}_{\bar{s}s}. \tag{B5}$$

The minimal soliton-breather form factor can be obtained combining Eqs. (2.23), (4.19), and (4.20) of Ref. 51, which can be summarized as

$$S(\theta) = \exp\left\{\int_0^\infty dt f(t)\sinh\left(\frac{t\theta}{i\pi}\right)\right\} \Rightarrow F^{\min}(\theta) = \exp\left\{\int_0^\infty dt f(t)\frac{1-\cosh\left[t\left(1+\frac{\theta}{i\pi}\right)\right]}{2\sinh(t)}\right\}.$$

The soliton-breather S matrix Eq. (B3) then gives rise to the minimal form factor

$$F^{\min}_{sb_n}(\theta) = \mathcal{R}_{sb_n}(\theta)\exp\left\{\int_0^\infty \frac{dt}{t}\frac{\cosh(\xi t)\sinh(n\xi t)}{\cosh(t)\sinh(\xi t)} \times \frac{1-\cosh\left[2t\left(1+\frac{\theta}{i\pi}\right)\right]}{\sinh(2t)}\right\}, \tag{B6}$$

where $\mathcal{R}_{sb_n}(\theta)$ is given by

$$R_{sb_{2n}}(\theta) = 1,$$

$$R_{sb_{2n+1}}(\theta) = i\sinh(\theta/2). \tag{B7}$$

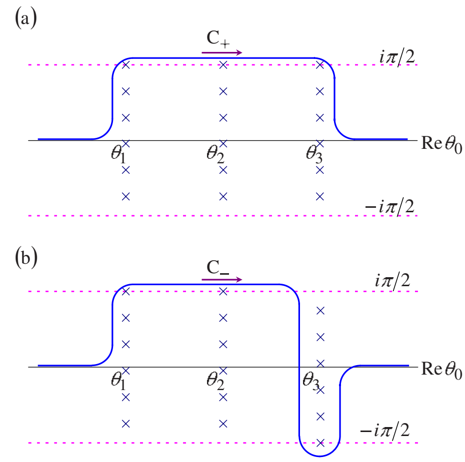

FIG. 10. (Color online) Integration contours C_+ [panel (a)] and C_- [panel (b)]. Both the contours are located in the strip $-\pi/2-0 < \Im\theta_0 < \pi/2+0$.

3. Soliton-breather form factors

We will calculate the full form factor using the residue condition,[56,58]

$$ig^{b_n}_{s\bar{s}}F^{1a}_{sb_n}(\theta_s,\theta_b) = \operatorname{Res}_{\delta=0}F^{1a}_{ss\bar{s}}\left(\theta_s, \theta_b - \frac{iu^{\bar{s}s}_{b_n}}{2}, \theta_b + \delta + \frac{iu^{\bar{s}s}_{b_n}}{2}\right), \tag{B8}$$

where $u^{\bar{s}s}_{b_n} = \pi(1-n\xi)$, and

$$g^{b_n}_{\bar{s}s} = (-1)^n g^{b_n}_{s\bar{s}} = \left| 2\cot\left(\frac{n\pi\xi}{2}\right)\prod_{l=1}^{n-1}\cot^2\left(\frac{l\pi\xi}{2}\right)\right|^{1/2}. \tag{B9}$$

The three particle form factor involving two solitons and one antisoliton is[56]

$$F^{1a}_{ss\bar{s}}(\theta_1,\theta_2,\theta_3) = \frac{i\mathcal{C}_2\sqrt{Z_1(a)}}{4\mathcal{C}_1}e^{i\pi a/2\beta}e^{(a/\beta)(\theta_1+\theta_2+\theta_3)+\theta_3/\xi}G(\theta_{12})G(\theta_{13})G(\theta_{23}) \times\left[e^{i\pi/2\beta^2}\int_{C_+}\frac{d\theta_0}{2\pi}e^{-(2a/\beta+1/\xi)\theta_0}W(\theta_{10})W(\theta_{20})W(\theta_{30}) - e^{-i\pi/2\beta^2}\int_{C_-}\frac{d\theta_0}{2\pi}e^{-(2a/\beta+1/\xi)\theta_0}W(\theta_{10})W(\theta_{20})W(\theta_{03})\right], \tag{B10}$$

where $\theta_{jk} = \theta_j - \theta_k$,

$$G(\theta) = i\mathcal{C}_1\sinh\left(\frac{\theta}{2}\right)\exp\left\{-\int_0^\infty \frac{dt}{t}\frac{\sinh[(1-\xi)t]\sinh^2\left[t\left(1-\frac{i\theta}{\pi}\right)\right]}{\sinh(2t)\cosh(t)\sinh(\xi t)}\right\}, \tag{B11}$$

$$W(\theta)=\frac{-2}{\cosh(\theta)}\times\exp\left\{-2\int_0^\infty\frac{dt}{t}\frac{\sinh[t(\xi-1)]\sinh^2[t(1-i\theta/\pi)]}{\sinh(2t)\sinh(t\xi)}\right\},\tag{B12}$$

$$\mathcal{C}_1=\exp\left\{-\int_0^\infty\frac{dt}{t}\frac{\sinh^2(t/2)\sinh[t(\xi-1)]}{\sinh(2t)\sinh(t\xi)\cosh(t)}\right\},\tag{B13}$$

$$\mathcal{C}_2=\exp\left\{4\int_0^\infty\frac{dt}{t}\frac{\sinh^2(t/2)\sinh[t(\xi-1)]}{\sinh(2t)\sinh(t\xi)}\right\}.\tag{B14}$$

The integration contours C_+ and C_- are constructed as follows. The contour C_+ runs from $-\infty$ to ∞ in the complex θ_0 plane, passing above the poles at $\theta_p+i\pi/2$, $p=1,2,3$. Similarly, the contour C_- runs above the points $\theta_p+i\pi/2$, $p=1,2$, and then below $\theta_3-i\pi/2$ (see Fig. 10).

Let us consider the form factor Eq. (B10) for rapidities $\theta_1=\theta_s$, $\theta_2=\theta_b-\frac{iu^{\bar{s}\bar{s}}_{b_n}}{2}$, and $\theta_3=\theta_b+\delta+\frac{iu^{\bar{s}\bar{s}}_{b_n}}{2}$. The function $W(\theta)$ has poles in the strip $|\mathrm{Im}\ \theta|<\frac{\pi}{2}$ of the complex θ-plane at the points $\theta=iv_k$, where

$$v_k=\pi\left(k\xi-\frac{1}{2}\right),\quad 0\le k<\left[\frac{1}{\xi}\right].$$

As a result the function $W(\theta_{10})W(\theta_{20})W(\theta_{03})$ has poles at $\theta_0=\theta_1-i\pi(k\xi-\frac{1}{2})$, $\theta_0=\theta_b+\frac{i\pi\xi}{2}(n-2k)$, and $\theta_0=\theta_b+\delta-\frac{i\pi\xi}{2}(n-2k)$, $0\le k<\frac{n}{2}+\frac{1}{2\xi}$. By construction the contour C_- runs between $n+1$ pairs of poles at $\theta_0=\theta_b+\frac{i\pi\xi}{2}(n-2k)$, and $\theta_0=\theta_b+\delta+\frac{i\pi\xi}{2}(n-2k)$, $0\le k\le n$, with only an infinitesimal separation δ between them (see Fig. 11). As a result the integral over θ_0 exhibits a simple pole for $\delta\to0$. In order to extract the residue of this pole, we deform the "singular" contour C_- into a "regular" contour C plus closed contours including one pole from each pair. C is chosen such that the integral over it is finite in the limit $\delta\to0$. The contours C and C_- are shown for $n=1$ in Fig. 11.

For general n we then find that

$$\int_{C_-}\frac{d\theta_0}{2\pi}e^{-(2a/\beta+1/\xi)\theta_0}W(\theta_{10})W(\theta_{20})W(\theta_{03})=\sum_{k=0}^{n}ie^{-(2a/\beta+1/\xi)(\theta_b+i\pi\xi(n-2k)/2)}W\left(\theta_{1b}-\frac{i\pi\xi(n-2k)}{2}\right)\times W_{\mathrm{res}}(iv_k)W(-\delta+iv_{n-k})+\text{regular part},\tag{B15}$$

where $W_{\mathrm{res}}(iv_k)$ denotes the residue of the function $W(\theta)$ taken at the point $\theta=iv_k$. We note that $W(-\delta+iv_{n-k})$ has a simple pole at $\delta=0$.

The regular part of the integral does not contribute to the residue in the right hand side of Eq. (B8) and in the following will be ignored. Similarly, the integral over C_+ has a finite limit $\delta\to0$.

In order to proceed we need to analytically continue the function $W(\theta)$, which can be done using the relation[51]

$$W(\theta\pm i\pi\xi)=\frac{\sin\left[\frac{i}{2}\left(\theta\mp\frac{i\pi}{2}\right)\right]}{\sin\left[\frac{i}{2}\left(\theta\pm i\pi\xi\pm\frac{i\pi}{2}\right)\right]}W(\theta).\tag{B16}$$

Using Eq. (B16) the residues of $W(\theta)$ are readily calculated

$$W_{\mathrm{res}}(iv_k)=\frac{2(-1)^{k-1}}{\sqrt{\mathcal{C}_2}\sin\left(\frac{k\pi\xi}{2}\right)}\prod_{j=1}^{k-1}\cot\left(\frac{j\pi\xi}{2}\right),\quad k\ge1,$$

$$W_{\mathrm{res}}(iv_0)=-\frac{2}{\sqrt{\mathcal{C}_2}}.\tag{B17}$$

The soliton-breather form factors can now be determined from the residue condition (B8)

$$ig^{b_n}_{\bar{s}\bar{s}}F^{1a}_{sb_n}(\theta_s,\theta_b)=-\frac{i\mathcal{C}_2\sqrt{Z_1(a)}}{4\mathcal{C}_1}e^{i\pi a/2\beta+a\theta_s/\beta}G(-iu^{\bar{s}\bar{s}}_{b_n})\times G\left(\theta_{sb}+\frac{iu^{\bar{s}\bar{s}}_{b_n}}{2}\right)G\left(\theta_{sb}-\frac{iu^{\bar{s}\bar{s}}_{b_n}}{2}\right)\times\sum_{k=0}^{n}(-1)^{n-k}e^{-i\pi a\xi(n-2k)/\beta}W_{\mathrm{res}}(iv_k)\times W_{\mathrm{res}}(iv_{n-k})W\left(\theta_{sb}-i\frac{\pi\xi(n-2k)}{2}\right).\tag{B18}$$

The soliton-breather form factor can be expressed in terms of the minimal form factor [Eq. (B6)] as

$$F^{1a}_{sb_n}(\theta_s,\theta_b)=N^a_{sb_n}\sqrt{Z_1(a)}e^{i\pi a/2\beta+a\theta_s/\beta}K^a_{sb_n}(\theta_{sb})F^{\min}_{sb_n}(\theta_{sb}).\tag{B19}$$

Here $N^a_{sb_n}$ is a normalization constant given by

$$N^a_{sb_n}=\frac{e^{i\pi n\xi a/\beta}}{ig^s_{sb_n}\mathrm{Res}_{\theta=iu^{sb_n}_s}[K^a_{sb_n}(\theta)]F^{\min}_{sb_n}(iu^{sb_n}_s)},\tag{B20}$$

where

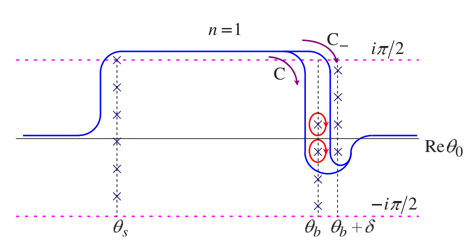

FIG. 11. (Color online) Integration contour C_- for $\xi=0.174\,371$ and $n=1$. The contour C_- is transformed into the contour C and the closed contours around the poles.

$$u_s^{sb_k} = \frac{\pi}{2}(k\xi + 1). \tag{B21}$$

The "pole functions" $K^a_{sb_n}(\theta)$ have somewhat different forms for even and odd n, respectively, and are given by

$$K^a_{sb_{2m}}(\theta) = \frac{1}{\cosh\theta}\prod_{l=1}^{m-1}\frac{1}{\cosh\left(\frac{\theta}{2}+\frac{iu_s^{sb_{2l}}}{2}\right)\cosh\left(\frac{\theta}{2}-\frac{iu_s^{sb_{2l}}}{2}\right)} \times\left\{[W_{\rm res}(iv_m)]^2 - \sum_{k=1}^{m} W_{\rm res}(iv_{m-k})W_{\rm res}(iv_{m+k}) \times[e^{-2i\pi ka\xi/\beta}\Psi_{2k}(\theta) + e^{2i\pi ka\xi/\beta}\Psi_{2k}(-\theta)]\right\}, \tag{B22}$$

$$K^a_{sb_{2m+1}}(\theta) = \frac{1}{\sinh\left(\frac{\theta}{2}\right)}\prod_{l=0}^{m-1}\frac{1}{\cosh\left(\frac{\theta}{2}+\frac{iu_s^{sb_{2l+1}}}{2}\right)\cosh\left(\frac{\theta}{2}-\frac{iu_s^{sb_{2l+1}}}{2}\right)} \times\sum_{k=0}^{m} W_{\rm res}(iv_{m-k})W_{\rm res}(iv_{m+k+1})[e^{-i\pi a(2k+1)\xi/\beta}\Psi_{2k+1}(\theta) + e^{i\pi a(2k+1)\xi/\beta}\Psi_{2k+1}(-\theta)], \tag{B23}$$

where

$$\Psi_{2k}(\theta) = \frac{\sin\left(\frac{i\theta}{2}-\frac{\pi}{4}\right)}{\sin\left(\frac{i\theta}{2}+\frac{u_s^{sb_{2k}}}{2}\right)}\prod_{j=1}^{k-1}\cot\left(\frac{i\theta}{2}+\frac{u_s^{sb_{2j}}}{2}\right), \tag{B24}$$

$$\Psi_{2k+1}(\theta) = \frac{1}{\sin\left(\frac{i\theta}{2}+\frac{u_s^{sb_{2k+1}}}{2}\right)}\prod_{j=0}^{k-1}\cot\left(\frac{i\theta}{2}+\frac{u_s^{sb_{2j+1}}}{2}\right). \tag{B25}$$

APPENDIX C: FORM FACTORS OF exp[$ia\Theta$]

The operator $\exp[ia\Theta]$ carries zero topological charge. Hence the nonvanishing form factors with less than three particles involve a single breather, a soliton-antisoliton pair, or two breathers. In this appendix we construct these one and two particle form factors.

1. S matrices and minimal form factors

The breather-breather S matrix is[57]

$$S_{b_kb_l}(\theta) = \exp\left\{4\int_0^\infty \frac{dt}{t}\frac{\sinh\left(\frac{2\theta t}{i\pi}\right)}{\cosh(t)\sinh(\xi t)} \times\cosh(\xi t)\sinh(k\xi t)\cosh[(1-l\xi)t]\right\},\quad k<l, \tag{C1}$$

$$S_{b_kb_k}(\theta) = -\exp\left\{2\int_0^\infty \frac{dt}{t}\frac{\sinh\left(\frac{2\theta t}{i\pi}\right)}{\cosh(t)\sinh(\xi t)} \times\{\cosh(\xi t)\sinh[(2k\xi-1)t] + \sinh[(1-\xi)t]\}\right\}. \tag{C2}$$

Evaluating the integrals gives

$$S_{b_kb_l}(\theta) = \tanh\left(\frac{\theta+iu^{bb}_{l+k}}{2}\right)\coth\left(\frac{\theta-iu^{bb}_{l+k}}{2}\right) \times\tanh\left(\frac{\theta+iu^{bb}_{l-k}}{2}\right)\coth\left(\frac{\theta-iu^{bb}_{l-k}}{2}\right) \times\prod_{j=1}^{k-1}\left\{\tanh^2\left(\frac{\theta+iu^{bb}_{l-k+2j}}{2}\right) \times\coth^2\left(\frac{\theta-iu^{bb}_{l-k+2j}}{2}\right)\right\}, \tag{C3}$$

where now $k\le l$, and

$$u_n^{bb} = \frac{n\pi\xi}{2}. \tag{C4}$$

The simple pole in $S_{b_kb_l}(\theta)$ at $\theta=iu^{bb}_{k+l}$ corresponds to the formation of a b_{k+l} breather bound state. The corresponding residue is

$$S_{\rm res}(iu^{bb}_{k+l}) = 2i\tan\left(\frac{(k+l)\pi\xi}{2}\right)\tan\left(\frac{l\pi\xi}{2}\right)\cot\left(\frac{k\pi\xi}{2}\right) \times\prod_{j=1}^{k-1}\cot^2\left(\frac{j\pi\xi}{2}\right)\prod_{j=l+1}^{l+k-1}\tan^2\left(\frac{j\pi\xi}{2}\right). \tag{C5}$$

The corresponding three-particle coupling is

$$g^{b_{k+l}}_{b_kb_l} = \left|2\cot\left(\frac{k\pi\xi}{2}\right)\tan\left(\frac{l\pi\xi}{2}\right)\tan\left(\frac{(k+l)\pi\xi}{2}\right)\right|^{1/2} \times\prod_{j=1}^{k-1}\left|\cot\left(\frac{j\pi\xi}{2}\right)\tan\left(\frac{(l+j)\pi\xi}{2}\right)\right|. \tag{C6}$$

The minimal form factor for two different breathers is then

$$F^{\min}_{b_k b_l}(\theta) = \exp\left\{-2\int_0^\infty \frac{dt}{t}\frac{\cosh(\xi t)\cosh[(1-l\xi)t]}{\cosh(t)} \times \frac{\sinh(k\xi t)}{\sinh(\xi t)}\frac{\cosh\left[2t\left(1-\frac{i\theta}{\pi}\right)\right]-1}{\sinh(2t)}\right\}. \tag{C7}$$

The minimal form factor $F^{\min}_{b_k b_k}(\theta)$ involving two breathers of the same type is given by

$$F^{\min}_{b_k b_k}(\theta) = i\sinh\left(\frac{\theta}{2}\right)\exp\left\{-2\int_0^\infty \frac{dt}{t}\frac{\sinh^2\left[t\left(1-\frac{i\theta}{\pi}\right)\right]}{\sinh(2t)} \times \frac{\cosh(\xi t)\sinh[(2k\xi-1)t]+\sinh[(1-\xi)t]}{\cosh(t)\sinh(\xi t)}\right\}. \tag{C8}$$

2. Soliton-antisoliton and one-breather form factors

The soliton-antisoliton form factors for the operators $\cos(\beta\Theta)$, $\sin(\beta\Theta)$, and Θ,

$$\Theta = -i\lim_{a\to 0}\partial_a e^{ia\Theta}, \tag{C9}$$

are[59]

$$F^{\cos(\beta\Theta)}_{s\bar{s}}(\theta) = \frac{\mathcal{G}_\beta}{2}\frac{G(\theta)}{\mathcal{C}_1}\cot\left(\frac{\pi\xi}{2}\right)\frac{8i\cosh\left(\frac{\theta}{2}\right)}{\xi\sinh\left(\frac{\theta-i\pi}{\xi}\right)} \times \cosh\left(\frac{\theta-i\pi}{2\xi}\right), \tag{C10}$$

$$F^{\sin(\beta\Theta)}_{s\bar{s}}(\theta) = -\frac{\mathcal{G}_\beta}{2}\frac{G(\theta)}{\mathcal{C}_1}\cot\left(\frac{\pi\xi}{2}\right)\frac{8\cosh\left(\frac{\theta}{2}\right)}{\xi\sinh\left(\frac{\theta-i\pi}{\xi}\right)} \times \sinh\left(\frac{\theta-i\pi}{2\xi}\right), \tag{C11}$$

$$F^{\Theta}_{s\bar{s}}(\theta) = -\frac{G(\theta)}{\mathcal{C}_1}\frac{\pi}{\beta\cosh\left(\frac{\theta-i\pi}{2\xi}\right)\cosh\left(\frac{\theta}{2}\right)}, \tag{C12}$$

where $G(\theta)$ and $\mathcal{C}_1$ are given by Eqs. (B11) and (B13), respectively, and

$$\mathcal{G}_a \equiv \langle e^{ia\Theta}\rangle = \left[\frac{a_0\Delta\sqrt{\pi}\,\Gamma\left(\frac{1}{2-2\beta^2}\right)}{v2\Gamma\left(\frac{\beta^2}{2-2\beta^2}\right)}\right]^{2a^2} \times \exp\left\{\int_0^\infty \frac{dt}{t}\left[-2a^2e^{-2t} + \frac{\sinh^2(2a\beta t)}{2\sinh(t\beta^2)\sinh(t)\cosh(t(1-\beta^2))}\right]\right\}. \tag{C13}$$

The single-particle form factors $F^\beta_{b_n}$ and $F^\Theta_{b_n}$ for the operators $e^{i\beta\Theta}$ and Θ, respectively, can be obtained from the residue condition for the soliton-antisoliton form factor $F^\beta_{s\bar{s}}(\theta)$ and $F^\Theta_{s\bar{s}}(\theta)$,

$$g^{b_n}_{s\bar{s}}F^a_{b_n} = \mathrm{Res}_{\theta=-iu^{s\bar{s}}_{b_n}}F^a_{s\bar{s}}(\theta), \quad u^{s\bar{s}}_{b_n} = \pi(1-n\xi),$$

where $a=\beta$, Θ. Using Eqs. (C10)–(C12), we can write

$$F^\beta_{b_n} = \frac{2\cot\left(\frac{\pi\xi}{2}\right)\sin(n\pi\xi)(-i)^n}{\left[2\cot\left(\frac{\pi\xi n}{2}\right)\prod_{l=1}^{n-1}\cot^2\left(\frac{\pi j\xi}{2}\right)\right]^{1/2}}\mathcal{G}_\beta \times \exp\left[\int_0^\infty \frac{dt}{t}\frac{\sinh[t(\xi-1)]\sinh^2(tn\xi)}{\sinh(2t)\cosh(t)\sinh(t\xi)}\right], \tag{C14}$$

$$F^\Theta_{b_{2m-1}} = i(-1)^{m-1}\frac{G\{i\pi[(2m-1)\xi-1]\}}{g^{b_{2m-1}}_{s\bar{s}}\mathcal{C}_1}\frac{\pi\xi}{\beta\sin\left[\frac{(2m-1)\pi\xi}{2}\right]}. \tag{C15}$$

3. Breather-breather form factors of exp(*ia*Θ)

To calculate two-breather form factor $F^a_{b_k b_l}(\theta_{12})$, we will start with the formulas for n-breather ($n=k+l$) form factor $F^a_{\underline{b_1}}(\underline{\gamma})$ from Ref. 60,

$$F^a_{\underline{b_1}}(\underline{\gamma}) = \frac{\mathcal{G}_a}{2^{n/2}}K^a_n(\underline{\gamma})\prod_{1\le i<j\le n}R(\gamma_{ij}), \tag{C16}$$

$$R(\gamma) = \frac{\mathcal{N}F^{\min}_{b_1 b_1}(\gamma)}{\sinh\left[\frac{1}{2}(\gamma-i\pi\xi)\right]\sinh\left[\frac{1}{2}(\gamma+i\pi\xi)\right]}, \tag{C17}$$

$$K^a_n(\underline{\gamma}) = \sum_{l_1=0}^{1}\cdots\sum_{l_n=0}^{1}(-1)^{l_1+\cdots+l_n}p^a_n(\underline{l}) \times \prod_{1\le i<j\le n}\left[1+(l_i-l_j)\frac{i\sin(\pi\xi)}{\sinh(\gamma_{ij})}\right], \tag{C18}$$

$$p_n^a(\underline{l}) = \left(\frac{2}{R(-i\pi)\sin(\pi\xi)}\right)^{n/2} \prod_{i=1}^{n} e^{(i\pi\xi a/\beta)(-1)^{l_i}}, \quad \text{(C19)}$$

where $\underline{\gamma}=(\gamma_1,\ldots,\gamma_n)$, $\underline{l}=(l_1,\ldots,l_n)$, and $\gamma_{ij}=\gamma_i-\gamma_j$,

$$\mathcal{N} = -\exp\left\{2\int_0^\infty \frac{dt}{t}\frac{\sinh(\xi t)\sinh[(1-\xi)t]}{\cosh(t)\sinh(2t)}\right\}.$$

The normalization factor $\mathcal{G}_a/2^{n/2}$ is introduce in Ref. 59.

Form factor $F_{b_k b_l}(\theta_1,\theta_2)$ can be calculated as follows:

(1) First step, we calculate the residues of the form factor at the point $\gamma_{n-1}-\gamma_n=-i\pi\xi$ ($\gamma_{n-1}=\gamma'_{n-1}-\frac{i\pi\xi}{2}$, $\gamma_n=\gamma'_{n-1}+\delta_1+\frac{i\pi\xi}{2}$). As a result, we obtain the form factor for $n-2$ breathers b_1 and one breather b_2.

(2) Second step, we calculate the residue of the $k+l-1$-particle form factor obtained at the point $\gamma_{n-2}-\gamma'_{n-1}=\frac{3i\pi\xi}{2}$ ($\gamma_{n-2}=\gamma'_{n-2}-i\pi\xi$, $\gamma'_{n-1}=\gamma'_{n-2}+\delta_2+\frac{i\pi\xi}{2}$). As a result, we obtain the form factor for $n-3$ breathers b_1 and one breather b_3.

(3) Step number $l-1$, we calculate the residue of the $k+2$-particle form factor obtained at the point $\gamma_{k+1}-\gamma'_{k+2}=\frac{ki\pi\xi}{2}$ ($\gamma_{k+1}=\gamma'_{k+1}-\frac{i(l-1)\pi\xi}{2}$, $\gamma'_{k+2}=\gamma'_{k+1}+\delta_{l-1}+\frac{i\pi\xi}{2}$). As a result, we obtain the form factor for k breathers b_1 and one breather b_l.

(4) Finally, taking $\gamma'_{k+1}\equiv\theta_2$, we can write

$$\gamma_{k+m} = \theta_2 + \sum_{j=l-m+1}^{l-1}\delta_j - \frac{i(l-2m+1)\pi\xi}{2}, \quad \text{(C20)}$$

$m=1,2,\ldots,l$, and δ_j are infinitesimal parameters.

Similar calculations performed with the variables γ_j, $j=1,2,\ldots,k$, give

$$\gamma_m = \theta_1 + \sum_{j=k-m+1}^{k-1}\epsilon_j - \frac{i(k-2m+1)\pi\xi}{2}, \quad \text{(C21)}$$

$m=1,2,\ldots,k$, and ϵ_j are infinitesimal parameters.

It should be noted that the order of calculation of residues predicts the rules

$$|\delta_1| \ll |\delta_2| \ll \cdots \ll |\delta_{k-1}| \ll |\theta_{12}|,$$

$$|\epsilon_1| \ll |\epsilon_2| \ll \cdots \ll |\epsilon_{l-1}| \ll |\theta_{12}|. \quad \text{(C22)}$$

The n-particle ($n=k+l$) form factor [Eq. (C16)] depends on $\gamma_i-\gamma_j$, $1\le i\le j\le n$. Taking into account Eqs. (C20)–(C22), we can write

$$\gamma_{ij} = \begin{cases} -\epsilon_{k-j} - i(j-i)\pi\xi & \text{if } (i,j)\in A_1 \\ -\delta_{l-j} - i(j-i)\pi\xi & \text{if } (i,j)\in A_2 \\ \theta_{12} - i\left(\frac{l-k}{2}+j-m\right) & \text{if } (i,j)\in A_3, \end{cases} \quad \text{(C23)}$$

where the manifolds $A_{1,2,3}$ are constructed as following:

$$A_1: 1\le i\le j\le k,$$

$$A_2: k+1\le i\le j\le n,$$

$$A_3: 1\le i\le k, k+1\le j\le n.$$

Then we obtain the following expression for the two-particle form factor,

$$F^a_{b_k b_l}(\theta_{12}) = N^a_{b_k b_l} K^a_{b_k b_l}(\theta_{12}) F^{\min}_{b_k b_l}(\theta_{12}), \quad \text{(C24)}$$

where the minimal form factor $F^{\min}_{b_k b_l}(\theta_{12})$ is given by Eq. (C7) for $k<l$, and Eq. (C8) for $k=l$,

$$K^a_{b_k b_l}(\theta) = K^a_n(\underline{\gamma}) \times \prod_{\nu=(l-k/2)+1}^{l+k/2} \frac{1}{\sinh\left[\frac{1}{2}(\theta-i\pi\xi\nu)\right]\sinh\left[\frac{1}{2}(\theta+i\pi\xi\nu)\right]}. \quad \text{(C25)}$$

The normalization constant $N^a_{b_k b_l}$ can be calculated as

$$N^a_{b_k b_l} = \frac{i g_{kl}^{k+l} F^a_{b_{k+l}}}{K^{\text{res}}_{b_k b_l} F^{\min}_{b_k b_l}\left(-\frac{i\pi\xi}{2}(k+l)\right)},$$

$$K^{\text{res}}_{b_k b_l} = \text{Res}_{\delta=0}\left[K^a_{b_k b_l}\left(-\delta - \frac{i\pi\xi}{2}(k+l)\right)\right],$$

the one-particle form factor F_{b_n} is given by Eq. (C14).

In particular, the pole function for the few lowest breathers are

$$K^a_{b_1 b_1}(\theta) = \frac{(a)^2}{\sinh\left[\frac{1}{2}(\theta-i\pi\xi)\right]\sinh\left[\frac{1}{2}(\theta+i\pi\xi)\right]},$$

$$K^a_{b_1 b_2}(\theta) = \frac{(a)}{\sinh\left[\frac{1}{2}\left(\theta-\frac{3i\pi\xi}{2}\right)\right]\sinh\left[\frac{1}{2}\left(\theta+\frac{3i\pi\xi}{2}\right)\right]}\left\{(a)^2 + \frac{1}{8\cos\left(\frac{\pi\xi}{2}\right)\cosh\left[\frac{1}{2}\left(\theta+\frac{i\pi\xi}{2}\right)\right]\cosh\left[\frac{1}{2}\left(\theta-\frac{i\pi\xi}{2}\right)\right]}\right\},$$

$$K^a_{b_2b_2}(\theta) = \prod_{k=1}^{2} \frac{1}{\sinh\left[\frac{1}{2}(\theta - ik\pi\xi)\right]\sinh\left[\frac{1}{2}(\theta + ik\pi\xi)\right]}(a)^2\left\{(a)^2 + \frac{1}{2\cosh\left[\frac{1}{2}(\theta + i\pi\xi)\right]\cosh\left[\frac{1}{2}(\theta - i\pi\xi)\right]}\right\},$$

$$K^a_{b_1b_3}(\theta) = \frac{(a)^2}{\sinh\left[\frac{1}{2}(\theta - 2i\pi\xi)\right]\sinh\left[\frac{1}{2}(\theta + 2i\pi\xi)\right]}\left\{(a)^2 + \frac{1}{4\cos(\pi\xi)[1+\cos(\pi\xi)]} + \frac{1+2\cos(\pi\xi)}{8\cos(\pi\xi)\cosh\left[\frac{1}{2}(\theta + i\pi\xi)\right]\cosh\left[\frac{1}{2}(\theta - i\pi\xi)\right]}\right\}.$$

where

$$(a) = \frac{\sin\left(\frac{\pi\xi a}{\beta}\right)}{\sin(\pi\xi)}.$$

4. Breather-breather form factors of Θ

Equation (C9) allows us to express the operator Θ in terms of exponential operator $e^{ia\Theta}$. Therefore the form factors $F^{\Theta}_{b_kb_l}(\theta)$ are expressed in terms of the form factors of the exponential fields. Taking into account that the pole function $K^a_{b_kb_l}(\theta)$ Eq. (C25) goes to zero as a^2 when $k+l$ is even and linearly with a when $k+l$ is odd, we can conclude that only form factors $F^{\Theta}_{b_kb_l}(\theta)$ with $k+l$ being odd are nontrivial. These form factors are written as

$$F^{\Theta}_{b_kb_l}(\theta) = N^{\Theta}_{b_kb_l}K^{\Theta}_{b_kb_l}(\theta)F^{\min}_{b_kb_l}(\theta), \tag{C26}$$

where the pole function $K^{\Theta}_{b_kb_l}(\theta)$ is given by,

$$K^{\Theta}_{b_kb_l}(\theta) = -i\lim_{a\to 0}\partial_a K^a_{b_kb_l}(\theta),$$

the normalization factor $N^{\Theta}_{b_kb_l}$ is determined as

$$N^{\Theta}_{b_kb_l} = \lim_{a\to 0} N^a_{b_kb_l},$$

and the minimal form factor is defined by Eq. (C7).

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