Dynamical Correlations of the Spin-\(\frac{1}{2}\) Heisenberg XXZ Chain in a Staggered Field

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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.

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I. INTRODUCTION

The field-induced gap problem in anisotropic quasi one dimensional spin-\(\frac{1}{2}\) Heisenberg antiferromagnets has attracted much experimental\(^3\)\(^–\)\(^15\) 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\(^1\)\(^–\)\(^6\), CDC \([\text{CuCl}_2\cdot 2((\text{CD}_3)_2\text{SO})]\)\(^7\), Copper-Pyrimidine\(^8\)\(^–\)\(^12\) and \(\text{Yb}_4\text{As}_3\)\(^13\)\(^,\)\(^14\). 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 \(H\) induces a staggered field perpendicular to \(H\). 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\(^16\)

\[
\mathcal{H} = J \sum_j \mathbf{S}_j \cdot \mathbf{S}_{j+1} - H \sum_j S_j^z + h \sum_j (-1)^j S_j^x , \quad (1)
\]

where \(h = \gamma H\). The constant \(\gamma\) 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,

\[
\mathcal{H} = J \sum_j \left[ S_j^x S_{j+1}^x + S_j^y S_{j+1}^y + \delta S_j^z S_{j+1}^z \right] - H \sum_j S_j^z + h \sum_j (-1)^j S_j^x . \quad (2)
\]

In what follows we will consider the region \(-1 < \delta \leq 1\) 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 section II we construct the continuum limit of the model (2). In section III we derive a spectral representation of the dynamical structure factor at low energies. In section IV we present the calculations for retarded two-point correlation functions. In section 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 appendices: 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. Appendices B and C present results for the form factors of the operators entering the calculation of the dynamical structure factor.

II. CONTINUOUS 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\(^33\)\(^–\)\(^36\)

\[
\mathcal{H}_{h=0} = \frac{\nu}{16\pi} \int dx \left[ (\partial_x \Phi)^2 + (\partial_x \Theta)^2 \right] , \quad (3)
\]
where the field $\Phi(x)$ and its dual field $\Theta(x)$ are compactified

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

The commutation relation between $\Phi$ and $\Theta$ reads

$$
\left[\Theta(x), \Phi(x')\right] = 8\pi i \delta_H(x-x'),
$$

where $\delta_H(x)$ is the Heaviside step function, equal to 0 for $x < 0$, 1 for $x > 0$ and 1/2 for $x = 0$. The parameters $v$, $\beta$ and $k_F$ (see below) in the low-energy theory can be calculated directly from the Bethe ansatz solution on the XXZ chain. How this is done is briefly reviewed in Appendix A. The results 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

$$
S^a_j = \sum_{a=1}^3 e^{iQ^a_a x} S^a_0(x) + \ldots,
$$

where $x = ja_0$ and $a_0$ is the lattice spacing. The wavenumbers $Q^a_0$ are

$$
\begin{align*}
Q^x_1 &= -Q^x_3 = Q = \frac{\pi}{a_0} - 2k_F, \quad Q^z_2 = \frac{\pi}{a_0}, \\
Q^y_2 &= Q^x_2, \\
Q^z_1 &= 0, \quad Q^z_3 = -Q^z_2 = 2k_F,
\end{align*}
$$

where the Fermi momentum is given by

$$
k_F = \frac{\pi}{2a_0}(1 - 2\langle S^z_j \rangle).
$$

Here $\langle S^z_j \rangle$ is the magnetization per site. The continuum fields $S^a_j$ are given in terms of the canonical boson $\Phi$ and its dual field $\Theta$ as

$$
\begin{align*}
S^x_1(x) &= \frac{1}{2} A(H) \left( O^1_3(x) + O^{-1}_{-3}(x) \right), \\
S^y_2(x) &= c(H) \cos \left( \beta \Theta(x) \right), \\
S^z_2(x) &= \left( S^y_2(x) \right)^\dagger, \\
S^y_3(x) &= \frac{1}{2i} A(H) \left[ O^1_3(x) - O^1_{-3}(x) \right], \\
S^y_4(x) &= c(H) \sin \left( \beta \Theta(x) \right), \\
S^y_3(x) &= \left( S^y_4(x) \right)^\dagger, \\
S^z_1(x) &= \frac{a_0}{8\pi\beta} \partial_x \Phi(x), \\
S^z_2(x) &= \left( S^z_1(x) \right)^\dagger + \frac{1}{2i} a(H) C^1_0(x),
\end{align*}
$$

where

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

We are using normalizations such that

$$
\langle O^1_a(\tau, x)O^{-1}_a(0, 0) \rangle = \left[ \frac{v\tau + ix}{v\tau - ix} \right]^\dagger \left[ \frac{a_0^2}{v^2\tau^2 + x^2} \right]^{2a_0^2 + \frac{8\pi^2}{x^2}}.
$$

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

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

where $\mu(h, H) = \frac{h}{h_c(H)}$. 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.

\section{A. Elementary Excitations}

The sine-Gordon model is integrable and its spectrum and scattering matrix are known exactly. In the relevant range of the parameter $\beta$ ($0 < \beta < 1$) the spectrum of elementary excitations consists of a soliton–anti-soliton doublet and several soliton–anti-soliton bound states called “breathers”. There are altogether $\lfloor 1/\xi \rfloor$ breathers, where $[x]$ denotes the integer part of $x$ and $\xi = \frac{a_0}{2\pi\beta}$. In order to distinguish the various single-particle states we introduce labels $s$ and $\bar{s}$ for solitons and anti-solitons 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 $\theta$ as

$$
vP_e = \Delta_s \sinh(\theta), \quad E_e = \Delta_s \cosh(\theta),
$$

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

$$
\frac{\Delta}{J} = \frac{2v}{J_{a_0}\sqrt{\pi} \Gamma(\frac{1+\xi}{2})} \left[ J_{a_0} \frac{c(H)\pi}{2} \frac{\Gamma(\frac{1+\xi}{2})}{\Gamma(\frac{1+\xi}{2})} \right] \frac{1}{J}. \quad (23)
$$

When $\delta \approx 1$ and the magnetization is small the leading irrelevant perturbation to the Gaussian model needs to be taken into account, leading to

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

where $B = 0.422169$. 


B. Scattering States

It is useful to introduce creation and annihilation operators $A^\dagger_n(\theta)$ and $A_n(\theta)$ for the elementary excitations. Here $s = s, s_1, \ldots, s_{|\theta|}$. The creation/annihilation operators fulfill the so-called Faddeev-Zamolodchikov (FZ) algebra

\[
A_n(\theta_1)A_b(\theta_2) = S_{ab}^{\theta_1\theta_2}(\theta_1 - \theta_2)A_b(\theta_2)A_n(\theta_1);
\]
\[
A^\dagger_n(\theta_1)A^\dagger_b(\theta_2) = S_{ab}^{\theta_1\theta_2}(\theta_1 - \theta_2)A^\dagger_b(\theta_2)A^\dagger_n(\theta_1);
\]
\[
A^\dagger_n(\theta_1)A_b(\theta_2) = S_{ab}^{\theta_1\theta_2}(\theta_1 - \theta_2)A_b(\theta_1)A^\dagger_n(\theta_1) + 2\pi \delta_{ab} \delta(\theta_1 - \theta_2).
\]  

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

\[
|\{\epsilon_n, \theta_n\}\rangle = A^\dagger_n(\theta_n) \cdots A^\dagger_{\epsilon_1}(\theta_1)|0\rangle.
\]  

Energy and momentum of these states are

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

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

\[
I = \sum_{n=0}^{\infty} \sum_{\{\epsilon\}} \int \frac{d\theta_1 \cdots d\theta_n}{n!(2\pi)^n} |\{\epsilon_n, \theta_n\}\rangle \langle \{\epsilon_n, \theta_n\}|.
\]  

C. Discrete Symmetries

The Hamiltonian is invariant with respect to charge conjugation

\[
C C^{-1} = -\Theta, \quad C \Phi C^{-1} = -\Phi.
\]  

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

\[
C|0\rangle = |0\rangle, \quad CA^\dagger_n(\theta)C^{-1} = A^\dagger_{-n}(\theta), \quad CB_k(\theta)C^{-1} = (-1)^k B_{-k}(\theta).
\]

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

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

is a conserved quantity. We will use the conventions in which soliton/antisoliton and breathers have topological charge $\mp 1$ and zero respectively.

| $m$ | $A$ | $a$ | $c$ | $v/J_{g0}$ | $\beta$ | $H/J$ |
|---|---|---|---|---|---|---|
| 0.02 | 0.3044 | 0.3953 | 0.5257 | 1.1804 | 0.386192 | 0.090093 |
| 0.04 | 0.3065 | 0.3913 | 0.5268 | 1.1714 | 0.385821 | 0.18186 |
| 0.06 | 0.3096 | 0.3867 | 0.5256 | 1.1582 | 0.385332 | 0.2598 |
| 0.08 | 0.3130 | 0.3817 | 0.5240 | 1.1373 | 0.384573 | 0.35073 |
| 0.10 | 0.3173 | 0.3769 | 0.5219 | 1.1142 | 0.383768 | 0.42867 |
| 0.12 | 0.3226 | 0.3713 | 0.5194 | 1.0807 | 0.38265 | 0.5196 |
| 0.14 | 0.3284 | 0.3661 | 0.5164 | 1.0460 | 0.381535 | 0.59754 |
| 0.16 | 0.3354 | 0.3610 | 0.5129 | 1.0124 | 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 | 1.1691 |
| 0.36 | 0.5342 | 0.3193 | 0.4367 | 0.456492 | 0.365244 | 1.19508 |
| 0.38 | 0.588 | 0.3166 | 0.4222 | 0.39204 | 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 | 0.358389 | 1.28276 |
| 0.46 | 1.214 | 0.3127 | 0.3279 | 0.122936 | 0.356722 | 1.29251 |
| 0.48 | 1.89 | 0.3142 | 0.2796 | 0.044871 | 0.354713 | 1.299 |

III. DYNAMICAL STRUCTURE FACTOR

The central object of our study is the inelastic neutron scattering intensity, which is proportional to\textsuperscript{46}

\[
I(\omega, k) \propto \sum_{\alpha, \alpha'} \left( \delta^{\alpha\alpha'} - \frac{k^\alpha k'^{\alpha'}}{k^2} \right) S^{\alpha\alpha'}(\omega, k).
\]  

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

\[
S^{\alpha\alpha'}(\omega, k) = \frac{1}{L} \sum_{l,l'} \int_{-\infty}^{\infty} dt e^{i\omega t - ik(l-l')} \langle 0| S^\alpha_l(t) S^{\alpha'}_{l'}(0) |0\rangle.
\]  

Substituting the low-energy expressions (6) into (32) we obtain

\[
S^{\alpha\alpha'}(\omega, k) = \sum_{a,b=1}^{3} \int_{-\infty}^{\infty} dt e^{i\omega t - i(k-\Omega_n^a)l + i(k+\Omega_n^b)l'} \times \langle 0| S^a_{\epsilon}(t, x) S^{\alpha'}_{\epsilon}(0, y) |0\rangle.
\]
where \( x = l a_0, y = l' a_0 \) and \( S_0^a(x) \) are the leading terms in the low energy limits (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 (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 (28) between the operators in (33) and using

\[
\langle 0| S_a^a(t, x) |\{\epsilon_n, \theta_n\}\rangle = e^{-iE_n t + iP_n z} \langle 0| S_a^a(0, 0) |\{\epsilon_n, \theta_n\}\rangle,
\]

we arrive at

\[
S^a_a(\omega, Q_a^a + q) = \frac{2\pi}{a_0} \sum_{n=1}^{\infty} \sum_{\{\epsilon_n\}} \sum_{b=1}^{3} \delta_{Q_a^a, 0} \int d\theta_1 \ldots d\theta_n \left( \frac{Q_a^a}{n!(2\pi)^n} \right) \langle 0| S_a^a |\{\epsilon_n, \theta_n\}\rangle \langle \{\epsilon_n, \theta_n\}|S_b^a' |0\rangle \delta(q - P_n) \delta(\omega - E_n). \tag{35}
\]

| \(Q\) | 1 | 0 | 1 | 1 | 1 | 1 |
|---|---|---|---|---|---|---|
| \(C\) | + | | | | | |

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

Here \( q \) is assumed to be sufficiently small \((q \sim \frac{\Delta}{a_0} \ll k_F, \frac{\Delta}{a_0})\). Due to energy-momentum conservation only a finite number of intermediate states contributes to the correlator (35). Moreover, at low energies contributions of intermediate states with large numbers of particles to the correlator (35) are generally small\(^48,49\). We therefore restrict our following analysis to one and two particle contributions. Many matrix elements in (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 \(S_a^a\) are summarized in Table II. Using these properties we furthermore conclude that at low energies the non-vanishing 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 \(k = \frac{x}{a_0}\);

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 \(n \leq 2\) in the spectral representation (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

\[
G^{AB}(\omega, q) = \frac{2\pi v}{a_0} \sum_{n=1}^{\infty} \sum_{\{\epsilon_n\}} \int d\theta_1 \ldots d\theta_n n!(2\pi)^n \left\{ \langle 0| A |\{\epsilon_n, \theta_n\}\rangle \langle \{\epsilon_n, \theta_n\}|B|0\rangle \frac{\delta(vq - P_n)}{\omega - E_n + i\eta} - \langle 0| B |\{\epsilon_n, \theta_n\}\rangle \langle \{\epsilon_n, \theta_n\}|A|0\rangle \frac{\delta(vq + P_n)}{\omega + E_n + i\eta} \right\}. \tag{36}
\]

Here \(\eta\) is a positive infinitesimal, \(|\{\epsilon_n, \theta_n\}\rangle\) are \(n\)-particle scattering states of solitons, antisolitons and breathers (26) with energies and momenta are given by (27) and

\[(22)\) respectively. The leading contribution to the spectral sum in (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 $G_{1p}^{AB}$

\[
G_{1p}^{AB}(\omega, q) = \frac{v}{a_0} \sum_a \int d\theta \left[ \langle 0|A|\theta_a \rangle \langle \theta_a |B|0 \rangle \frac{\delta(vq - \Delta_a \sinh \theta)}{\omega - \Delta_a \cosh \theta + i\eta} - \langle 0|B|\theta_a \rangle \langle \theta_a |A|0 \rangle \frac{\delta(vq + \Delta_a \sinh \theta)}{\omega + \Delta_a \cosh \theta + i\eta} \right]
\]

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

\[
\varepsilon_a(q) = \sqrt{\Delta_a^2 + v^2 q^2}, \quad (38)
\]

\[
\theta_0^a = \text{arcsinh} \left( \frac{vq}{\Delta_a} \right). \quad (39)
\]

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 $\theta = (\theta_1 + \theta_2)/2$. Resolving the momentum conservation delta function then gives

\[
G_{2p}^{AB}(\omega, q) = \frac{v}{a_0} \sum_{a_1, a_2} \int \frac{d\theta_1 d\theta_2}{2(2\pi)^2} \left[ \langle 0|A|\theta_1, \theta_2 \rangle \langle \theta_1, \theta_2 |B|0 \rangle \frac{\delta(vq - \sum_{j=1}^{2} \Delta_{aj} \sinh \theta_j)}{\omega - \sum_{j=1}^{2} \Delta_{aj} \cosh \theta_j + i\eta} \right.
\]

\[
- \langle 0|B|\theta_1, \theta_2 \rangle \langle \theta_1, \theta_2 |A|0 \rangle \frac{\delta(vq + \sum_{j=1}^{2} \Delta_{aj} \sinh \theta_j)}{\omega + \sum_{j=1}^{2} \Delta_{aj} \cosh \theta_j + i\eta}
\]

\[
= \frac{v}{a_0} \sum_a \int \frac{d\theta}{2\pi} \left[ \frac{\langle 0|A|\theta^b_0 - \theta_-, \theta_0^b - \theta_- \rangle_{ba} \langle \theta^b_0 + \theta_- \rangle_{ba} \langle \theta^b_0 + \theta_- |A|0 \rangle}{\varepsilon_{ab}(q, \theta_-) (\omega - \varepsilon_{ab}(q, \theta_-) + i\eta) \varepsilon_{ab}(q, \theta_-) (\omega + \varepsilon_{ab}(q, \theta_-) + i\eta)} \right], \quad (40)
\]

where

\[
\varepsilon_{ab}(q, \theta) = \left[ v^2 q^2 + \Delta_a^2 + \Delta_b^2 \right],
\]

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

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

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

Carrying out the $\theta_-$ integral using the delta functions we obtain

\[
s^2 = \omega^2 - v^2 q^2, \quad (42)
\]

\[
\theta_{ab}(s) = \text{arccosh} \left[ \frac{s^2 - \Delta_a^2 - \Delta_b^2}{2\Delta_a \Delta_b} \right]. \quad (43)
\]
\[-\frac{1}{\pi} \text{Im} \mathcal{G}_{2p}^{AB}(\omega > 0, q) = \frac{v}{2\pi a_0} \sum_{a,b} \sum_{\sigma = \pm} \langle 0 | \theta_{ba}^\sigma(\omega, q), \theta_{ab}^\sigma(\omega, q)_{ba, ab} \theta_{ba}^{-\sigma}(\omega, q), \theta_{ba}^{-\sigma}(\omega, q) | B(0) \rangle \theta_H (s - \Delta_a - \Delta_b), \]

where \( \theta_H(x) \) is the Heaviside function and

\[ \theta_{ab}^\sigma(\omega, q) = \text{arcsinh} \left[ \frac{1}{2s} \left( \sqrt{s^2 + (\Delta_a^2 - \Delta_b^2)} + \right. \right. \]
\[ \left. \left. \pm \omega \sqrt{\left(s^2 - (\Delta_a - \Delta_b)^2\right) \left(s^2 - (\Delta_a + \Delta_b)^2\right)} \right] \right], \]

\[ \theta_{ab}^\sigma(\omega, q) - \theta_{ba}^{-\sigma}(\omega, q) = \sigma \theta_{ab}(s). \]

The two terms in (44) arise from the two delta functions in (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 \( S^{\alpha \beta}(\omega, Q^a + q) \) (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 cut-off 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

\[ \gamma = \frac{\hbar}{\hbar} = 0.01191, \quad \delta = 0.3, \quad H = 0.2598J. \]

These correspond to a magnetization per site of \( \langle S^z \rangle = 0.06 \) (see Table I) and \( \xi = 0.174371 \). The spectrum consists of soliton and antisoliton with gap \( \Delta \approx 0.04897J \)

\[ S^{xx} (\omega > 0, -Q + q) \approx \frac{2vA^2 e^2 q^2}{\Delta^2} \delta (s^2 - \Delta^2) + \frac{vA^2}{4\pi a_0} \sum_{k=1}^{1/\xi} \left( a_{sbk} \right)^2 \frac{1}{\sqrt{s^2 - (\Delta - \Delta k)^2}} \left( s^2 - (\Delta + \Delta k)^2 \right) \times \]
\[ \times \sum_{\sigma = \pm} \left[ K_{sbk}^\sigma (\sigma \theta_{sbk}(s)) e^{\theta_{sbk}(\omega, q)} + K_{sbk}^{-\sigma} (\sigma \theta_{sbk}(s)) e^{-\theta_{sbk}(\omega, q)} \right]^2. \]

where \( s \) is the Mandelstam variable (42), the overall normalization is

\[ \hat{A} = A(H) \left( Z_1(\beta) \right)^{1/2}, \]

and five breathers with gaps

\[ \Delta_1 = 0.54098\Delta, \quad \Delta_2 = 1.04162\Delta, \quad \Delta_3 = 1.46461\Delta, \quad \Delta_4 = 1.77841\Delta, \quad \Delta_5 = 1.95962\Delta. \]

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

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

In the continuum limit \( S^{xx}(\omega, k) \) is non-vanishing in the vicinity of the points \( k = \pm Q \) and \( \pm \pi/\xi \). 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 \( k \approx -Q = -\frac{2\pi}{\xi} (S^z_j) \)

In the continuum limit \( S^{xx}(\omega, -Q + q) \) with \( q \ll Q \) is given by the two-point function of \( S^z_j \) with \( S^z_i \) (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 section IV to carry out the rapidity integrals we arrive at the following expression for \( S^{xx}(\omega, -Q + q) \) within the two-particle approximation

Here \( s \) is the Mandelstam variable (42), the overall normalization is

\[ \hat{A} = A(H) \left( Z_1(\beta) \right)^{1/2}, \]
tions \(K_{\pm \delta_{\phi}}(\theta)\) by equation (B22) for \(k\) even and (B23) for \(k\) odd, the normalization factor \(N_{\delta_{\phi}}^\beta\) by equation (B20) and the functions \(\theta_{\phi}(s)\) and \(\theta_{\phi}(\omega, q)\) are presented in equations (43) and (45), respectively.

We note that \(S^{xx}(\omega, -Q + \Delta/\nu)\) as a function of \(\omega\) for \(\delta = 0.3\) and \(H = 0.2598J\). The delta-function peak (pink) has been broadened to make it visible.

![Figure 1](image)

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

In Fig. 2 we plot the dynamical structure factor (51) as a function of frequency. We note that because \(S^x\)

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

where \(\nu = 2(\beta + \frac{1}{2})^2 > 1\). For large \(\omega\) 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 (48) has divergence for \(\omega \to \sqrt{(\Delta + \Delta_k)^2 + v^2 q^2}\) \((k = 1, 2, \ldots, [1/\xi])\), 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 \(S^{xx}(\omega, \pi/a_0 + q)\) with \(qa_0 \ll \pi\) is given by the two-point function of the charge neutral operator \(S^x_2\) (13). Using Table II and (30) we find that the following intermediate states with at most two particles contribute to the two-point function of \(S^x_2\)

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

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 section IV, we obtain the following expression in the two-particle approximation

\[
S^{xx}\left(\omega > 0, \frac{\pi}{a_0} + q\right) \approx \frac{vq^2}{\pi a_0} \left\{ 2\pi \sum_{k=1}^{[1/\xi]} \left| F_{b_k}^\beta \right|^2 \delta(s^2 - \Delta^2_{2k}) + \frac{|F_{s_k}^\beta(\theta_{s_k}(s))|^2 \partial H(s - 2\Delta)}{s\sqrt{s^2 - 4\Delta^2}} + \sum_{k,k' = 1}^{[1/\xi]} \delta_{k+k'} \left| F_{b_k b_{-k'}}^\beta(\theta_{b_k b_{-k'}}(s)) \right|^2 \partial H(s - \Delta_k - \Delta_{k'}) \right\}, \quad (51)
\]

Here the single-breather form factors \(F_{b_k}^\beta\) are given by equation (C14), the soliton-antisoliton form factor \(F_{s_k}^\beta(\theta)\) by (C10) and the breather-breather form factors \(F_{b_k b_{-k'}}^\beta(\theta)\) by (C24) respectively. The function \(\theta_{s}(s)\) is given by (43) and

\[
\delta_{k}^{\text{even}} = \begin{cases} 
1, & \text{if } k \text{ is even}, \\
0, & \text{otherwise}.
\end{cases} \quad (52)
\]

In Fig. 2 we plot the dynamical structure factor (51) as a function of frequency. We note that because \(S^x_2\) is a scalar operator \(S^{xx}(\omega, \pi/a_0 + q)\) depends only on the Mandelstam variable \(s\) (42) rather than on \(\omega\) and \(q\) separately. The first peak in \(S^{xx}(\omega, \pi/a_0 + q)\) is due to the \(b_2\) single-breather excitation (blue line). At \(\omega = \Delta_1\) there is a second single-breather contribution, due to \(b_1\). Above \(\omega = 2\Delta_1\) a strong \(b_1 b_1\) two-breather continuum occurs (pink line). Around \(\omega = 2\Delta\) contributions from soliton-antisoliton and \(b_1 b_3\) and \(b_2 b_2\) two-breather continua are visible. We note that the thresholds of \(b_1 b_3, s s\) and \(b_2 b_2\) continua all occur around \(2\Delta\) is a peculiarity of the pa-
vanishing in the vicinity of the points $k = \pm Q$ and $\frac{\pi}{a_0}$. We will consider both cases in turn.

I. Momenta $k \approx -Q = -\frac{2\pi}{a_0} (S^y_j)$

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

1. Single-soliton states.

2. Two-particle states containing one soliton and one breather.

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

$S^{yy}(\omega > 0, -Q + q) \approx \frac{2vA^2 \nu^2 \eta^2 + \Delta^2}{\Delta^2} \delta(s^2 - \Delta^2) + \frac{2vA^2}{4\pi a_0} \sum_{k=1}^{[1/\xi]} \left( \frac{\nu^{2} s_{\text{min}}^2}{\Delta^2} \right)^{1/2} \vartheta_{H}(s - \Delta - \Delta_{k}) \times \sum_{\sigma = \pm} \left[ K^\sigma_{sbk}(\sigma \theta_{sbk}(s)) e^{\theta_{sbk}(\omega,q)} - K^\sigma_{sbk}(-\sigma \theta_{sbk}(s)) e^{-\theta_{sbk}(\omega,q)} \right]^{2}.$

(53)

Here the overall normalization $\tilde{A}$ is given by equation (49), the minimal form factor $F_{sbk}^{\text{min}}(\theta)$ by (B6), the pole function $K^\sigma_{sbk}(\theta)$ by (B22) for $k$ even and (B23) for $k$ odd, the functions $\theta_{sbk}(s)$ and $\theta_{sbk}(\omega,q)$ by (43) and (45), respectively.

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

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

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

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

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

We plot $S^{yy}(\omega, -Q + \Delta/v)$ as a function of $\omega$ in Figure 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 at energy at $\Delta \sqrt{2}$. At higher energies breather-soliton continua appear. Their contributions grow with increasing $\omega$ because $S^y_j$ is an irrelevant operator.

Next we turn to the $yy$-component of the dynamical structure factor. In the continuum limit $S^{yy}(\omega, k)$ is non-

\[ S^{yy}(\omega > 0, -Q + q) \approx \frac{2vA^2 \nu^2 \eta^2 + \Delta^2}{\Delta^2} \delta(s^2 - \Delta^2) + \frac{2vA^2}{4\pi a_0} \sum_{k=1}^{[1/\xi]} \left( \frac{\nu^{2} s_{\text{min}}^2}{\Delta^2} \right)^{1/2} \vartheta_{H}(s - \Delta - \Delta_{k}) \times \sum_{\sigma = \pm} \left[ K^\sigma_{sbk}(\sigma \theta_{sbk}(s)) e^{\theta_{sbk}(\omega,q)} - K^\sigma_{sbk}(-\sigma \theta_{sbk}(s)) e^{-\theta_{sbk}(\omega,q)} \right]^{2}. \]

(53)
Using the results of section IV, we obtain the following expression in the two-particle approximation

\[
S_{yy}^{zz} (\omega > 0, \frac{\pi}{a_0} + q) \approx \frac{ve^2(H)}{\pi a_0} \left\{ 2\pi \sum_{k=1}^{[1/\xi]} \delta_{k}^{\text{odd}} |F_{b_{b_{k}}}^{b_{b_{k}}}|^2 \delta(s^2 - \Delta_k^2) + \frac{|F_{ss}^{\sin(\beta\Theta)}(\theta_{ss}(s))|^2 \partial_H(s - 2\Delta)}{s\sqrt{s^2 - 4\Delta^2}} + \right. \\
\left. + \sum_{k,k'=1}^{[1/\xi]} \delta_{k+k'}^{\text{odd}} |F_{b_{b_{k}}}^{b_{b_{k'}}}(\theta_{b_{b_{k}}}b_{b_{k'}}(s))|^2 \frac{\partial_H(s - \Delta_k - \Delta_{k'})}{\sqrt{(s^2 - (\Delta_k - \Delta_{k'})^2)(s^2 - (\Delta_k + \Delta_{k'})^2)}} \right\}.
\]

Here the single-breather form factors \(F_{b_{k}}^{b_{k}}\) are given by (C14), the soliton-antisoliton form factor \(F_{ss}^{\sin(\beta\Theta)}(\theta)\) by (C11), the two-breather form factors \(F_{b_{b_{k}}}^{b_{b_{k}}}\) by (C24), the function \(\theta_{ss}(s)\) by (43) and

\[
\delta_k^{\text{odd}} = \begin{cases} 
1, & \text{if } k \text{ is odd}, \\
0, & \text{otherwise}.
\end{cases}
\]

![FIG. 4: One and two-particle contributions to \(S_{yy}^{zz}(\omega, \frac{\pi}{a_0})\) as a function of \(\omega\) for \(A = 0.3\) and \(H = 0.2598 J\). Delta-function peaks (blue) have been broadened to make them visible. Insert: the soliton-antisoliton and breather-breather two-particle contributions.](image)

We plot \(S_{yy}^{zz}(\omega, \frac{\pi}{a_0})\) as a function of \(\omega\) 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 \(b_1b_2, ss\) and \(b_1b_4\) 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 non-vanishing 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 \(qa_0 < \pi\) is given by the two-point function of the charge neutral operator \(S_z^z(17)\). Using Table II and (30) we find that the following intermediate states with at most two particles contribute to the two-point function of \(S_z^z\):

1. Single breather states odd under charge conjugation, i.e. \(B_{2n+1}^z(\theta)|0\).
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 section IV, we obtain the following expression in the two-particle approximation

\[
S_{zz}(\omega > 0, q) \approx \frac{2a_0\bar{q}\omega^2}{v} \sum_{k=1}^{[1/\xi]} \delta_{k}^{\text{odd}} |F_{b_{b_{k}}}^{b_{b_{k}}}|^2 \delta(s^2 - \Delta_k^2) + \frac{a_0\bar{q}\omega^2}{v} |F_{ss}^{\sin(\beta\Theta)}(\theta_{ss}(s))|^2 \frac{\partial_H(s - 2\Delta)}{s\sqrt{s^2 - 4\Delta^2}} + \\
\left. + \sum_{k,k'=1}^{[1/\xi]} \delta_{k+k'}^{\text{odd}} |F_{b_{b_{k}}}^{b_{b_{k'}}}(\theta_{b_{b_{k}}}b_{b_{k'}}(s))|^2 \frac{\partial_H(s - \Delta_k - \Delta_{k'})}{\sqrt{(s^2 - (\Delta_k - \Delta_{k'})^2)(s^2 - (\Delta_k + \Delta_{k'})^2)}} \right).
\]
The dynamical structure factor \( S^{zz}(\omega, q) \) is given by equation (56), which is shown in Figure 5. Note that since \( \mathcal{S}_1 \) is a scalar operator, \( S^{zz}(\omega, q) \) depends on the Mandelstam variable \( s \) (42) rather than on \( \omega \) and \( q \) separately. In order to broaden the delta function contributions we introduce a small imaginary part in \( \omega \). The dominant peak in \( S^{zz}(\omega, q) \) is due to a \( b_1 \) breather contribution. The contributions due to \( b_2 \) and \( b_3 \) breather states are much smaller. The soliton-antisoliton and breather-breather contributions to \( S^{zz}(\omega, q) \) are barely visible in the figure.

**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. 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 dynamical response and determined for the first time all mediate states with at most two particles contribute to the two-point function of

\[
S^{zz}(\omega > 0, -2k_F + q) \approx \frac{v^2}{\alpha_0} \delta(s^2 - \Delta^2) + \frac{v^2}{2\pi\alpha_0} \sum_{k=1}^{1/2} \left( N_{abk}^0 \right)^2 \left( K_{abk}^0(\theta_{abk}(s)) \right)^2 \frac{\left| F_{abk}^{\min}(\theta_{abk}(s)) \right|^2 \varphi_H(s - \Delta - \Delta_k)}{\sqrt{(s^2 - (\Delta - \Delta_k)^2)(s^2 - (\Delta + \Delta_k)^2)}}. \tag{58}
\]

Here the minimal form factor \( F_{abk}^{\min}(\theta) \) is given by (B6), the pole function \( K_{abk}^0(\theta) \) by (B22) for \( k \) even and (B23) for \( k \) odd, the function \( \theta_{abk}(s) \) by (43), the overall normalization is

\[
\tilde{a} = a(H) \sqrt{\frac{Z(0)}{2}}. \tag{59}
\]

The dynamical structure factor (58) is shown in Figure 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.
VII. ACKNOWLEDGMENT

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APPENDIX A: SPIN VELOCITY, FERMI MOMENTUM AND COMPACTIFICATION RADIUS

In this appendix we summarize how to determine the parameters of the Gaussian model (3), (4) that describes the continuum limit of the Heisenberg XXZ chain in a magnetic field from the Bethe ansatz solution. 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 \( Z(\lambda) \)

\[
\begin{align*}
\varepsilon(\lambda) &= -\frac{2\pi}{a_0} \int_{-\Lambda}^{\Lambda} \frac{d\mu}{2\pi} K(\lambda - \mu) \varepsilon(\mu) = \frac{J \sin^2 \gamma}{\cosh 2\lambda - \cos \gamma}, \\
p(\lambda) &= 2\pi a_0 \int_{0}^{\Lambda} \frac{d\mu}{2\pi} \rho(\mu), \\
\rho(\lambda) &= \frac{2}{\pi} \int_{-\Lambda}^{\Lambda} \frac{d\mu}{2\pi} K(\lambda - \mu) \rho(\mu) = \frac{2 \sin \gamma}{\pi(\cosh 2\lambda - \cos \gamma)}, \\
Z(\lambda) &= \frac{2}{\pi} \int_{-\Lambda}^{\Lambda} \frac{d\mu}{2\pi} K(\lambda - \mu) Z(\mu) = 1.
\end{align*}
\]

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

\[
K(\lambda) = -2 \sin 2\gamma / (\cosh 2\lambda - \cos 2\gamma).
\]

The integration boundary \( \Lambda \) is fixed by the condition

\[
\varepsilon(\pm \Lambda) = 0.
\]

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

\[
\langle S^z \rangle = \frac{1}{2} - \frac{1}{2} \int_{-\Lambda}^{\Lambda} d\lambda \rho(\lambda).
\]

The Fermi momentum is equal to

\[
k_F = p(\Lambda) = \frac{2\pi}{a_0} \int_{0}^{\Lambda} d\lambda \rho(\lambda) = \frac{\pi}{a_0} \left[ 1 - \langle S^z \rangle \right] = \frac{1}{2} \int_{-\Lambda}^{\Lambda} d\lambda \rho(\lambda).
\]

Finally, the dressed charge is related to \( \beta \) by

\[
\beta = \frac{1}{\sqrt{8\pi Z(\Lambda)}}.
\]

In order to determine \( v \) and \( \beta \) we solve (A1) numerically, which is easily done to very high precision as the equations are linear. The results are shown in Fig. 7, 8 and 9.

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

The exponential field \( O^{-1}_a \) (19) has topological charge +1. Hence it has non-vanishing matrix elements between
the ground state $|0\rangle$ and one soliton states, two-particle soliton-breather $s_{b_n}$ 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\(^{56}\)

$$F^{1a}_s(\theta) = \sqrt{Z_1(a)} e^{\frac{i\theta}{\hbar c}} e^{\frac{a^2}{\hbar^2}},$$  \hspace{1cm} (B1)

where

$$\sqrt{Z_1(a)} = \left(\frac{C_2}{2C_1^2}\right)^{1/4} \left(\frac{\xi C_2}{16}\right)^{-1/8} \left[\sqrt{\pi} A \frac{\Gamma((3 + \xi)/2)}{v \Gamma(\xi/2)}\right]^{2a^2+1/8/\beta^2} \times \exp\left\{\int_0^\infty \frac{dt}{t} \left(\frac{\cosh(4c\xi at/\beta) e^{-(1+\xi)t} - 1}{4\sinh(\xi t) \sinh(\xi (t+1)) \cosh(t)} + \frac{1}{4\sinh(\xi t)} - \left(2a^2 + \frac{1}{8\beta^2}\right) e^{-2t}\right)\right\}. \hspace{1cm} (B2)$$

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

The soliton-breather S-matrix is given by\(^{57}\)
\[ S_{sb_n}(\theta) = (-1)^n \exp \left\{ 2 \int_0^\infty \frac{dt}{t} \frac{\cosh(\xi t) \sinh(n \xi t)}{\cosh(t) \sinh(\xi t)} \sinh \left( \frac{2\theta t}{i\pi} \right) \right\} = \prod_{j=1}^n \frac{\sinh \left( \theta + i \frac{\pi (n+1-2j)}{2} \right) + i \cos \left( \frac{\pi j}{2} \right)}{\sinh \left( \theta - i \frac{\pi (n+1-2j)}{2} \right) - i \cos \left( \frac{\pi j}{2} \right)} . \]  

\]

The corresponding soliton-breather 3-particle coupling is

\[ g_{sb_n}^b = \left( \frac{n \pi \xi}{2} \right) \prod_{i=1}^{n-1} \cot \left( \frac{\pi \xi}{2} \right) \right]^{1/2} . \quad \text{(B4)} \]

Note that by crossing symmetry we must have

\[ g_{sb_n}^b = g_{ss}^s . \quad \text{(B5)} \]

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

\[ S(\theta) = \exp \left\{ \int_0^\infty dt f(t) \sinh \left( \frac{t \theta}{i\pi} \right) \right\} . \]

\[ \Rightarrow F_{\text{min}}(\theta) = \exp \left\{ \int_0^\infty dt f(t) \left( 1 - \cosh[t(1 + \frac{\theta}{\pi})] \right) \right\} . \]

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

\[ F_{\text{min}}^{\text{sb}}(\theta) = R_{\text{sb}_n}(\theta) \exp \left\{ \int_0^\infty dt \frac{\cosh(\xi t) \sinh(n \xi t)}{t} \times \prod_{i=1}^{n-1} \cot \left( \frac{\pi \xi}{2} \right) \right\} , \quad \text{(B6)} \]

where \( R_{\text{sb}_n}(\theta) \) is given by

\[ R_{\text{sb}_n}(\theta) = 1 , \quad R_{\text{sb}_{n+1}}(\theta) = i \sinh(\theta/2) . \quad \text{(B7)} \]

### 3. Soliton-breather form factors

We will calculate the full form factor using the residue condition:\textsuperscript{56,58}

\[ ig_{sb}^{b_n} F_{ss}^{1a}(\theta_s, \theta_b) = \text{Res}_{\delta = 0} F_{ss}^{1a}(\theta_s, \theta_b - \frac{i \delta \xi_{bs}}{2}, \theta_b + \delta + \frac{i \delta \xi_{bs}}{2}) , \quad \text{(B8)} \]

where \( \xi_{bs} = \pi(1 - n \xi) \), and

\[ g_{ss}^b = (-1)^n g_{ss}^s = \left| 2 \cot \left( \frac{n \pi \xi}{2} \right) \prod_{i=1}^{n-1} \cot \left( \frac{l \pi \xi}{2} \right) \right|^{1/2} . \quad \text{(B9)} \]

The three particle form factor involving two solitons and one antisoliton is:\textsuperscript{56}

\[ F_{ss}^{1a}(\theta_1, \theta_2, \theta_3) = \frac{i C_2 \sqrt{Z_2(\alpha)}}{4C_1} e^{\frac{i \pi \xi}{2} + \frac{i \pi \xi}{2} + \frac{i \pi \xi}{2} + \frac{i \pi \xi}{2}} G(\theta_{12})G(\theta_{13})G(\theta_{23}) \]

\[ \times \left[ \frac{-e^{-2 \pi \xi \theta_3}}{2\pi} \int_{C_+} \frac{d\theta_0}{2\pi} e^{-(\frac{\pi \xi}{2} + \frac{i \pi \xi}{2}) \theta_0} W(\theta_{10})W(\theta_{20})W(\theta_{30}) - e^{\frac{2 \pi \xi \theta_3}{2}} \int_{C_-} \frac{d\theta_0}{2\pi} e^{-\left(\frac{\pi \xi}{2} + \frac{i \pi \xi}{2}\right) \theta_0} W(\theta_{10})W(\theta_{20})W(\theta_{30}) \right] . \quad \text{(B10)} \]

where \( \theta_{jk} = \theta_j - \theta_k \),

\[ G(\theta) = i C_1 \sinh \left( \frac{\theta}{2} \right) \exp \left\{ - \int_0^\infty dt \frac{\sinh((1 - \xi) t) \sinh^2(t(1 - \frac{\theta}{\pi}))}{\sinh(2t) \cosh(t) \sinh(\xi t)} \right\} . \]

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

\[ C_1 = \exp \left[ - \int_0^\infty \frac{dt \sinh^2(t/2) \sinh(t(\xi - 1))}{t \sinh(2t) \sinh(t \xi) \cosh(t)} \right] , \quad \text{(B13)} \]

\[ C_2 = \exp \left[ 4 \int_0^\infty \frac{dt \sinh^2(t/2) \sinh(t(\xi - 1))}{t \sinh(2t) \sinh(t \xi)} \right] . \quad \text{(B14)} \]

The integration contours \( C_+ \) and \( C_- \) are constructed as follows. The contour \( C_+ \) runs from \(-\infty\) to \(\infty\) in the
complex $\theta_0$ 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 figure 10).

Let us consider the form factor (B10) for rapidities $\theta_1 = \theta_s$, $\theta_2 = \theta_b - \frac{i\pi \nu}{2}$, $\theta_3 = \theta_b + \delta + \frac{i\pi \nu}{2}$, $0 \leq k < \frac{1}{2}$. The function $W(\theta)$ has poles in the strip $\text{Im} \theta < -\pi$ of the complex $\theta$-plane at the points $\theta = i\nu_k$, where

$$v_k = \frac{\pi(k - \frac{1}{2})}{2}, \quad 0 < k < \frac{1}{2}.$$ 

As a result the function $W(\theta_0)W(\theta_2)W(\theta_3)$ has poles at $\theta_0 = \theta_s - \frac{i\pi \nu}{2}$, $\theta_0 = \theta_b + \frac{i\pi \nu}{2}(n - 2k)$, and $\theta_0 = \theta_s + \frac{i\pi \nu}{2}(n - 2k)$, $0 \leq k \leq \frac{n}{2} - \frac{1}{2}$. By construction the contour $C_-$ runs between $n + 1$ pairs of poles at $\theta_0 = \theta_s + \frac{i\pi \nu}{2}(n - 2k)$, and $\theta_0 = \theta_s + \frac{i\pi \nu}{2}(n - 2k)$, $0 \leq k \leq \frac{n}{2} + \frac{1}{2}$, with only an infinitesimal separation $\delta$ between them (see Fig. 11). As a result the integral over $\theta_0$ exhibits a simple pole for $\delta \to 0$. 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 $\delta \to 0$. The contours $C$ and $C_-$ are shown for $n = 1$ in Fig. 11.

For general $n$ we then find that

$$\int_{C_-} \frac{d\theta_0}{2\pi} e^{-i(2\pi + \frac{i\pi}{2})\theta_0} W(\theta_1)W(\theta_2)W(\theta_3) = \sum_{k=0}^{n} i e^{-i(2\pi + \frac{i\pi}{2})\theta_0 + i\pi \nu(n - 2k)} W(\theta_1 - \frac{i\pi \nu(n - 2k)}{2}) \times W_{\text{res}}(i\nu_k)W(-\delta + i\nu_{n-k}) + \text{regular part,} \tag{B15}$$

where $W_{\text{res}}(i\nu_k)$ denotes the residue of the function $W(\theta)$ taken at the point $\theta = i\nu_k$. We note that $W(-\delta + i\nu_{n-k})$ 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 equation (B8) and in the following will be ignored. Similarly, the integral over $C_+$ has a finite limit $\delta \to 0$.

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

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

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

$$W_{\text{res}}(i\nu_k) = \frac{2(-1)^{k-1}}{\sqrt{C_2}} \prod_{j=1}^{k-1} \cot \left( \frac{j\pi \xi}{2} \right), \quad k \geq 1, \tag{B17}$$

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

$$i\nu_s e_{s1}^{\alpha} F_s(\theta_s, \theta_0) = - \frac{i C_2 \sqrt{Z_1(\alpha)}}{4C_1} e^{i\pi \nu_s/2 + 2\alpha} G(i\nu_s^{\alpha}) \times G(\theta_s + i\nu_s^{\alpha}) G(\theta_s - i\nu_s^{\alpha}) \times \sum_{k=0}^{n} (-1)^{n-k} e^{-i\pi \nu(n - 2k)} W_{\text{res}}(i\nu_k)W_{\text{res}}(i\nu_{n-k}) \times W(\theta_s - \frac{i\pi \nu(n - 2k)}{2}). \tag{B18}$$

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

$$F_{s1}^{\alpha} F_{s1}^{\alpha} = N_{s2}^{\alpha} \sqrt{Z_1(\alpha)} e^{i\pi \nu_s/2 + 2\alpha} K_{s2}^{\alpha}(\theta_s) \times \times F_{s2}^{\alpha}(\theta_s). \tag{B19}$$

Here $N_{s2}^{\alpha}$ is a normalization constant given by

$$N_{s2}^{\alpha} = \frac{e^{i\pi \nu_s/2}}{i g_{s2}^{\alpha} \text{Res}_{\theta = i\nu_s^{\alpha}} [K_{s2}^{\alpha}(\theta)] F_{s2}^{\alpha}(i\nu_s^{\alpha})}, \tag{B20}$$
where
\[ u_s^{sb} = \frac{\pi}{2} (k \xi + 1). \] (B21)

\[ K_{s_{2m}}^a(\theta) = \frac{1}{\cosh \theta} \prod_{l=1}^{m-1} \frac{1}{\cosh \left( \frac{\theta}{2} + i u_s^{sb_l} \right) \cosh \left( \frac{\theta}{2} - i u_s^{sb_l} \right)} \]
\[ \times \left\{ W_{\text{res}}(iv_m) - \sum_{k=1}^{m} W_{\text{res}}(iv_{m-k}) W_{\text{res}}(iv_{m+k}) \right\} e^{-\frac{\pi i k \xi a}{\theta}} \Psi_{2k}(\theta) + e^{\frac{\pi i k \xi a}{\theta}} \Psi_{2k+1}(\theta), \] (B22)

\[ K_{s_{2m+1}}^a(\theta) = \frac{1}{\sinh \left( \frac{\theta}{2} \right)} \prod_{l=0}^{m-1} \frac{1}{\cosh \left( \frac{\theta}{2} + i u_s^{sb_{l+1}} \right) \cosh \left( \frac{\theta}{2} - i u_s^{sb_{l+1}} \right)} \]
\[ \times \sum_{k=0}^{m} W_{\text{res}}(iv_{m-k}) W_{\text{res}}(iv_{m+k+1}) \left\{ e^{-\frac{\pi i k \xi a}{\theta}} \Psi_{2k+1}(\theta) + e^{\frac{\pi i k \xi a}{\theta}} \Psi_{2k+1}(\theta) \right\}, \] (B23)

where
\[ \Psi_{2k}(\theta) = \frac{\sin \left( \frac{\theta}{2} - \frac{\pi}{2} \right)}{\sin \left( \frac{\theta}{2} + \frac{\pi}{2} \right)} \prod_{j=1}^{k-1} \cosh \left( \frac{i \theta}{2} + u_s^{sb_{2j}} \right), \] (B24)

\[ \Psi_{2k+1}(\theta) = \frac{1}{\sin \left( \frac{\theta}{2} + \frac{\pi}{2} \right)} \prod_{j=0}^{k-1} \cosh \left( \frac{i \theta}{2} + u_s^{sb_{2j+1}} \right). \] (B25)

\section*{APPENDIX C: FORM FACTORS OF \( e^{ia\Theta} \)}

The operator \( e^{ia\Theta} \) carries zero topological charge. Hence the non-vanishing 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.

\subsection*{1. S-matrices and minimal form factors}

The breather-breather S-matrix is\(^5\)
\[ S_{bb}(\theta) = \exp \left\{ \int_{0}^{\infty} \frac{dt}{t} \sinh \left( \frac{2\theta t}{\pi} \right) \cosh(\theta t) \sinh(\xi t) \right\} \times \cosh(\xi t) \sinh(k \xi t) \cosh((1-l \xi t)), \] \( k < l, \) (C1)

\[ S_{bb}(\theta) = -\exp \left\{ \int_{0}^{\infty} \frac{dt}{t} \sinh \left( \frac{2\theta t}{\pi} \right) \cosh(\theta t) \sinh(\xi t) \right\} \times \left[ \cosh(\xi t) \sinh((2k \xi - 1) t) + \sinh((1 - \xi t)) \right]. \] (C2)

The corresponding three-particle coupling is
\[ g_{bb}(l \xi, k \xi, 1 \xi) = \left[ 2 \cot \left( \frac{k \pi \xi}{2} \right) \tan \left( \frac{l \pi \xi}{2} \right) \tan \left( \frac{(l + j) \pi \xi}{2} \right) \right]^{\frac{1}{2}} \times \prod_{j=1}^{k-1} \cot \left( \frac{j \pi \xi}{2} \right) \tan \left( \frac{(l + j) \pi \xi}{2} \right). \] (C6)
The minimal form factor for two different breathers is then

\[
F_{b_i b_k}^{\text{min}}(\theta) = \exp\left\{ -2 \int_0^\infty \frac{dt}{t} \frac{\cosh(\xi t) \cosh((1-l\xi)t)}{\cosh(t)} \right. \\
\left. \times \frac{\sinh(k\xi t)}{\sinh(\xi t)} \frac{\cosh(2t(1-\frac{m}{2})) - 1}{\sinh(2t)} \right\},
\]

(C7)

The minimal form factor \( F_{b_i b_k}^{\text{min}}(\theta) \) involving two breathers of the same type is given by

\[
F_{b_i b_k}^{\text{min}}(\theta) = i \sinh\left( \frac{\theta}{2} \right)\exp\left\{ -2 \int_0^\infty \frac{dt}{t} \frac{\sinh^2(t(1-\frac{m}{2}))}{\sinh(2t)} \right. \\
\left. \times \cosh(\xi t) \sinh((2k\xi - 1)t) + \sinh((1-\xi)t) \right\},
\]

(C8)

2. Soliton-antisoliton and one-breather form factors

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

\[
\Theta = -i \lim_{a \to 0} \partial_a e^{ia\theta},
\]

are\(^{59}\)

\[
F_{ss}^{\cos(\beta \Theta)}(\theta) = \frac{G_\beta G(\theta)}{C_1} \cot\left( \frac{\pi \xi}{2} \right) \frac{8 \cosh(\frac{\theta}{2})}{\xi \sinh(\frac{\theta - \pi n}{2})} \times \cosh\left( \frac{\theta - i\pi}{2\xi} \right),
\]

(C10)

\[
F_{ss}^{\sin(\beta \Theta)}(\theta) = -\frac{G_\beta G(\theta)}{C_1} \cot\left( \frac{\pi \xi}{2} \right) \frac{8 \cosh(\frac{\theta}{2})}{\xi \sinh(\frac{\theta - \pi n}{2})} \times \sinh\left( \frac{\theta - i\pi}{2\xi} \right),
\]

(C11)

\[
F_{ss}^{\Theta}(\theta) = -\frac{G(\theta)}{C_1} \beta \cosh(\frac{\theta - \pi n}{2}) \cosh(\frac{\theta}{2}),
\]

(C12)

where \( G(\theta) \) and \( C_1 \) are given by eqs. (B11) and (B13), respectively, and

\[
G_a = \langle e^{ia\theta} \rangle = \left[ \frac{a_0 \Delta \sqrt{\Gamma(\frac{1}{2})}}{\Gamma(\frac{3}{2})} \right]^{2a^2} \exp\left\{ \int_0^\infty \frac{dt}{t} \left[ -2a^2 e^{-2t} + \frac{\sinh^2(2a\beta t)}{2 \sinh(t(2\beta^2)) \cosh(t(1-\beta^2))} \right] \right\},
\]

(C13)

The single-particle form factors \( F_{b_n}^\alpha \) and \( F_{b_n}^\Theta \) for the operators \( e^{i\alpha \Theta} \) and \( \Theta \), respectively, can be obtained from the residue condition for the soliton-antisoliton form factor \( F_{ss}^{\Theta}(\theta) \) and \( F_{ss}^{\Theta}(\theta) \)

\[
g_{ss}^{b_n} F_{a s}(\theta) = \text{Res}_{\theta = -i\nu_{n}^s} F_{ss}^{\alpha}(\theta), \quad \nu_{b_n}^{\alpha} = \pi(1 - n\xi),
\]

The single-particle form factors \( F_{b_n}^\beta \) and \( F_{b_n}^\Theta \) can be calculated using the formulas

\[
F_{b_n}^\beta = \frac{2 \cot\left( \frac{\pi \xi}{2} \right) \sin(n\pi\xi)(-1)^n}{\left[ 2 \cot\left( \frac{n\xi}{2} \right) \prod_{m=1}^{n-1} \cot^2\left( \frac{m\xi}{2} \right) \right]} G_\beta \exp\left[ \int_0^\infty \frac{dt}{t} \frac{\sinh(t(\xi - 1)) \sinh^2(tn\xi)}{\sinh(2t) \cosh(t) \sinh(t(\xi))} \right],
\]

(C14)

\[
F_{b_{2m-1}}^\Theta = i(-1)^{m-1} \frac{G(\pi(2m-1)\xi - 1)}{g_{ss}^{b_{2m-1}} C_1} \frac{\pi \xi}{\beta \sin\left( \frac{(2m-1)\pi \xi}{2} \right)}.
\]

(C15)

3. Breather-breather form factors of \( e^{ia\Theta} \)

To calculate two breather form factor \( F_{b_i b_k}^{\alpha}(\theta_{12}) \), we will start with the formulas for \( n \)-breather \( (n = k + l) \) form factor \( F_{b_i}^\alpha(\gamma) \) from Ref.\(^{60}\)

\[
F_{b_i}^\alpha(\gamma) = \frac{G_a}{2^m/2} \frac{K_n^a(\gamma)}{\prod_{1 \leq i < j \leq n} R(\gamma_{ij})},
\]

(C16)
\[ R(\gamma) = \frac{N F_{b_1b_2}^{\text{min}}(\gamma)}{\sinh \left( \frac{1}{2} (\gamma - i\pi \xi) \right) \sinh \left( \frac{1}{2} (\gamma + i\pi \xi) \right)} \]  
(C17)

\[ K_n^a(\gamma) = \frac{1}{\pi} \sum_{l_0}^{1} \sum_{l_n=0}^{1} (-1)^{l_1+\ldots+l_n} \gamma_n^a(l) \times \prod_{1 \leq i < j \leq n} \left[ 1 + (l_i - l_j) \frac{i \sin(\pi \xi)}{\sinh(\gamma_{ij})} \right] \]  
(C18)

\[ f_n^a(l) = \frac{2}{\pi^2} \sum_{\ell=1}^{\infty} \prod_{i=1}^{\ell} e^{\frac{i \pi \xi}{2} (-1)^i} \]  
(C19)

where \( \gamma = (\gamma_1, \ldots, \gamma_n), l = (l_1, \ldots, l_n), \gamma_{ij} = \gamma_i - \gamma_j, \)\n
\[ N' = -\exp \left\{ 2 \int_0^\infty dt \frac{\sinh(\xi t)}{\cosh(t) \sinh(2t)} \right\}. \]

The normalization factor \( G_n/2^n/2 \) is introduced in Ref. 50. Form factor \( F_{b_1b_2}(\theta_1, \theta_2) \) can be calculated as follows.

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

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

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

Finally, taking \( \gamma_{k+1} = \theta_2 \), we can write

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

\( m = 1, 2, \ldots, l \), and \( \delta_j \) are infinitesimal parameters.

Similar calculations performed with the variables \( \gamma_j \), \( j = 1, 2, \ldots, k \), give

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

\( \epsilon_j \) are infinitesimal parameters.

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

\[ |\delta_1| \ll |\delta_2| \ll \cdots \ll |\delta_{k-1}| \ll |\theta_1|, \]  
(C22)

The \( n \)-particle \( (n = k + l) \) form factor \( (C16) \) depends on \( \gamma_i - \gamma_j, 1 \leq i < j < n \). Taking into account equations \( (C21), (C20), \) and \( (C22) \), we can write

\[ \gamma_{ij} = \begin{cases} -\epsilon_{k-j} - i (j - i) \pi \xi, & \text{if } (i, j) \in A_1, \\ -\delta_{k-j} - i (j - i) \pi \xi, & \text{if } (i, j) \in A_2, \\ \theta_{l-1} - i \left( \frac{l-1}{2} + j - m \right), & \text{if } (i, j) \in A_3, \end{cases} \]  
(C23)

where the manifolds \( A_{1,2,3} \) are constructed as following,

\( A_1 : 1 \leq i < j \leq k \),

\( A_2 : k + 1 \leq i < j \leq n \),

\( A_3 : 1 \leq i \leq k, k + 1 \leq j \leq n \).

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

\[ F_{b_1b_2}^m(\theta_12) = N_{b_1b_2}^a K_{b_1b_2}^a(\theta_12) F_{b_1b_2}^{\text{min}}(\theta_12). \]  
(C24)

where the minimal form factor \( F_{b_1b_2}^{\text{min}}(\theta_12) \) is given by equation \( (C7) \) for \( k < l \), and equation \( (C8) \) for \( k = l \),

\[ K_{b_1b_2}^a(\theta) = K_n^a(\gamma) \times \prod_{\nu=k-l+1}^{k+l} \frac{1}{\sinh \left( \frac{1}{2} (\theta - i \pi \nu) \right) \sinh \left( \frac{1}{2} (\theta + i \pi \nu) \right)}. \]  
(C25)

The normalization constant \( N_{b_1b_2}^a \) can be calculated as

\[ N_{b_1b_2}^a = \frac{i \theta_{k+l} F_{b_1b_2}^a}{K_{b_1b_2}^{\text{res}} F_{b_1b_2}^{\text{min}}(-\frac{i \pi \xi}{2}(k + l))}, \]

\[ K_{b_1b_2}^{\text{res}} = \text{Res}_{\delta=0}[K_{b_1b_2}^a(-\delta - \frac{i \pi \xi}{2}(k + l))], \]

the one-particle form factor \( F_{b_1} \) is given by equation \( (C14) \).

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

\[ [a] = \frac{\sin(\frac{\pi \tilde{a}}{2})}{\sin(\pi \tilde{a})}. \]

4. Breather-breather form factors of Θ

Equation (C9) allows us to express the operator Θ in terms of exponential operator \( e^{ia\tilde{a}} \). Therefore the form factors \( F_{b,b}^{\tilde{a}}(\theta) \) are expressed in terms of the form factors of the exponential fields. Taking into account that the pole function \( K_{b,b}^{\tilde{a}}(\theta) \) (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 \( F_{b,b}^{\tilde{a}}(\theta) \) with \( k + l \)

being odd are nontrivial. These form factors are written as

\[ F_{b,b}^{\tilde{a}}(\theta) = N_{b,b}^{\tilde{a}} K_{b,b}^{\tilde{a}}(\theta) F_{b,b}^{\min}(\theta), \]

where the pole function \( K_{b,b}^{\tilde{a}}(\theta) \) is given by,

\[ K_{b,b}^{\tilde{a}}(\theta) = -i \lim_{\tilde{a} \to 0} \partial_{\tilde{a}} K_{b,b}^{\tilde{a}}(\theta), \]

the normalization factor \( N_{b,b}^{\tilde{a}} \) is determined as

\[ N_{b,b}^{\tilde{a}} = \lim_{\tilde{a} \to 0} N_{b,b}^{\tilde{a}}, \]

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

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