

Many-body theory of magnetoelasticity in one dimension

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We construct a many-body theory of magnetoelasticity in one dimension and show that the dynamical correlation functions of the quantum magnet, connecting the spins with phonons, involve all energy scales. Accounting for all magnetic states nonperturbatively via the exact diagonalization techniques of Bethe ansatz, we find that the renormalization of the phonon velocity is a nonmonotonous function of the external magnetic field and identify a new mechanism for attenuation of phonons—via hybridization with the continuum of excitations at high energy. We conduct ultrasonic measurements on a high-quality single crystal of the frustrated spin-1/2 Heisenberg antiferromagnet Cs_2CuCl_4 in its nearly one-dimensional regime and confirm the theoretical predictions, demonstrating that ultrasound can be used as a powerful probe of strong correlations in one dimension.

DOI: [10.1103/PhysRevB.95.045120](https://doi.org/10.1103/PhysRevB.95.045120)**I. INTRODUCTION**

Magnetic insulators present a good example of interacting quantum systems where phonons can serve as an intrinsic probe of the strongly-correlated spins [1]. The first microscopic theory of magnetoelasticity was developed at finite temperatures [2,3], where the static and the dynamic correlation functions of the spins were shown to couple to phonons with the same strength in the perturbative regime. At low temperature, assuming existence of a spin-liquid regime in two- and three-dimensional Heisenberg antiferromagnets, phonons were shown to measure the mass and lifetime of the spin-liquid quasiparticles [4,5]. In one dimension (1D)—where interacting magnons form a spin-Luttinger liquid at low energy—the theory remains largely unexplored. At the same time such 1D systems are readily accessible in experiments on Cs_2CuCl_4 [6,7], CsNiCl_3 [8], KCuF_3 [9], and a metal organic coordination polymer $\text{Cu(II)-2,5-bis(pyrazol-1-yl)-1,4-dihydroxybenzene}$ [10].

In this paper we construct a microscopic theory of magnetoelasticity in 1D using the diagonalization methods of Bethe ansatz [11]. We derive the matrix elements for the four-point correlation function that couples the strongly-correlated spins to phonons dynamically and show that Luttinger liquid at low energy contributes comparably with the high-energy excitations that we are able to account for due to the hierarchy of modes [12–14]. The contribution of the static correlation function to the renormalization of the sound velocity is parametrically larger than the dynamical correlation functions. The resonant decay of phonons in the many-body spin continuum vanishes very fast, as the fourth power of the length in large systems. However we identify another mechanism, hybridization with the excitations at high energy via the dynamical correlation function, that remains

finite in the thermodynamic limit. This work advances the many-body diagonalization tools in 1D [15–19] in to the field of magnetoelasticity, which is beginning to receive attention also in spintronics [20–23].

To test our theory we conduct ultrasonic measurements on a high-quality single crystal of Cs_2CuCl_4 in its nearly 1D regime, i.e., at temperatures of 0.7–2.1 K and magnetic fields up to 9 T [24,25]. The observed dependencies of the sound velocity and attenuation of the sound wave on the magnetic field agree well with all theoretical predictions. We find that the magnetic-field dependent part of the attenuation is governed by the hybridization mechanism. Our results demonstrate that ultrasonic investigations, besides neutron-scattering experiments [6,9,26], can be used as a powerful probe of correlation functions of the many-body system in 1D in magnetic insulators, just as tunneling spectroscopy in semiconductor heterostructures [27,28].

The paper is organized as follows. Section II contains the definition of the magnetostrictive interactions between the Heisenberg model and the phonon models in one dimension and the diagonalization of the isolated Heisenberg model by means of Bethe ansatz. In Sec. III we study renormalization of sound velocity by evaluating microscopically the dynamical correlation function of the spins that couples to the phonons (Sec. III A) and by analyzing it using the hierarchy of interacting modes (Sec. III B). In Sec. IV we consider different mechanisms of attenuation of phonons. In Sec. V we conduct an ultrasound experiment on Cs_2CuCl_4 in its nearly one-dimensional regime and confirm the theoretical predictions. In Appendix A we derive the quantization equation for the pi-pairs' solutions of Bethe equations in the XY limit. In Appendix B we quote the normalization factor of the Bethe states together with the algebraic Bethe ansatz method. In Appendix C we derive the matrix element of the spin operator needed for the magnetostrictive interaction.

II. MODEL

Theoretically, we consider phonons interacting with 1/2 spins on a 1D lattice of length L via a magnetostrictive

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interaction as [2,3]

$$H = H_m + H_{\text{ph}} + V, \quad (1)$$

where

$$H_m = \sum_{j=1}^L (J \mathbf{S}_j \cdot \mathbf{S}_{j+1} + B S_j^z), \quad H_{\text{ph}} = \sum_k \omega_k a_k^\dagger a_k, \quad (2)$$

$$V = \sum_{j=1}^L [J_1(x_{j+1} - x_j) + J_2(x_{j+1} - x_j)^2] \mathbf{S}_j \cdot \mathbf{S}_{j+1} \quad (3)$$

are the Heisenberg model of spins, the free phonon model, and the interaction between them, respectively, \mathbf{S}_j are the spin-1/2 operators, J is the exchange interaction between spins when the atoms are in equilibrium, and B is the external magnetic field in energy units. Here a_k are Bose operators of the phonons, $\omega_k = 2\omega_D |\sin(k/2)|$ is the phonon dispersion, ω_D is Debye energy, $x_j = \sum_k \sqrt{\frac{\hbar b}{m v_0 |k| L}} (a_k + a_{-k}^\dagger) e^{-ikj}$ is the position operator of an atom with the mass m at lattice site j , and v_0 is the sound velocity. Phononic excitations modulate the exchange integrals resulting in a set of magnetoelastic constants $J_n = \partial_x^n J(x)|_{x=b}/n!$ that quantify the magnetoelastic interaction, where b is the lattice parameter. We assume the periodic boundary condition: $\mathbf{S}_{j+L} = \mathbf{S}_j$ and $x_{j+L} = x_j$.

The spin Hamiltonian in Eq. (2) is diagonalized by N -magnon states parameterized with a set of N quasimomenta $\mathbf{q} = (q_1 \dots q_N)$ that satisfy the nonlinear Bethe equations [11]

$$q_j L - \sum_{l \neq j} \varphi_{jl} = 2\pi I_j, \quad (4)$$

where the two-body scattering phases are

$$e^{i\varphi_{ij}} = -\frac{e^{i(q_i+q_j)} + 1 - 2\Delta e^{iq_i}}{e^{i(q_i+q_j)} + 1 - 2\Delta e^{iq_j}}, \quad (5)$$

$\Delta = 1$, and I_j is a set of nonequal integers. Solutions of Bethe equations can be found via numerical deformation from the XY point $\Delta = 0$ (where $\varphi_{ij} = \pi$ gives the solutions $q_j = 2\pi I_j/L$) to the Heisenberg point $\Delta = 1$ [29]. However, Bethe equations remain nonlinear, $\alpha L - \Phi(\alpha, \mathbf{q}) = 2\pi I_j$, for some solutions that contain at least a pair of quasimomenta satisfying the condition $q_i + q_j = \pm\pi$ in the $\Delta = 0$ limit—see derivation in Appendix A. Here $q_i = \pm\pi - \alpha$, $q_j = \alpha$, the scattering phase

$$e^{i\Phi(\alpha, \mathbf{q})} = -\frac{i \frac{2\lambda}{L} \sum_{j=1}^{N-2r} \frac{1 - \sin q_j \sin \alpha}{\sin q_j - \sin \alpha} + e^{i\alpha}}{i \frac{2\lambda}{L} \sum_{j=1}^{N-2r} \frac{1 - \sin q_j \sin \alpha}{\sin q_j - \sin \alpha} - e^{-i\alpha}} \quad (6)$$

depends on another quasimomenta, n is the number of such pi-pairs, and $\lambda = 1$. Solutions for α can be obtained again via deformation from the $\lambda = 0$ to the $\lambda = 1$ point. The eigenenergy of H_m corresponding to the state \mathbf{q} is

$$\varepsilon = \sum_{j=1}^N (J \cos q_j - J + B) + \left(\frac{J}{2} - B\right) \frac{L}{2} \quad (7)$$

and the total momentum—preserved by the translational invariance—is $Q = \sum_{j=1}^N q_j$.

We consider renormalization of phonons by spins via the magnetostrictive interaction V perturbatively. The perturbation series for the eigenenergy of H is

$$E(k) = \varepsilon_0 + \omega_k + \langle k|V|k \rangle + \sum_{\{\mathbf{k}, \mathbf{q}\}} \frac{|\langle \mathbf{k}, \mathbf{q}|V|k \rangle|^2}{\varepsilon_0 + \omega_k - \varepsilon_{\mathbf{q}} - \omega_{\mathbf{k}}}, \quad (8)$$

where ε_0 is the ground state energy of H_m , ω_k is an eigenenergy of H_{ph} parameterized by M momenta $\mathbf{k} = (k_1, \dots, k_M)$. The unperturbed state $|k\rangle = |k\rangle_{\text{ph}}|0\rangle_m$ is a direct product of a single phonon $|k\rangle_{\text{ph}}$ and the spin ground state $|0\rangle_m$ and $|\mathbf{k}, \mathbf{q}\rangle = |\mathbf{k}\rangle_{\text{ph}}|\mathbf{q}\rangle_m$ are the intermediate states.

III. RENORMALIZATION OF SOUND VELOCITY

Change of the sound velocity is given by a derivative of $E(k)$ as

$$\delta v = \delta v_1 + \delta v_2, \quad (9)$$

where evaluation of the phononic matrix elements leaves the spin correlation functions split into the static and the dynamic parts,

$$\delta v_1 = \frac{J_2 b^2 \hbar}{2m v_0} \langle 0|\mathbf{S}_1 \cdot \mathbf{S}_2|0\rangle_m, \quad (10)$$

$$\delta v_2 = \frac{J_1^2 b^2 \hbar}{m v_0} \sum_{\{\mathbf{q}; Q=p\}} \frac{L |\langle \mathbf{q}|\mathbf{S}_1 \cdot \mathbf{S}_2|0\rangle_m|^2 (\varepsilon_0 - \varepsilon_{\mathbf{q}})}{(\varepsilon_0 - \varepsilon_{\mathbf{q}})^2 - (\omega_D p)^2}. \quad (11)$$

Here $\hbar p/b = 2\pi \hbar/(bL)$ is the quantum of the momentum and the sum over all of the many-magnon states, $\{\mathbf{q}\}$, and is restricted by momentum conservation to the states with $Q = p$. The static correlation function in δv_1 is immediately obtained from ε_0 using the translational invariance

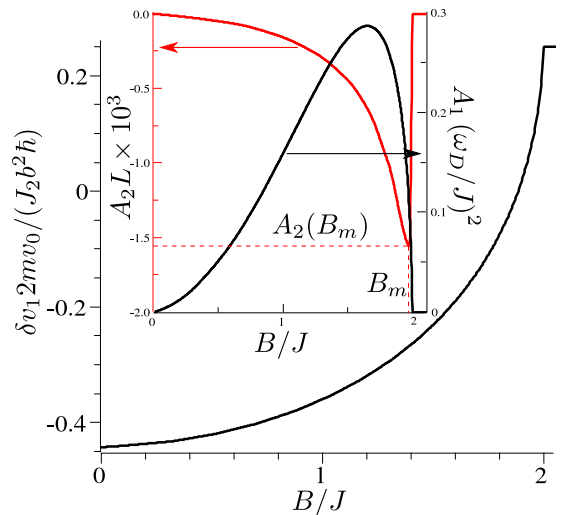


FIG. 1. The static spin correlation function from Eq. (10) as a function of the magnetic field B , calculated using Bethe ansatz. Inset is the dynamic correlation function from Eq. (11) calculated using the matrix element in Eq. (13): The black line is the Luttinger liquid contribution in Eq. (20), and the red line is the high-energy contribution in Eq. (21).

as [30]

$$\langle 0|\mathbf{S}_1 \cdot \mathbf{S}_2|0\rangle_m = \frac{\varepsilon_0 - B(N - \frac{L}{2})}{JL}. \quad (12)$$

Its dependence on the magnetic field, changing from the ferromagnetic value of 0.25 at high fields to the antiferromagnetic $\simeq -0.44$ in zero field, is shown in Fig. 1.

A. Dynamical correlation function of spins

The dynamical part in δv_2 is a fourth-order correlation function. We evaluate the needed matrix element using the algebraic Bethe ansatz [31] and obtain it as a sum over determinants of $N \times N$ matrices, see Appendix C for details,

$$\begin{aligned} \langle \mathbf{q}|\mathbf{S}_1 \cdot \mathbf{S}_2|0\rangle &= (\sqrt{\langle 0|0\rangle} \langle \mathbf{q}|\mathbf{q}\rangle)^{-1} \left\{ \frac{\prod_i \text{ch}(v_j + \eta)}{\prod_{i<j} \text{sh}(v_i - v_j)} \sum_y (-1)^y \frac{\prod_{i,j:j \neq y} \text{sh}(u_j - v_i)}{\prod_j \text{ch}^2(u_j - \eta)} \prod_{l:l \neq y} \frac{\text{sh}(u_l - u_y + 2\eta)}{\text{sh}(u_l - u_y)} \right. \\ &\quad \times \left[\det \hat{K}^{(y)} - \left(1 - \frac{2 \text{sh}(2\eta) \text{sh} \eta \text{sh} u_y \prod_{j:j \neq y} \text{ch}(u_j + \eta)}{\prod_{i<j \neq y} \text{sh}(u_i - u_j)} \right) \det \hat{G}^{(y)} \right] \\ &\quad \left. - \frac{\prod_j \text{ch}(u_j + \eta) \prod_j \text{ch}(v_j + \eta)}{\prod_j \text{ch}^2(u_j - \eta) \prod_{i<j} \text{sh}(v_i - v_j)} \det \hat{K} \right\}, \end{aligned} \quad (13)$$

where the matrix elements are

$$K_{ab} = T_{ab} + \frac{(-1)^b \text{sh}^3(2\eta) \text{sh} u_b \prod_{l:l \neq b} \text{sh}(u_l - u_b + 2\eta) \text{sh} \eta \prod_{j,i:i \neq b} \text{sh}(u_i - v_j) \left[\frac{\text{sh} u_b}{\text{ch} \eta} + \sum_l \frac{\text{sh}(2\eta) \text{ch}(u_b + \eta)}{\text{ch}(v_l - \eta) \text{ch}(v_l + \eta)} \right]}{\prod_{i<j \neq b} \text{sh}(u_i - u_j) \prod_{l:l \neq b} \text{sh}(u_l - u_b) \text{ch}(u_b + \eta) \text{ch}(u_b - \eta) \text{ch}(v_a - \eta) \text{ch}(v_a + \eta)}, \quad (14)$$

$$\begin{aligned} K_{ab}^{(y)} &= T_{ab} + \frac{(-1)^b \text{sh}^3(2\eta) \text{sgn}(y - b) \text{ch}(u_y - \eta) \text{ch}(u_b + \eta) \prod_{l:l \neq y,b} \text{sh}(u_l - u_b + 2\eta)}{\text{ch}(v_a - \eta) \text{ch}(v_a + \eta) \prod_i \text{sh}(u_b - v_i) \prod_{i<j \neq y,b} \text{sh}(u_i - u_j) \prod_{l:l \neq y,b} \text{sh}(u_l - u_b)} \\ &\quad \times \left[\frac{\text{ch}(u_b - \eta)}{\text{ch}(u_b + \eta)} - \frac{\text{sh}(u_y - u_b + 2\eta)}{\text{sh}(u_y - u_b - 2\eta)} + \frac{\text{sh} 2\eta \text{ch}(u_b - 2\eta) \text{sh} u_y}{\text{ch}(u_y - \eta) \text{ch}(u_b + \eta)} \right], \end{aligned} \quad (15)$$

when $b \neq y$ and

$$K_{ay}^{(y)} = \frac{\text{sh}(2\eta) \text{sh}(2v_a)}{\text{ch}^2(v_a - \eta) \text{ch}^2(v_a + \eta)}, \quad (16)$$

$G_{ab}^{(y)} = T_{ab}$ when $b \neq y$ and $G_{ay}^{(y)} = K_{ay}^{(y)}$,

$$T_{ab} = \frac{\text{ch}^L(v_b - \eta) \text{sh}(2\eta)}{\text{ch}^L(v_b + \eta) \text{sh}^2(v_b - u_a)} \prod_{j:j \neq a} \frac{\text{sh}(v_b - u_j + 2\eta)}{\text{sh}(v_b - u_j)} - \frac{\text{sh}(2\eta)}{\text{sh}^2(u_a - v_b)} \prod_{j:j \neq a} \frac{\text{sh}(u_j - v_b + 2\eta)}{\text{sh}(u_j - v_b)}. \quad (17)$$

The normalization factors of Bethe states [32,33] $\langle 0|0\rangle$ and $\langle \mathbf{q}|\mathbf{q}\rangle$ are quoted in Appendix B in terms of a determinant of an $N \times N$ matrix. Here $\eta = (\text{acosh} 1)/2$,

$$u_j = \ln \left(\frac{\sqrt{1 - e^{iq_j^0 - 2\eta}}}{\sqrt{1 - e^{-iq_j^0 - 2\eta}}} \right) - i \frac{q_j^0}{2} \quad (18)$$

are the quasimomenta of the ground state \mathbf{q}^0 in Orbach parametrization, and v_j is obtained from u_j by $q_j^0 \rightarrow q_j$ where \mathbf{q} are the excited states [11].

B. Hierarchy of modes

The excitations in the sum over \mathbf{q} in Eq. (11) have the same number of quasimomenta as the ground state at a given magnetic field. They are constructed by removing a quasimomentum from the ground state distribution and promoting it to an empty position, see sketch in Fig. 2. We will label these excitations as $\psi \psi^*$ pairs.

The whole dynamical correlation function in Eq. (11) exhibits a hierarchy of modes governed by their spectral strength [12–14]. The excitations split into groups according to $n = 1, 2, 3, \dots$ $\psi \psi^*$ pairs that have progressively smaller amplitudes of their matrix elements, $|\langle \mathbf{q}|\mathbf{S}_1 \cdot \mathbf{S}_2|0\rangle|^2 \sim 1/L^{2n}$. We keep the first three levels of the hierarchy,

$$\delta v_2 = \frac{J_1^2 b^2 \hbar}{m v_0 J} (A_1 + A_2 + A_3). \quad (19)$$

The first level consists of only one pair with the minimally possible momentum $Q = p$,

$$A_1(B) = \frac{v_m J L^2 |\langle p|\mathbf{S}_1 \cdot \mathbf{S}_2|0\rangle_m|^2}{2\pi \omega_D^2}, \quad (20)$$

where $v_m = (\varepsilon_p - \varepsilon_0)/p$ is the renormalized velocity of Luttinger liquid and we have used smallness of the exchange energy compared with Debye energy $J/\omega_D \sim 10^{-3}$ for general material parameters [34]. The only matrix element in Eq. (20) can be obtained using the bosonic modes of Luttinger liquid [35], where the dispersion is almost linear. We, however,

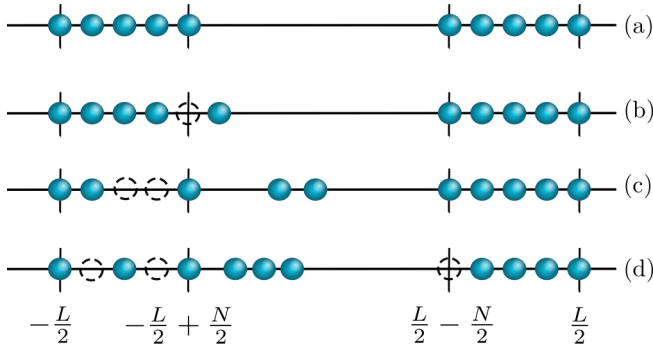


FIG. 2. Configurations of nonequal integer numbers I_j that correspond to the solutions of the Bethe equations for the model H_m : (a) the ground state, (b) one $\psi\psi^*$ -pair excitation, (c) two $\psi\psi^*$ -pair excitations, (d) three $\psi\psi^*$ -pair excitations. These eigenstates include complex solutions at $\Delta = 1$, which are obtained via numerical deformation of Bethe equations from the $\Delta = 0$ to the $\Delta = 1$ point.

use a more general Bethe ansatz approach here. Solutions of Bethe equations give v_m directly that, together with the matrix element in Eq. (13), gives the magnetic field dependence of $A_1(B)$ shown in the inset (right axis) in Fig. 1.

There are polynomially many states in the second and in the third levels of the hierarchy,

$$A_{2(3)}(B) = \sum_{\{\mathbf{q}\}:Q=p} \frac{L|\langle \mathbf{q} | \mathbf{S}_1 \cdot \mathbf{S}_2 | 0 \rangle_m|^2}{\varepsilon_{\mathbf{q}} - \varepsilon_0}, \quad (21)$$

where the summand in Eq. (11) was expanded in a Taylor series in $\omega_D p / (\varepsilon_0 - \varepsilon_{\mathbf{q}}) \ll 1$ since the sum over \mathbf{q} accumulates dominantly at high energy. Contribution of the low-energy excitations (for which $(\varepsilon_0 - \varepsilon_{\mathbf{q}}) / \omega_D p \ll 1$) has an additional small factor J^2 / ω_D^2 , like in Eq. (20). At intermediate energies, $(\varepsilon_0 - \varepsilon_{\mathbf{q}}) \simeq \omega_D p$, the perturbation theory for $E(k)$ becomes inapplicable since these magnetic excitations are in resonance with the acoustic phonon. However, the width of the anticrossing [36] $\lesssim J_1 \sqrt{\hbar b \omega_D^2 / (m J^3 L^5)}$ is much smaller than the many-magnon level spacing J/L that is still in the Luttinger liquid regime. The nonperturbative contribution of these levels is of the order of the anticrossing width and vanishes in large systems.

We obtain the magnetic field dependence of A_2 numerically as a sum over the two $\psi\psi^*$ pairs in Eq. (21), see inset in Fig. 1. At high fields A_2 is small since there are only a few excitations, the strength of which is small as $1/L^4$ at the second level of the hierarchy, and at small fields A_2 is again small since the majority of the excitations belongs to the class of pi-pairs close to the half filling of the magnetic band, which makes their amplitudes even weaker than $1/L^4$ due to Eq. (6). At the intermediate fields the $1/L^4$ smallness is partially compensated by a large number of the excitations, whose majority does not have pi-pairs yet. The position of the maximum of $|A_2(B)|$ is identified from numerics at $B_m = 2J - 9\pi^2 J / (2L^2)$. The value of the function at this point is $A_2(B_m) = -0.0016/L$ for large systems, see scaling of $A_2(B_m)$ in Fig. 3, which is small in a different parameter compared with A_1 .

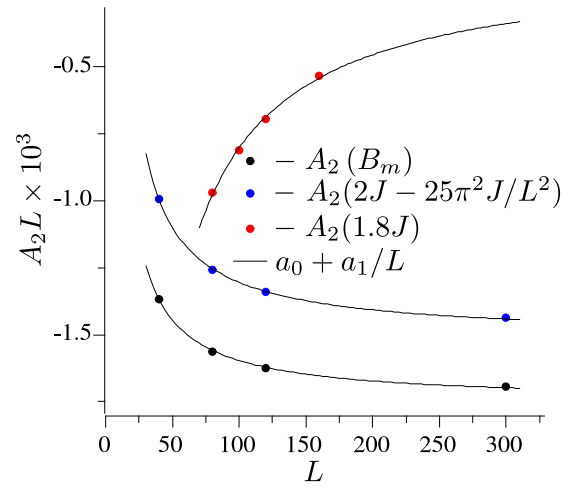


FIG. 3. Scaling of $A_2 L$ defined in Eq. (21) with the system length at three values of the magnetic field $B = B_m, 2J - 25\pi^2 J/L^2, 1.8J$. The fitting of finite size corrections, $A_2 L = a_0 + a_1/L$, gives $(a_0, a_1) \times 10^2 = (-0.17, 1.51), (-0.15, 2.04), (-0.01, -6.95)$ for the three magnetic fields, respectively.

For typical values of material parameters, A_1 and A_2 are of the same order, e.g., $1/L \sim 10^{-6}$ and $(\omega_D/J)^2 \sim 10^{-6}$ for ultrasonic measurements in a magnetic insulator [1]. The three $\psi\psi^*$ -pairs contribution A_3 is smaller than A_2 due to an additional $1/L^2$ in accord with the hierarchy of modes [12–14] for the whole range of magnetic fields, see Fig. 4.

IV. ATTENUATION OF PHONONS

Next let us analyze decay of the phonons into the spin excitations. The excitation spectrum of Heisenberg model in Eq. (2) is continuous which always has some states in resonance with the single phonon energy $\omega_D p$ providing a channel for the direct relaxation, unlike the previous phenomenological approaches [37,38]. The rate of such a

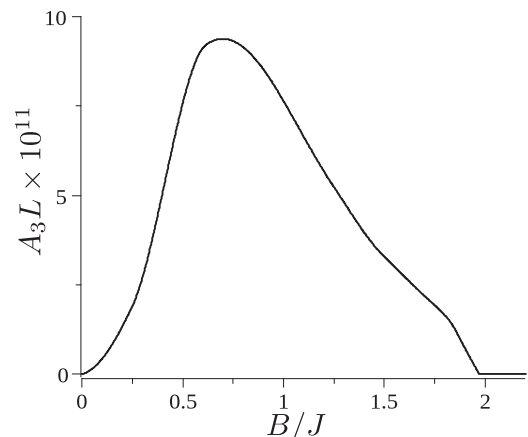


FIG. 4. Contribution of the third level of the hierarchy of modes to δv_2 defined in Eq. (21); $L = 40$. It is small compared with A_2 in the inset of Fig. 1 for the whole range of magnetic fields.

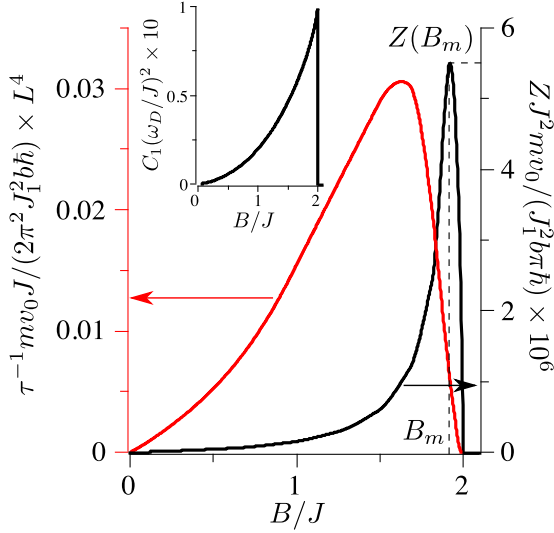


FIG. 5. Two mechanisms of the sound attenuation: the red line is the relaxation rate τ^{-1} calculated using the Fermi golden rule in Eq. (22), while the black line is the degree of hybridization Z of a sound phonon with the magnetic excitations dominated by high energies in Eq. (24). Inset is the low energy contribution to Eq. (24).

process is given by the Fermi golden rule,

$$\tau^{-1} = \frac{2\pi^2 J_1^2 b}{mv_0} \sum_{\{\mathbf{q}\}; Q=p} |\langle \mathbf{q} | \mathbf{S}_1 \cdot \mathbf{S}_2 | 0 \rangle_m|^2 \delta(\Delta E), \quad (22)$$

where $\Delta E = \varepsilon_{\mathbf{q}} - \varepsilon_0 - \omega_p$ and the contribution of the J_2 term in Eq. (3) is zero due to $\delta(\Delta E)$. The principal value of the sum in Eq. (22) is accumulated by the second level of the hierarchy, which we evaluate numerically—see the magnetic field dependence of τ^{-1} in Fig. 5. Its maximum value has the same small prefactor $1/L^4$ as the matrix element in Eq. (13) making the direct relaxation extremely slow in large systems.

However, the amplitude of the free phonons can also be reduced via hybridization with the magnetic excitations, similarly to the δv_2 renormalization of their velocity. The first order in perturbation theory for the wave function,

$$|\Psi_{\mathbf{k}}\rangle = |k\rangle + \sum_{\{\mathbf{k}, \mathbf{q}\}} \frac{\langle \mathbf{k}, \mathbf{q} | V | k \rangle}{\varepsilon_0 + \omega_{\mathbf{k}} - \varepsilon_{\mathbf{q}} - \omega_{\mathbf{k}}} |\mathbf{k}\rangle_{\text{ph}} |\mathbf{q}\rangle_m, \quad (23)$$

gives suppression at low momenta, $Z = 1 - |\langle p | \Psi_p \rangle|^2$, as

$$Z = \frac{J_1^2 b \pi \hbar^2}{mv_0} \sum_{\{\mathbf{q}\}; Q=p} \frac{|\langle \mathbf{q} | \mathbf{S}_1 \cdot \mathbf{S}_2 | 0 \rangle_m|^2}{(\varepsilon_0 - \varepsilon_{\mathbf{q}} - \omega_D p)^2}, \quad (24)$$

which we analyze using the hierarchy of modes:

$$Z = \frac{J_1^2 b \pi \hbar^2}{J^2 m v_0} (C_1 + C_2 + C_3), \quad (25)$$

where

$$C_1 = \frac{(J/\omega_D)^2 L^2 |\langle p | \mathbf{S}_1 \cdot \mathbf{S}_2 | 0 \rangle_m|^2}{(2\pi)^2} \quad (26)$$

and

$$C_{2(3)} = \sum_{\{\mathbf{q}\}; Q=p} \frac{|\langle \mathbf{q} | \mathbf{S}_1 \cdot \mathbf{S}_2 | 0 \rangle_m|^2}{(\varepsilon_0 - \varepsilon_{\mathbf{q}})^2}, \quad (27)$$

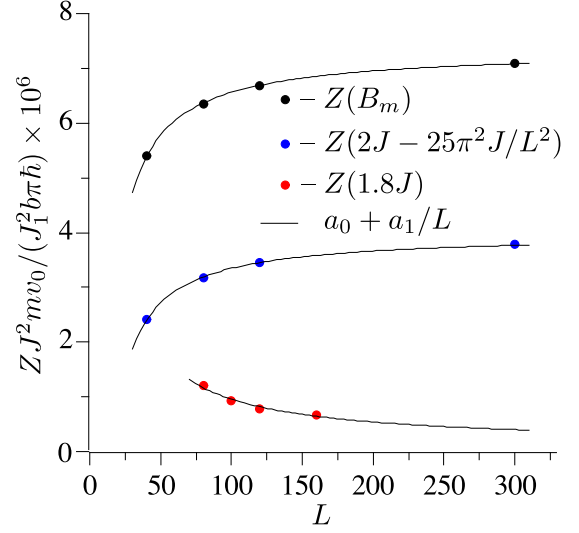


FIG. 6. Scaling of Z defined in Eq. (24) with the system length at three values of the magnetic field $B = B_m, 2J - 25\pi^2 J/L^2, 1.8J$. The fitting of finite size corrections, $Z J^2 m v_0 / (J_1^2 b \pi \hbar^2) = a_0 + a_1/L$, gives $(a_0, a_1) \times 10^5 = (0.73, -7.8), (0.40, -6.3), (0.012, 8.4)$ for the three magnetic fields, respectively.

like in the analysis of Eq. (11) before. The first level contribution C_1 is small in J^2/ω_D^2 like A_1 , see inset in Fig. 5. But C_2 , shown in Fig. 5, remains finite in the thermodynamic limit (see scaling in Fig. 6) unlike A_2 above, and C_3 is small in $1/L^2$ compared with C_2 , see Fig. 7. This hybridization mechanism can be distinguished from other nonmagnetic channels of relaxation via its magnetic field dependence and from the exponential decay into the resonant magnetic states described by Eq. (22) since it is constant in the temporal and spatial domains.

V. ULTRASOUND EXPERIMENT ON Cs_2CuCl_4

Finally, we discuss our experimental results. High-quality single crystals of several mm size of the frustrated spin-1/2 antiferromagnet Cs_2CuCl_4 were grown from an aqueous solution by an evaporation technique [39]. A pair of

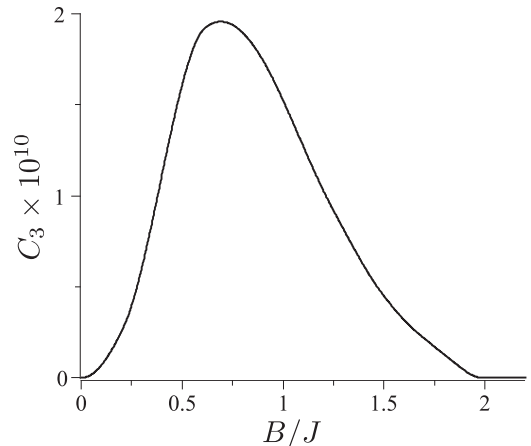


FIG. 7. Contribution of the third level of the hierarchy of modes to Z defined in Eq. (27); $L = 40$. It is small compared with C_2 in Fig. 5 for the whole range of magnetic fields.

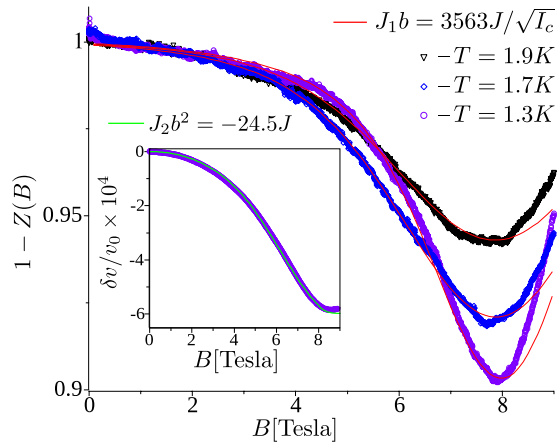


FIG. 8. Experimental results (open triangles, diamonds, and circles) of the renormalized amplitude $1 - Z$ of the longitudinal ultrasound wave propagating along the [010] axis of Cs_2CuCl_4 at $T = (1.900 \pm 0.005)$ K, $T = (1.700 \pm 0.005)$ K, and $T = (1.300 \pm 0.005)$ K. The red lines represent the results of Eq. (24) with $J_1b = 3563J/\sqrt{I_c}$. The inset shows data (open circles) of the corresponding normalized sound velocity at $T = (1.300 \pm 0.005)$ K. The green line shows the result of Eq. (10) using $J_2b^2 = -24.5J$. Additional data are presented in Fig. 9.

piezoelectric polymer-foil transducers was glued to opposite parallel surfaces perpendicular to the [010] direction for the generation and the detection of the ultrasound waves. These longitudinal waves propagate along the [010] direction that corresponds to the elastic mode c_{22} . Changes of the sound velocity δv and the renormalized amplitude of the sound wave $1 - Z$ were measured as functions of magnetic field at constant temperatures, using the experimental set up described in detail in Ref. [40].

In Fig. 8 we compare the experimental data for the sound velocity with the theoretical results expressed in Eqs. (10) and (11). By fitting the static correlation function given by Eq. (10), we extract $J_2b^2 = -24.5J$, with the magnetic coupling constant $J = 0.375$ meV taken from Ref. [6]—see inset in Fig. 8. We find no signatures of the dynamical correlation functions represented by Eq. (11)—which are parametrically small—down to the noise level of our experiment. This defines an upper bound to the other microscopic constant $J_1b \leq 1.25 \times 10^4 J$.

Analyzing the attenuation of the amplitude of the sound wave Z , we find that its functional dependence on the magnetic field is in good agreement with the dynamic hybridization mechanism represented by Eq. (24)—see Fig. 8 and additional data in Fig. 9. By fitting its amplitude, we extract the other microscopic parameter as $J_1b = 3563J/\sqrt{I_c}$, where I_c is the

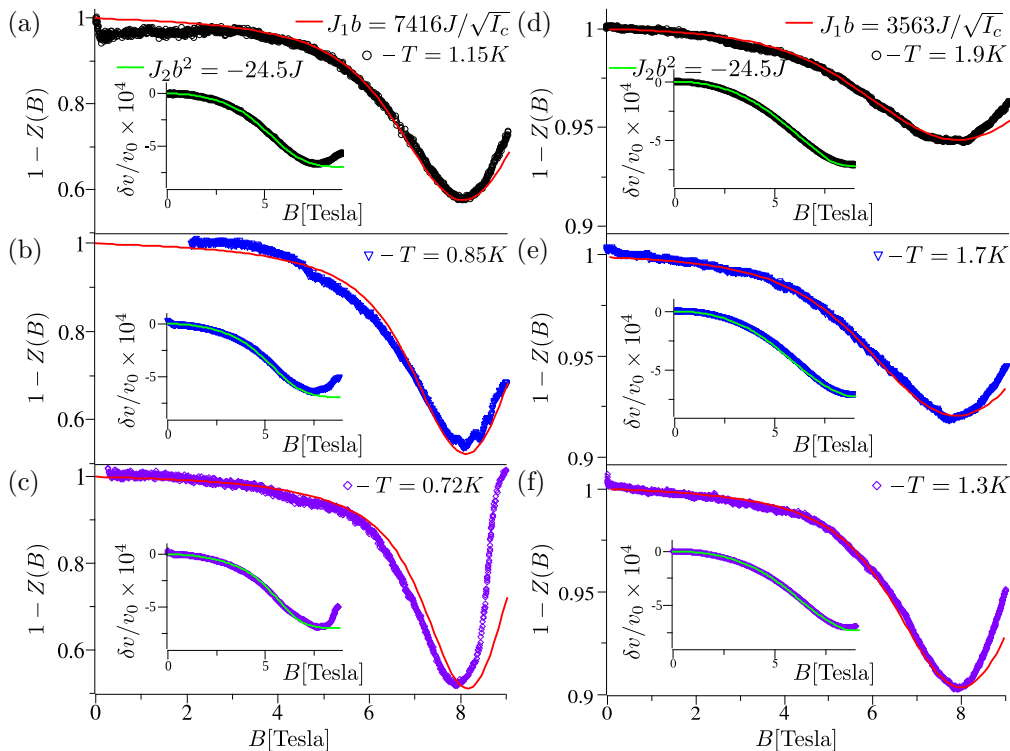


FIG. 9. Experimental results (open circles, triangles, and diamonds) of the renormalized amplitude $1 - Z$ of the longitudinal ultrasound wave propagating along the [010] axis of Cs_2CuCl_4 at the temperatures of (a) $T = (1.150 \pm 0.005)$ K, (b) $T = (0.850 \pm 0.005)$ K, (c) $T = (0.720 \pm 0.005)$ K, (d) $T = (1.900 \pm 0.005)$ K, (e) $T = (1.700 \pm 0.005)$ K, and (f) $T = (1.300 \pm 0.005)$ K. The red lines represent the results of Eq. (24) with $J_1b = 7416J/\sqrt{I_c}$ for (a)–(c) and with $J_1b = 3563J/\sqrt{I_c}$ for (d)–(f). The data in (d)–(f) were taken in a different cryostat system using upgraded electronics and a better quality sample compared with the data in (a)–(c) leading to a decrease of the nonmagnetic losses by a factor of $I_c(a,b,c)/I_c(d,e,f) \approx 4.3$. The insets show data of the corresponding normalized sound velocities at the same temperatures. The green lines show the result of Eq. (10) using $J_2b^2 = -24.5J$. The results of our ultrasound experiments are still relatively close to the 1D regime at the temperature of $T = (0.720 \pm 0.005)$ K, at which the system is already in a transitional state between the 1D and a 2D regime.

degree of nonmagnetic losses. A quantitative determination of these losses is not possible since they consist of various extrinsic (e.g., coupling and diffraction losses, nonparallel alignment of the sample, etc.) and intrinsic attenuation mechanisms like direct scattering at defects or dislocation damping [41]. However, even for $I_c = 1$ this value of $J_1 b$ is consistent with the bound from the measurement of the sound velocity.

The values of the microscopic constants are significantly different from the values measured along the a axis in Ref. [42] manifesting an anisotropy of Cs_2CuCl_4 . Our very good fit of the magnetic field dependencies by the purely one-dimensional theory in Figs. 8 and 9 gives a further argument that the interchain interactions in Cs_2CuCl_4 in the finite temperature regime are negligible despite only a moderate degree of the exchange anisotropy of ~ 3 in the a - b plane [43].

VI. CONCLUSIONS

In conclusion, constructing a microscopic theory of magnetoelasticity in 1D we have shown that the necessary correlation functions involve the many-body excitations at all energy scales and have identified a new mechanism of sound attenuation. Our theoretical predictions agree with our ultrasound experiments in the 1D regime of Cs_2CuCl_4 .

ACKNOWLEDGMENT

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APPENDIX A: DERIVATION OF THE QUANTIZATION EQUATION FOR PI-PAIRS

The XXZ model is a generalization of Heisenberg model that introduces the interaction strength between magnons $J\Delta$ as a model parameter, which breaks the rotational symmetry of the spin-spin interaction term $\mathbf{S}_j \cdot \mathbf{S}_{j+1}$. In one dimension the model reads

$$H_m = \sum_{j=1}^L \left(J \frac{S_j^- S_{j+1}^+ + S_j^+ S_{j+1}^-}{2} + J\Delta S_j^z S_{j+1}^z + B S_j^z \right), \quad (\text{A1})$$

where $S_j^\pm = S_j^x \pm i S_j^y$. For $\Delta = 1$ this model becomes the model in Eq. (2). The N -magnon eigenstates of this Hamiltonian can be found by solving a set of Bethe equations,

$$q_j L - \sum_{l \neq j} \varphi_{jl} = 2\pi I_j, \quad (\text{A2})$$

for N quasimomenta q_j , where the two-magnon scattering phases are given by

$$e^{i\varphi_{ij}} = - \frac{e^{i(q_i+q_j)} + 1 - 2\Delta e^{iq_i}}{e^{i(q_i+q_j)} + 1 - 2\Delta e^{iq_j}} \quad (\text{A3})$$

and I_j is a set of N nonequal integer numbers.

In the free magnon limit $\Delta = 0$ the two-body phase shifts φ_{ij} become independent of quasimomenta and equal to the shifts of free fermions or hard-core bosons, $\varphi_{ij} = \pi$ that is immediately obtained by taking the $\Delta \rightarrow 0$ limit of Eq. (A3) giving $\exp(i\varphi_{ij}) = -1$. This result restores the plain wave

quantization condition for each magnon independently, $q_j = 2\pi(I_j + 1/2)/L$ [44], from the system of nonlinear Bethe equations in Eq. (A2). Alternatively, the free magnon result can be obtained by setting $\Delta = 0$ in the Hamiltonian in Eq. (A1) and then by diagonalizing the resulting XY model directly [45].

However, the noninteracting limit becomes ambiguous when at least one pair of quasimomenta in an N magnon state satisfies the condition $q_i + q_j = 2\pi(I_i + I_j + 1)/L = \pm\pi$ at $\Delta = 0$. In evaluating the $\Delta = 0$ limit of Eq. (A3), the leading order of $e^{i(q_i+q_j)} + 1$ is zero in the Taylor series around the $\Delta = 0$ point, both in the numerator and in the denominator. Thus, higher order coefficients have to be calculated, $e^{i(q_i+q_j)} + 1 = c_1\Delta + c_2\Delta^2 + \dots$, that requires, in general, solving the whole set of N Bethe equation in Eq. (A2) in a nonlinear fashion, i.e., c_1, c_2, \dots depend on all q_l —not just q_i and q_j —since Δ is still finite, which requires solving all N Bethe equations for all q_l simultaneously in taking the limit. This issue was noted in Refs. [46,47] but was never resolved. Here we start from a finite but small Δ , for which all scattering phase are well behaved, and then take the limit $\Delta \rightarrow 0$ systematically.

Let us consider a N -magnon solution of Bethe equations that contains $2r$ quasimomenta that satisfy the $q_{2j} + q_{2j+1} = \pm\pi$ condition (we will call these pairs of quasimomenta pi-pairs below) and $N - 2r$ quasimomenta that do not have a pi-pair. For a finite but small $\Delta \ll 1$ the quasimomenta of a pi-pair can be parameterized as

$$q_{2j} = \pm\pi - \alpha_j + \frac{\delta_j}{2}, \quad j \leq r, \quad (\text{A4})$$

$$q_{2j+1} = \alpha_j + \frac{\delta_j}{2}, \quad (\text{A5})$$

where α_j is an unknown parameter of the j th pi-pair that has a nonzero value, since Bethe equations for this pair cannot be solved due to the unknown (at the moment) phase shift $\varphi_{2j,2j+1}$ at $\Delta = 0$, and δ_j is a parameter that vanishes at $\Delta = 0$. On the other hand, the remaining quasimomenta $j > 2r$ can be found immediately for $\Delta = 0$ since all of their scattering phases in Eq. (A3) for these quasimomenta are well behaved, $\varphi_{ij} = \pi$. Thus at a finite $\Delta \ll 1$ we can write

$$q_j = \frac{2\pi(I_j + \frac{1}{2})}{L} + \epsilon_j, \quad j > 2r, \quad (\text{A6})$$

where ϵ_j are small corrections due to a finite Δ that depend on all other quasimomenta and vanish for $\Delta = 0$. Conservation of the total momentum of N magnons, $\sum_{j=1}^N q_j = 2\pi \sum_{j=1}^N I_j/L$ including the pi-pairs, is independent of the interactions and imposes an additional constraint on δ_j and ϵ_j ,

$$\sum_{j=2r+1}^N \epsilon_j = - \sum_{j=1}^r \delta_j. \quad (\text{A7})$$

It is obtained as a sum of all equations in Eq. (A2) after substitution of Eqs. (A4)–(A6).

Since α_j cannot be obtained directly from its own Bethe equation due to the undefined scattering phase within the corresponding pi-pair, we are going to obtain an equation for α_j from the other $j > 2r$ Bethe equations that do not have this issue. We start from expanding φ_{ji} for $j > 2r$

magnons—which are defined at the point $\Delta = 0$ —up to the linear order in small Δ . Taking into account that ϵ_j is proportional to Δ and δ_j is linear (or a higher order) in Δ we obtain the following expansion of φ_{ji} between the j th magnon and a pi-pair and the j th magnon and another j' th magnons, which do not have a pi-pair, respectively,

$$\varphi_{j,2i} = \pi - 2\Delta \frac{\sin \frac{q_j - \alpha_i}{2}}{\cos \frac{q_j + \alpha_i}{2}}, \quad (\text{A8})$$

$$\varphi_{j,2i+1} = \pi - 2\Delta \frac{\cos \frac{q_j + \alpha_i}{2}}{\sin \frac{q_j - \alpha_i}{2}}, \quad (\text{A9})$$

$$\varphi_{jj'} = \pi - 2\Delta \frac{\sin \frac{q_j - q_{j'}}{2}}{\cos \frac{q_j + q_{j'}}{2}}. \quad (\text{A10})$$

Then we substitute these expansions in Eq. (A2) and sum all of them with $j > 2r$ obtaining a relation between δ_i and α_i that parameterizes the quasimomenta for $j \leq 2r$,

$$-L \sum_{i=1}^r \delta_i + 4\Delta \sum_{i=1}^r \sum_{j=2n+1}^N \frac{1 - \sin q_j \sin \alpha_i}{\sin q_j - \sin \alpha_i} = 0, \quad (\text{A11})$$

where the sum over j is taken over the remaining quasimomenta that do not have a pi-pair, given by Eq. (A6) with $\epsilon_j = 0$. Here we used Eq. (A7) to express ϵ_j through δ_j and canceled all $\varphi_{jj'}$ terms for both $j, j' > 2r$ due to the $\varphi_{jj'} = -\varphi_{j'j}$ symmetry of Eq. (A10)—note that the scattering phases are defined up to an arbitrary period 2π times an integer.

The equation in Eq. (A11) is a sum of r terms and each term depends only on two unknown variables δ_i and α_i . Thus Eq. (A11) splits into r independent equations and solving them separately we find

$$\delta_i = \frac{4}{L} \sum_{j=2r+1}^N \frac{1 - \sin q_j \sin \alpha_i}{\sin q_j - \sin \alpha_i} \Delta. \quad (\text{A12})$$

This result shows that the linear term in the Taylor expansion for δ_i in Δ does not vanish. However it depends on the still unknown parameter α_i . In order to find it, we take the $\Delta \rightarrow 0$ limit of Eq. (A3) for the two quasimomenta within the i th pi-pair and obtain

$$e^{i\varphi_{2i,2i+1}} = \frac{i \frac{2}{L} \sum_{j=2r+1}^N \frac{1 - \sin q_j \sin \alpha_i}{\sin q_j - \sin \alpha_i} - e^{-i\alpha_i}}{i \frac{2}{L} \sum_{j=2r+1}^N \frac{1 - \sin q_j \sin \alpha_i}{\sin q_j - \sin \alpha_i} + e^{i\alpha_i}}, \quad (\text{A13})$$

where

$$e^{i(q_{2i} + q_{2i+1})} + 1 = \frac{4}{L} \sum_{j=2r+1}^N \frac{1 - \sin q_j \sin \alpha_i}{\sin q_j - \sin \alpha_i} \Delta \quad (\text{A14})$$

was expanded up to the linear order in Δ , substituted in Eq. (A3), and Δ was canceled from the whole expression altogether. Substituting Eq. (A13) into each of the $2i$ th (or $2i + 1$ st) Bethe equation in Eq. (A2) in the exponential form we obtain an equation for each α_i independently in the $\Delta = 0$ limit,

$$-e^{iL\alpha_i} \frac{i \frac{2}{L} \sum_{j=2r+1}^N \frac{1 - \sin q_j \sin \alpha_i}{\sin q_j - \sin \alpha_i} - e^{-i\alpha_i}}{i \frac{2}{L} \sum_{j=2r+1}^N \frac{1 - \sin q_j \sin \alpha_i}{\sin q_j - \sin \alpha_i} + e^{i\alpha_i}} = 1. \quad (\text{A15})$$

This result does not coincide with the free wave quantization condition $\exp(i\alpha_i L) = -1$, being a nonlinear equation for α_i . Its solutions can be found by introducing an extra deformation parameter λ ,

$$-e^{iL\alpha} \frac{i \frac{2\lambda}{L} \sum_{j=2r+1}^N \frac{1 - \sin q_j \sin \alpha}{\sin q_j - \sin \alpha} - e^{-i\alpha}}{i \frac{2\lambda}{L} \sum_{j=2r+1}^N \frac{1 - \sin q_j \sin \alpha}{\sin q_j - \sin \alpha} + e^{i\alpha}} = 1, \quad (\text{A16})$$

where the subscript was omitted, $\alpha_i \rightarrow \alpha$, since the equation is the same for all indices i . The solutions can be classified in the limit $\lambda = 0$, like the Bethe equations, where Eq. (A16) is solved by $\alpha = 2\pi(I_j + 1/2)/(L - 2)$. Then a smooth deformation of the equation from $\lambda = 0$ to $\lambda = 1$ gives all solutions of the nonlinear Eq. (A15). The quantization equation of pi-pairs in the $\Delta = 0$ limit before Eq. (6) is Eq. (A16) in the logarithmic form.

The two-magnon solutions of Bethe equations that we identified as pi-pairs in Eq. (A16) at $\Delta = 0$ can account for the missing complex solutions, which instead remain real, of the XXZ model at $\Delta = 1$ found in Ref. [48]. For $N = 2$ the parameter δ in Eq. (A12) remains zero for any Δ making the scattering phase $\varphi_{12} = -2\alpha$ and Eq. (A2) independent of Δ as well, in this case. Thus this two-magnon solution remains real at $\Delta = 1$ and has to be removed from the class of complex conjugated quasimomenta. We also note that pi-pairs are still solutions of Bethe equations at any finite Δ in full accord with the arguments of Ref. [49]. It is only the limit $\Delta \rightarrow 0$ of these solutions that does not recover the single particle quantization rule $q_j = 2\pi(I_j + 1/2)/L$.

APPENDIX B: NORMALIZATION FACTORS OF BETHE STATES

The eigenstates of the XXZ model in Eq. (A1) are the Bethe states

$$|\Psi\rangle = \sum_{\mathcal{P}, j_1 < \dots < j_N} e^{i \sum_l q_{\mathcal{P}_l} j_l + i \sum_{l < l'} \varphi_{\mathcal{P}_l, \mathcal{P}_{l'}} / 2} S_{j_1}^+ \dots S_{j_N}^+ |\Downarrow\rangle, \quad (\text{B1})$$

where \mathcal{P} is a permutation of N quasimomenta q_j and $|\Downarrow\rangle$ is the ferromagnetic ground state. In this so-called coordinate representation the many-body states $|\Psi\rangle$ are not factorizable making calculations of scalar products and expectation values in this representation almost intractable. However, a calculation of the form factors needed in Eq. (13) becomes manageable using the algebraic form of Bethe ansatz [31], in which Bethe states are factorized in terms of operators with given commutation relations.

Following Ref. [31] we write down the many-body wave functions using operators that satisfy a Yang-Baxter algebra as

$$|\mathbf{u}\rangle = \prod_{j=1}^N C(u_j) |\Downarrow\rangle, \quad (\text{B2})$$

where u_j are N auxiliary parameters and $C(u)$ is one of the four matrix elements of the transition matrix

$$T(u) = \begin{pmatrix} A(u) & B(u) \\ C(u) & D(u) \end{pmatrix}, \quad (\text{B3})$$

which is defined in an auxiliary 2×2 space. This T -matrix satisfies the Yang-Baxter equation

$$R(u - v)(T(u) \otimes T(v)) = (T(v) \otimes T(u))R(u - v). \quad (\text{B4})$$

Here we use the following R -matrix that corresponds to the spin Hamiltonian in Eq. (A1),

$$R(u) = \begin{pmatrix} 1 & & & \\ & b(u) & c(u) & \\ & c(u) & b(u) & \\ & & & 1 \end{pmatrix}, \quad (\text{B5})$$

where $b(u) = \sinh(u)/\sinh(u + 2\eta)$ and $c(u) = \sinh(2\eta)/\sinh(u + 2\eta)$.

The entries of Eq. (B4) give commutation relations between the matrix elements of T . Here we write down four of them that will be used later,

$$[B_u, C_v] = \frac{c(u - v)}{b(u - v)}(A_u D_v - A_v D_u), \quad (\text{B6})$$

$$A_u C_v = \frac{1}{b(u - v)}C_v A_u - \frac{c(u - v)}{b(u - v)}C_u A_v, \quad (\text{B7})$$

$$D_u C_v = \frac{1}{b(v - u)}C_v D_u - \frac{c(v - u)}{b(v - u)}C_u D_v, \quad (\text{B8})$$

$$[A_u, D_v] = \frac{c(u - v)}{b(u - v)}(C_v B_u - C_u B_v). \quad (\text{B9})$$

We have introduced the subscript u and v as a shorthand of the argument, e.g. $A_u \equiv A(u)$, above.

The transfer matrix $\tau(u) = \text{Tr}T(u) = A(u) + D(u)$ contains all of the conserved quantities of the model in Eq. (A1) including the Hamiltonian. Thus if $|\mathbf{u}\rangle$ is an eigenstate of $\tau(u)$ then it is an eigenstate of the Hamiltonian. The eigenvalue equation, $\tau(u)|\mathbf{u}\rangle = \mathcal{T}_u|\mathbf{u}\rangle$ where \mathcal{T}_u is a scalar quantity—the corresponding eigenvalue, can be solved using the commutation relations in Eqs. (B6)–(B9). The results of acting with the A_u and D_u operators on the state $|\mathbf{u}\rangle$ in Eq. (B2) are obtained by commuting them from left to right through the product of $C(u_j)$ operators,

$$\begin{aligned} A_u \prod_{j=1}^N C(u_j)|0\rangle &= a_u \prod_{j=1}^N \frac{1}{b_{uj}} C(u_j)|0\rangle - \sum_{j=1}^N a_j \frac{c_{uj}}{b_{uj}} C(u) \\ &\times \prod_{l=1 \neq j}^N \frac{1}{b_{jl}} C(u_l)|\downarrow\rangle, \end{aligned} \quad (\text{B10})$$

$$\begin{aligned} D_u \prod_{j=1}^N C(u_j)|0\rangle &= d_u \prod_{j=1}^N \frac{1}{b_{ju}} C(u_j)|0\rangle + \sum_{j=1}^N d_j \frac{c_{uj}}{b_{uj}} C(u) \\ &\times \prod_{l=1 \neq j}^N \frac{1}{b_{lj}} C(u_l)|\downarrow\rangle, \end{aligned} \quad (\text{B11})$$

where the vacuum eigenvalues of the operators, $A_u|\downarrow\rangle = a_u|\downarrow\rangle$ and $D_u|\downarrow\rangle = d_u|\downarrow\rangle$, are

$$a_u = \frac{\cosh^L(u - \eta)}{\cosh^L(u + \eta)} \quad \text{and} \quad d_u = 1. \quad (\text{B12})$$

Since the right hand side of Eqs. (B10) and (B11) contains terms that are not proportional to the original state multiplied by a scalar, an arbitrary Bethe state is not an eigenstate of the transfer matrix τ for an arbitrary set of the auxiliary parameters u_j . However, the second terms in Eqs. (B10) and (B11) can be made zero by selecting specific sets of u_j that are solutions of the following set of nonlinear equations,

$$\frac{a_j}{d_j} = \prod_{l=1 \neq j}^N \frac{b_{jl}}{b_{lj}}, \quad (\text{B13})$$

where we have used the shorthand with the subscripts, i.e. $a_j \equiv a(u_j)$ and $b_{jl} \equiv b(u_j - u_l)$. Substitution of the expressions for a_j and d_j from Eq. (B12) and for b_{jl} from Eq. (B5) gives the following Bethe equation and the eigenvalue of the transfer matrix τ ,

$$\frac{\cosh(u_j - \eta)^L}{\cosh(u_j + \eta)^L} = \prod_{l=1 \neq j}^N \frac{\sinh(u_j - u_l - 2\eta)}{\sinh(u_j - u_l + 2\eta)}, \quad (\text{B14})$$

$$\mathcal{T}_u = a_u \prod_{j=1}^N \frac{1}{b_{uj}} + d_u \prod_{j=1}^N \frac{1}{b_{ju}}. \quad (\text{B15})$$

The Bethe ansatz equations—in the coordinate representation—are obtained under substitution of

$$u_j = \ln \left[\sqrt{\frac{1 - e^{iq_j - 2\eta}}{1 - e^{-iq_j - 2\eta}}} \right] - \frac{iq_j}{2} \quad (\text{B16})$$

and

$$\eta = \frac{\text{acosh}\Delta}{2} \quad (\text{B17})$$

into Eq. (B14).

The scalar product between two Bethe states $\langle \mathbf{v} |$ and $|\mathbf{u}\rangle$ can be calculated using the commutation relations in Eqs. (B6)–(B9). The multiplication of the bra and ket states in the form of Eq. (B2) is evaluated by commuting each operator $B(v_j)$ from left to right through the product of $C(u_j)$ operators and then by using the vacuum eigenvalues of the generated A and D operators from Eq. (B12). When u_j is a solution of Eq. (B14) and v_j is an arbitrary set of auxiliary parameters the result can be written in a compact form as a determinant of an $N \times N$ matrix—the so-called Slavnov's formula [50],

$$\langle \mathbf{v} | \mathbf{u} \rangle = \frac{\prod_{i,j=1}^N \sinh(v_j - u_i)}{\prod_{j < i} \sinh(v_j - v_i) \prod_{j < i} \sinh(u_j - u_i)} \det \hat{T}, \quad (\text{B18})$$

where matrix elements are $T_{ab} = \partial_{u_a} \mathcal{T}(v_b)$. Under substitution of $\mathcal{T}(u)$ from Eq. (B5) these matrix elements read

$$T_{ab} = \frac{\cosh^L(v_b - \eta)}{\cosh^L(v_b + \eta)} \frac{\sinh(2\eta)}{\sinh^2(v_b - u_a)} \prod_{j=1 \neq a}^N \frac{\sinh(v_b - u_j + 2\eta)}{\sinh(v_b - u_j)} - \frac{\sinh(2\eta)}{\sinh^2(u_a - v_b)} \prod_{j=1 \neq a}^N \frac{\sinh(u_j - v_b + 2\eta)}{\sinh(u_j - v_b)}. \quad (\text{B19})$$

The normalization factor of Bethe states in Eq. (B2) can be evaluated by taking the $\mathbf{v} \rightarrow \mathbf{u}$ limit of Eq. (B18) [32,33],

$$\langle \mathbf{u} | \mathbf{u} \rangle = \sinh^N(2\eta) \prod_{i \neq j=1}^N \frac{\sinh(u_j - u_i + 2\eta)}{\sinh(u_j - u_i)} \det \hat{M}, \quad (\text{B20})$$

where the matrix elements are

$$M_{ab} = \begin{cases} -L \frac{\sinh 2\eta}{\cosh(u_a + \eta) \cosh(u_a - \eta)} - \sum_{j \neq a} \frac{\sinh 4\eta}{\sinh(u_a - u_j - 2\eta) \sinh(u_a - u_j + 2\eta)}, & a = b, \\ \frac{\sinh 4\eta}{\sinh(u_b - u_a + 2\eta) \sinh(u_b - u_a - 2\eta)}, & a \neq b. \end{cases} \quad (\text{B21})$$

APPENDIX C: DERIVATION OF THE DYNAMICAL MATRIX ELEMENT FOR SPINS

In this section we will calculate the matrix element $\langle \mathbf{q} | \mathbf{S}_1 \cdot \mathbf{S}_2 | 0 \rangle$ —with respect to Bethe states of the spin Hamiltonian—that is needed for evaluating Eq. (11). We start by splitting the matrix element of the scalar product $\mathbf{S}_1 \cdot \mathbf{S}_2$ into three parts,

$$\langle \mathbf{q} | \mathbf{S}_1 \cdot \mathbf{S}_2 | 0 \rangle_m = G_{+-} + G_{-+} + G_{zz}, \quad (\text{C1})$$

where

$$G_{+-} = \frac{1}{2} \langle \mathbf{v} | S_1^+ S_2^- | \mathbf{u} \rangle, \quad (\text{C2})$$

$$G_{-+} = \frac{1}{2} \langle \mathbf{v} | S_1^- S_2^+ | \mathbf{u} \rangle, \quad (\text{C3})$$

$$G_{zz} = \langle \mathbf{v} | S_1^z S_2^z | \mathbf{u} \rangle, \quad (\text{C4})$$

u_j are the quasimomenta of the ground state $|0\rangle$, and v_j are the quasimomenta of an excited state $|\mathbf{q}\rangle$ with the same number of particles.

The local spin operators of the model in Eq. (A1) can be expressed in terms of the algebraic Bethe ansatz operators from Eq. (B3) as [15,16,51]

$$S_1^+ = C_\xi \tau_\xi^{L-1}, \quad S_2^+ = \tau_\xi C_\xi \tau_\xi^{L-2}, \quad (\text{C5})$$

$$S_1^- = B_\xi \tau_\xi^{L-1}, \quad S_2^- = \tau_\xi B_\xi \tau_\xi^{L-2}, \quad (\text{C6})$$

$$S_1^z = S_2^z \frac{A_\xi - D_\xi}{2} \tau_\xi^{L-1}, \quad S_2^z = \tau_\xi \frac{A_\xi - D_\xi}{2} \tau_\xi^{L-2}, \quad (\text{C7})$$

where $\xi = -i\pi/2 + \eta$.

Firstly, we evaluate the $+-$ correlation function. Under the substitution of Eqs. ((C5), (C6)) in to Eq. (C2) it reads

$$G_{+-} = \frac{1}{2} \langle \mathbf{v} | C_\xi B_\xi | \mathbf{u} \rangle. \quad (\text{C8})$$

Commuting of the B_ξ operator from left to right through a product of $C(u_j)$ operators by means of the commutation relations in Eqs. ((B6)–(B9)) gives

$$B_\xi \prod_{j=1}^N C_{u_j} | \Downarrow \rangle = \sum_{x=1}^{N+1} a_x c_{x\xi} \prod_{i=1 \neq x}^{N+1} \frac{1}{b_{xi}} \sum_{y=1 \neq x}^{N+1} c_{\xi y} \prod_{j=1 \neq x, y}^{N+1} \frac{1}{b_{jy}} \prod_{j=1 \neq x, y}^{N+1} C_{u_j} | \Downarrow \rangle, \quad (\text{C9})$$

where $u_{N+1} \equiv \xi$. Multiplying the above expression by C_ξ and evaluating the scalar product with the final state $\langle \mathbf{v} |$ we obtain

$$G_{+-} = \frac{1}{2} \sum_{x=1}^N a_x \frac{c_{x\xi}}{b_{x\xi}} \prod_{i=1 \neq x}^N \frac{1}{b_{xi}} \sum_{y=1 \neq x}^N \frac{c_{\xi y}}{b_{\xi y}} \prod_{j=1 \neq x, y}^N \frac{1}{b_{jy}} \langle u_{x-1, \xi}, u_{x+1}, u_{y-1, \xi}, u_{y+1} | \mathbf{v} \rangle + \frac{1}{2} \sum_{x=1}^N a_x \frac{c_{x\xi}}{b_{x\xi}} \prod_{i=1 \neq x}^N \frac{1}{b_{xi}} \prod_{j=1 \neq x}^N \frac{1}{b_{j\xi}} \langle u_{x-1, \xi}, u_{x+1} | \mathbf{v} \rangle. \quad (\text{C10})$$

Here the property $\langle \mathbf{v} | \mathbf{u} \rangle = \langle \mathbf{u} | \mathbf{v} \rangle$ where v_j satisfy the Bethe equations and u_j is an arbitrary set of auxiliary parameters [15,16] was used.

The remaining scalar product can be evaluated using the Slavnov's formula (B18). By substituting $\xi = -i\pi/2 + \eta$ into $\langle u_{x-1, \xi}, u_{x+1} | \mathbf{v} \rangle$ in the second line of Eq. (C10) explicitly we obtain

$$\langle u_{x+1, \xi}, u_{x-1} | \mathbf{v} \rangle = \frac{i(-1)^x \prod_j^N \cosh(v_j + \eta) \prod_{j, i \neq x}^N \sinh(u_i - v_j) \det \hat{T}^{(x)}}{\prod_{j \neq x}^N \cosh(u_j - \eta) \prod_{i < j} \sinh(v_i - v_j) \prod_{i < j \neq x} \sinh(u_i - u_j)}, \quad (\text{C11})$$

where the matrix elements are

$$T_{ab}^{(x)} = T_{ab}, \quad b \neq x, \quad (\text{C12})$$

$$T_{ax}^{(x)} = \frac{\sinh(2\eta)}{\cosh(v_a - \eta) \cosh(v_a + \eta)}, \quad b = x, \quad (\text{C13})$$

and T_{ab} are given in Eq. (B19).

Substitution of the two identical $u_j = u_{j'} = \xi$ into the scalar product $\langle u_{x-1}, \xi, u_{x+1}, u_{y-1}, \xi, u_{y+1} | \mathbf{v} \rangle$ in the first line in Eq. (C10) makes the prefactor in Eq. (B18) divergent, i.e. the prefactor has a pole of the first order as a function of $(u_{j'} - u_j)$. Simultaneously, the determinant in Eq. (B18) becomes zero under the same substitution $u_j = u_{j'} = \xi$ since two lines of the matrix in Eq. (B19) becomes identical. Thus, we will derive the explicit expression for the whole scalar product by substituting $u_j = \xi$ first, then, by taking the limit $u_{j'} = \bar{\xi} \rightarrow \xi$. Expanding the matrix elements in Eq. (B19) in a Taylor series in $(\bar{\xi} - \xi)$ and using general matrix identities we obtain

$$\begin{vmatrix} \dots & & & & \dots \\ & \mathbf{A}^T & & & \\ \dots & & \dots & & \\ \mathbf{A}^T + (\beta \mathbf{A}^T + \mathbf{X}^T)(\bar{\xi} - \xi) & & & & \\ \dots & & & & \dots \end{vmatrix} = (\bar{\xi} - \xi) \begin{vmatrix} \dots & & & & \dots \\ & \mathbf{A}^T & & & \\ \dots & & \dots & & \\ & & & & \mathbf{X}^T \\ \dots & & & & \dots \end{vmatrix}, \quad (\text{C14})$$

$$\langle u_{x-1}, \xi, u_{x+1}, u_{y-1}, \xi, u_{y+1} | \mathbf{v} \rangle = (-1)^{x+y} \frac{\prod_j \cosh^2(v_j + \eta)}{\prod_{j \neq x, y} \cosh^2(u_j - \eta)} \frac{\prod_{j, j', j' \neq x, y} \sinh(u_{j'} - v_j) \det \hat{T}^{(xy)}}{\prod_{j < j'} \sinh(v_i - v_j) \prod_{j < j' \neq x, y} \sinh(u_i - u_j)}, \quad (\text{C17})$$

where the matrix elements are

$$T_{ab}^{(xy)} = \begin{cases} T_{ab}, & b \neq x, y, \\ T_{ab}^{(b)}, & b = \min(x, y), \\ \frac{\sinh 2\eta \sinh 2v_a}{\cosh^2(v_a - \eta) \cosh^2(v_a + \eta)}, & b = \max(x, y). \end{cases} \quad (\text{C18})$$

Secondly, we turn to evaluating the $-+$ correlation function. Under the substitution of Eqs. (C5) and (C6) into Eq. (C3) it reads

$$G_{-+} = \frac{1}{2} \langle \mathbf{v} | B_\xi C_\xi | \mathbf{u} \rangle. \quad (\text{C19})$$

When B_ξ is commuted through the product of C_{u_j} operators using the general result in Eq. (C9), the first step of commuting B_ξ with C_ξ introduces a divergent denominator through the commutation relation in Eq. (B6). However, the operator

$$G_{-+} = \frac{1}{2} \langle \mathbf{v} | C_\xi B_\xi | \mathbf{u} \rangle + \frac{\sinh 2\eta}{2} \lim_{\bar{\xi} \rightarrow \xi} \partial_{\bar{\xi}} (\langle \mathbf{v} | A_{\bar{\xi}} D_\xi | \mathbf{u} \rangle - \langle \mathbf{v} | A_\xi D_{\bar{\xi}} | \mathbf{u} \rangle), \quad (\text{C20})$$

where $\langle \mathbf{v} | C_\xi B_\xi | \mathbf{u} \rangle$ has already been calculated in Eq. (C10).

The remaining two correlation functions under the derivative in Eq. (C20) can be calculated by successive use of the general result of commuting A_u and D_v operators through a product of $C(u_j)$ operators in Eqs. (B10) and (B11). The scalar product of $\langle \mathbf{v} |$ with the result of the commutation procedure gives

$$\begin{aligned} \langle \mathbf{v} | A_{\bar{\xi}} D_\xi | \mathbf{u} \rangle &= a_{\bar{\xi}} \prod_{l=1}^N \frac{1}{b_{l\bar{\xi}}} \prod_{j=1}^N \frac{1}{b_{\bar{\xi}j}} \delta_{\mathbf{u}, \mathbf{v}} - \prod_{l=1}^N \frac{1}{b_{l\bar{\xi}}} \sum_{j=1}^N a_j \frac{c_{\bar{\xi}j}}{b_{\bar{\xi}j}} \prod_{l=1 \neq j}^N \frac{1}{b_{jl}} \langle u_{j-1}, \bar{\xi}, u_{j+1} | \mathbf{v} \rangle \\ &+ \sum_{j=1}^N \frac{c_{\bar{\xi}j}}{b_{\bar{\xi}j}} \prod_{l=1 \neq j}^N \frac{1}{b_{lj}} a_{\bar{\xi}} \frac{1}{b_{\bar{\xi}\bar{\xi}}} \prod_{l=1 \neq j}^N \frac{1}{b_{\bar{\xi}l}} \langle u_{j-1}, \xi, u_{j+1} | \mathbf{v} \rangle - \sum_{j=1}^N \frac{c_{\bar{\xi}j}}{b_{\bar{\xi}j}} \prod_{l=1 \neq j}^N \frac{1}{b_{lj}} \sum_{j'=1 \neq j}^N a_{j'} \frac{c_{\bar{\xi}j'}}{b_{\bar{\xi}j'}} \frac{1}{b_{j'\bar{\xi}}} \\ &\times \prod_{l=1 \neq j, j'}^N \frac{1}{b_{j'l}} \langle u_{j-1}, \xi, u_{j+1}, u_{j'-1}, \bar{\xi}, u_{j'+1} | \mathbf{v} \rangle - \sum_{j=1}^N \frac{c_{\bar{\xi}j}}{b_{\bar{\xi}j}} \prod_{l=1 \neq j}^N \frac{1}{b_{lj}} a_{\bar{\xi}} \frac{c_{\bar{\xi}\bar{\xi}}}{b_{\bar{\xi}\bar{\xi}}} \prod_{l=1 \neq j}^N \frac{1}{b_{\bar{\xi}l}} \langle u_{j-1}, \bar{\xi}, u_{j+1} | \mathbf{v} \rangle, \quad (\text{C21}) \end{aligned}$$

where

$$A_a = \frac{\sinh(2\eta)}{\cosh(v_a - \eta) \cosh(v_a + \eta)} \prod_j^N \frac{\cosh(v_j + \eta)}{\cosh(v_j - \eta)} \quad (\text{C15})$$

is the j th row of Eq. (B19) under the substitution $u_j = \xi$,

$$X_a = \frac{\sinh 2\eta \sinh 2v_a}{\cosh^2(v_a - \eta) \cosh^2(v_a + \eta)} \prod_j^N \frac{\cosh(v_j + \eta)}{\cosh(v_j - \eta)}, \quad (\text{C16})$$

is the linear coefficient in the Taylor expansion of the j 'th row of Eq. (B19) around the point $u_j = \xi$, which is not collinear with A_a in the vector space, and β is the part of the linear coefficient that is collinear with A_a .

Cancellation of the $\bar{\xi} - \xi$ from the denominator in Eq. (C14) with the $1/(\bar{\xi} - \xi)$ from the prefactor in Eq. (B18) makes the whole scalar product finite. Contributions of the orders higher than one (in the expansion of the determinant) vanish in the limit $\bar{\xi} \rightarrow \xi$ and we obtain

factor in the numerator of Eq. (B6) becomes zero at the same time making the whole expression finite. Since the divergence occurs at the first step of commuting B_ξ through a product of $N + 1$ operators $C(u_j)$, taking the limit after using Eq. (C9), as it is done in Ref. [16], creates an extra and significant computation problems: the original divergence spreads through many terms under the sum in Eq. (C9) and cancelling them explicitly is a complicated problem.

Here we will do it in a different way by canceling this intermediate divergence from the beginning in Eq. (C19). Expanding the numerator and the denominator of the commutation relation in Eq. (B6) up to the linear order in $\bar{\xi} - \xi$, where $u \rightarrow \bar{\xi}$ and $v \rightarrow \xi$ auxiliary parameters were relabeled, we cancel the $\bar{\xi} - \xi$ with $1/(\bar{\xi} - \xi)$. Then, substituting the result of this procedure in Eq. (C19) we obtain

$$\begin{aligned}
\langle \mathbf{v} | A_{\xi} D_{\bar{\xi}} | \mathbf{u} \rangle &= a_{\bar{\xi}} \prod_{l=1}^N \frac{1}{b_{l\bar{\xi}}} \prod_{j=1}^N \frac{1}{b_{\bar{\xi}j}} \delta_{\mathbf{u}, \mathbf{v}} - \prod_{l=1}^N \frac{1}{b_{l\xi}} \sum_{j=1}^N a_j \frac{c_{\bar{\xi}j}}{b_{\bar{\xi}j}} \prod_{l=1 \neq j}^N \frac{1}{b_{jl}} \langle u_{j-1}, \bar{\xi}, u_{j+1} | \mathbf{v} \rangle \\
&+ \sum_{j=1}^N \frac{c_{\bar{\xi}j}}{b_{\bar{\xi}j}} \prod_{l=1 \neq j}^N \frac{1}{b_{lj}} a_{\bar{\xi}} \frac{1}{b_{\bar{\xi}\xi}} \prod_{l=1 \neq j}^N \frac{1}{b_{\bar{\xi}l}} \langle u_{j-1}, \xi, u_{j+1} | \mathbf{v} \rangle \\
&- \sum_{j=1}^N \frac{c_{\bar{\xi}j}}{b_{\bar{\xi}j}} \prod_{l=1 \neq j}^N \frac{1}{b_{lj}} \sum_{j'=1 \neq j}^N a_{j'} \frac{c_{\bar{\xi}j'}}{b_{\bar{\xi}j'}} \frac{1}{b_{j'\xi}} \prod_{l=1 \neq j, j'}^N \frac{1}{b_{jl}} \langle u_{j-1}, \xi, u_{j+1}, u_{j'-1}, \bar{\xi}, u_{j'+1} | \mathbf{v} \rangle
\end{aligned} \tag{C22}$$

for both terms in the second line of Eq. (C20), respectively. Then, after taking the derivative of Eqs. (C21) and (C22), with respect to $\bar{\xi}$ and the limit $\bar{\xi} \rightarrow \xi$, we substitute the results in to Eq. (C20) and obtain

$$\begin{aligned}
G_{-+} &= G_{+-} + \frac{\sinh 2\eta}{2} \left[\prod_{l=1}^N \frac{1}{b_{l\xi}} \sum_{j=1}^N \sum_{l=1}^N [\tanh(u_l + \eta) - \tanh(v_l - \eta)] a_j \frac{c_{j\xi}}{b_{j\xi}} \prod_{l=1 \neq j}^N \frac{1}{b_{jl}} \langle u_{j-1}, \xi, u_{j+1} | \mathbf{v} \rangle \right. \\
&+ \sum_{j=1}^N \frac{c_{j\xi}}{b_{j\xi}} \prod_{l=1 \neq j}^N \frac{1}{b_{lj}} \sum_{j'=1 \neq j}^N a_{j'} \frac{c_{\xi j'}}{b_{\xi j'}} (\tanh(u_{j'} + \eta) - \tanh(u_j - \eta)) \frac{1}{b_{j'\xi}} \prod_{l=1 \neq j, j'}^N \frac{1}{b_{jl}} \langle u_{j-1}, \xi, u_{j+1}, u_{j'-1}, \xi, u_{j'+1} | \mathbf{v} \rangle \\
&\left. + \prod_{l=1}^N \frac{1}{b_{l\xi}} \sum_{j=1}^N a_j \frac{c_{j\xi}}{b_{j\xi}} \prod_{l=1 \neq j}^N \frac{1}{b_{jl}} \langle u_{j-1}, \xi, u_{j+1} | \mathbf{v} \rangle' \right],
\end{aligned} \tag{C23}$$

where the derivative of $\langle u_{j-1}, \bar{\xi}, u_{j+1} | \mathbf{v} \rangle$ with respect to $\bar{\xi}$ results in an additional determinant,

$$\langle u_{x-1}, \xi, u_{x+1} | \mathbf{v} \rangle' = \frac{i(-1)^j \prod_{j'}^N \cosh(v_{j'} + \eta) \prod_{j', i \neq x}^N \sinh(u_i - v_{j'}) \det \hat{T}'^{(x)}}{\prod_{j' \neq x}^N \cosh(u_{j'} - \eta) \prod_{i < j'} \sinh(v_i - v_{j'}) \prod_{i < j' \neq x} \sinh(u_i - u_{j'})}, \tag{C24}$$

where the matrix elements are

$$T_{ax}^{(x)} = \frac{2 \sinh 2\eta \tanh(v_a - \eta)}{\cosh(v_a - \eta) \cosh(v_a + \eta)} - \frac{\sinh^2 2\eta}{\cosh(v_a - \eta) \cosh(v_a + \eta)} \sum_{j=1 \neq a}^N \frac{1}{\cosh(v_j - \eta) \cosh(v_j + \eta)} \tag{C25}$$

for $b = x$ and the remaining entries for $b \neq x$ are $T_{ab}^{(x)} \equiv T_{ab}$ from Eq. (B19).

Thirdly, we evaluate the zz correlation function. Under the substitution of Eq. (C7) in Eq. (C4) it reads

$$G_{zz} = \frac{1}{4} \langle \mathbf{v} | (A_{\xi} - D_{\xi})(A_{\bar{\xi}} - D_{\bar{\xi}}) | \mathbf{u} \rangle. \tag{C26}$$

Before proceeding with the commutation procedure as in the two previous cases we rewrite the above expression in a form more convenient for such a calculation using the definition of the transfer matrix, $A_{\xi} - D_{\xi} = 2A_{\xi} - \tau_{\xi}$, and its eigenvalue $\tau_{\xi} | \mathbf{u} \rangle = \mathcal{T}_{\xi} | \mathbf{u} \rangle$,

$$G_{zz} = \frac{1}{2} \langle \mathbf{v} | A_{\xi}^2 - \mathcal{T}_{\xi} A_{\xi} - D_{\xi} A_{\xi} | \mathbf{u} \rangle, \tag{C27}$$

where $\mathcal{T}_{\xi} = \prod_j b_{j\xi}^{-1}$ is given by Eq. (B15) and we have assumed that $\langle \mathbf{v} |$ and $| \mathbf{u} \rangle$ are a pair of orthogonal eigenstates, i.e., $\langle \mathbf{v} | \mathbf{u} \rangle = 0$.

The correlation function of A_{ξ} and $A_{\bar{\xi}}^2$ can be calculated using Eq. (B10) once and twice, respectively. The scalar products of $\langle \mathbf{v} |$ with the results of the commutation procedures are

$$\langle \mathbf{v} | A_{\xi} | \mathbf{u} \rangle = - \sum_{x=1}^N a_x \frac{c_{\xi x}}{b_{\xi x}} \prod_{l=1 \neq j}^N \frac{1}{b_{xl}} \langle u_{x+1}, \xi, u_{x-1} | \mathbf{v} \rangle, \tag{C28}$$

$$\langle \mathbf{v} | A_{\bar{\xi}}^2 | \mathbf{u} \rangle = 4 \sum_{x=1}^N a_x \frac{c_{\xi x}}{b_{\xi x}} \prod_{l: l \neq x}^N \frac{1}{b_{xl}} \sum_{y: y \neq x}^N a_y \frac{c_{\bar{\xi} y}}{b_{\bar{\xi} y}} \prod_{l: l \neq x, y}^N \frac{1}{b_{xl}} \frac{1}{b_{y\xi}} \langle u_{x-1}, \xi, u_{x+1}, u_{y-1}, \xi, u_{y+1} | \mathbf{v} \rangle, \tag{C29}$$

where the scalar products on the right hand sides are already given in Eqs. (C11) and (C17) in explicit form.

Evaluation of the remaining $D_{\xi} A_{\bar{\xi}}$ correlation function involves the same problem of taking the limit $v \rightarrow u = \xi$ in commutation relation Eq. (B9), as in the calculation of the $-+$ correlation function. Here we resolve it in the same way as we have already done in evaluating Eq. (C19). Expanding the numerator and the denominator of Eq. (B9) in $v - u \rightarrow 0$ we

rewrite the $D_{\xi}A_{\xi}$ correlation function as

$$\langle \mathbf{v} | D_{\xi} A_{\xi} | \mathbf{u} \rangle = \langle \mathbf{v} | \mathcal{T}_{\xi} A_{\xi} - A_{\xi}^2 | \mathbf{u} \rangle - \sinh 2\eta \lim_{\bar{\xi} \rightarrow \xi} \partial_{\bar{\xi}} \langle \mathbf{v} | C_{\xi} B_{\bar{\xi}} - C_{\bar{\xi}} B_{\xi} | \mathbf{u} \rangle. \quad (\text{C30})$$

We use the general result in Eq. (C9) and write the $C_{\xi}B_{\bar{\xi}}$ and $C_{\bar{\xi}}B_{\xi}$ correlation functions under the derivative as

$$\begin{aligned} \langle \mathbf{v} | C_{\bar{\xi}} B_{\xi} | \mathbf{u} \rangle &= \sum_{x=1}^N a_x \frac{c_{x\xi}}{b_{x\xi}} \prod_{i=1 \neq x}^N \frac{1}{b_{xi}} \sum_{y=1 \neq x}^N d_y \frac{c_{\xi y}}{b_{\xi y}} \prod_{j=1 \neq x, y}^N \frac{1}{b_{jy}} \langle u_{x-1}, \bar{\xi}, u_{x+1}, u_{y-1}, \xi, u_{y+1} | \mathbf{v} \rangle \\ &+ \sum_{x=1}^N a_x \frac{c_{x\xi}}{b_{x\xi}} \prod_{i=1 \neq x}^N \frac{1}{b_{xi}} \prod_{j=1 \neq x}^N \frac{1}{b_{j\xi}} \langle u_{x-1}, \bar{\xi}, u_{x+1} | \mathbf{v} \rangle, \end{aligned} \quad (\text{C31})$$

$$\begin{aligned} \langle \mathbf{v} | C_{\xi} B_{\bar{\xi}} | \mathbf{u} \rangle &= \sum_{x=1}^N a_x \frac{c_{x\bar{\xi}}}{b_{x\bar{\xi}}} \prod_{i=1 \neq x}^N \frac{1}{b_{xi}} \sum_{y=1 \neq x}^N d_y \frac{c_{\bar{\xi} y}}{b_{\bar{\xi} y}} \prod_{j=1 \neq x, y}^N \frac{1}{b_{jy}} \langle u_{x-1}, \xi, u_{x+1}, u_{y-1}, \bar{\xi}, u_{y+1} | \mathbf{v} \rangle \\ &+ \sum_{x=1}^N a_x \frac{c_{x\bar{\xi}}}{b_{x\bar{\xi}}} \prod_{i=1 \neq x}^N \frac{1}{b_{xi}} \prod_{j=1 \neq x}^N \frac{1}{b_{j\bar{\xi}}} \langle u_{x-1}, \xi, u_{x+1} | \mathbf{v} \rangle. \end{aligned} \quad (\text{C32})$$

Then, taking the derivative over $\bar{\xi}$, the limit $\bar{\xi} \rightarrow \xi$, and substituting the pair of the expressions above in Eqs. (C27) and (C30), together with the expressions in Eqs. (C28) and (C29), we obtain

$$\begin{aligned} G_{zz} &= \prod_j \frac{1}{b_{j\xi}} \sum_{j=1}^N a_j \frac{c_{\xi j}}{b_{\xi j}} \prod_{l=1 \neq j}^N \frac{1}{b_{jl}} \langle u_{j+1}, \xi, u_{j-1} | \mathbf{v} \rangle + \sum_{j=1}^N a_j \frac{c_{\xi j}}{b_{\xi j}} \prod_{l=1 \neq j}^N \frac{1}{b_{jl}} \sum_{j'=1 \neq j}^N a_{j'} \frac{c_{\xi j'}}{b_{\xi j'}} \prod_{l=1 \neq j, j'}^N \frac{1}{b_{j'l}} \\ &\times \frac{1}{b_{j'\xi}} \langle u_{j-1}, \xi, u_{j+1}, u_{j'-1}, \xi, u_{j'+1} | \mathbf{v} \rangle + \frac{\sinh 2\eta}{2} \left[\sum_{x=1}^N a_x \frac{c_{x\xi}}{b_{x\xi}} \prod_{i=1 \neq x}^N \frac{1}{b_{xi}} \sum_{y=1 \neq x}^N \frac{c_{\xi y}}{b_{\xi y}} \right. \\ &\times (\tanh(u_x - \eta) + \tanh(u_y - \eta)) \prod_{j=1 \neq x, y}^N \frac{1}{b_{jy}} \langle u_{x-1}, \xi, u_{x+1}, u_{y-1}, \xi, u_{y+1} | \mathbf{v} \rangle \\ &+ \sum_{x=1}^N a_x \frac{c_{x\xi}}{b_{x\xi}} \prod_{i=1 \neq x}^N \frac{1}{b_{xi}} \prod_{j=1 \neq x}^N \frac{1}{b_{j\xi}} \left[\tanh(u_x - \eta) + \tanh(v_x - \eta) \right. \\ &\left. + \sum_{j'=1 \neq x}^N [\tanh(v_{j'} - \eta) - \tanh(u_{j'} + \eta)] \right] \langle u_{x-1}, \xi, u_{x+1} | \mathbf{v} \rangle - \sum_{x=1}^N a_x \frac{c_{x\xi}}{b_{x\xi}} \prod_{i=1 \neq x}^N \frac{1}{b_{xi}} \prod_{j=1 \neq x}^N \frac{1}{b_{j\xi}} \langle u_{x-1}, \xi, u_{x+1} | \mathbf{v} \rangle' \left. \right], \end{aligned} \quad (\text{C33})$$

where all scalar products are already given in explicit form above.

Finally, we substitute Eqs. (C10), (C23), and (C33) in Eq. (C1), rewrite the result in a more compact form by collecting similar terms, and use a general matrix identity $\det \hat{T} + \sum_{x=1}^N \det \hat{T}^{(x)} = \det(\hat{T} + \hat{X})$, where the matrix $T^{(b)}$ is obtained by substitution of the x th column from the matrix \hat{X} and rank of \hat{X} is equal to one. After constructing the corresponding matrices \hat{X} for a single sum over x and for a sum over only one variable in the double sum over x, y we obtain

$$\begin{aligned} \langle \mathbf{q} | \mathbf{S}_1 \cdot \mathbf{S}_2 | 0 \rangle &= \frac{\prod_j^N \cosh(v_j + \eta)}{\prod_{i < j}^N \sinh(v_i - v_j)} \sum_{x=1}^N (-1)^x \frac{\prod_{i, j: j \neq x}^N \sinh(u_j - v_i)}{\prod_j^N \cosh^2(u_j - \eta)} \prod_{l=1 \neq x}^N \frac{\sinh(u_l - u_x + 2\eta)}{\sinh(u_l - u_x)} \\ &\times \left[\det \hat{K}^{(x)} - \left(1 - \frac{\sinh(2\eta) \sinh \eta \sinh u_x \prod_{j: j \neq x}^N \cosh(u_j + \eta)}{\prod_{i < j \neq x}^N \sinh(u_i - u_j)} \right) \det \hat{G}^{(x)} \right] \\ &- \frac{\prod_j \cosh(u_j + \eta) \prod_j \cosh(v_j + \eta)}{\prod_j \cosh^2(u_j - \eta) \prod_{i < j} \sinh(v_i - v_j)} \det \hat{K}, \end{aligned} \quad (\text{C34})$$

where the matrix elements are

$$K_{ab} = T_{ab} + (-1)^b \frac{\sinh^3(2\eta) \sinh \eta \sinh u_b}{\cosh(u_b + \eta)} \frac{\prod_{j,i \neq b}^N \sinh(u_i - v_j)}{\prod_{i < j \neq b} \sinh(u_i - u_j)} \prod_{l=1 \neq b}^N \frac{\sinh(u_l - u_b + 2\eta)}{\sinh(u_l - u_b)} \\ \times \frac{\frac{\sinh u_b}{\cosh(u_b + \eta) \cosh \eta} + \sum_{l=1}^N [\tanh(v_l + \eta) - \tanh(u_l + \eta)]}{\cosh(v_a - \eta) \cosh(v_a + \eta)}, \quad (\text{C35})$$

$$T_{ab} = \frac{\cosh^L(v_b - \eta)}{\cosh^L(v_b + \eta)} \frac{\sinh(2\eta)}{\sinh^2(v_b - u_a)} \prod_{j=1 \neq a}^N \frac{\sinh(v_b - u_j + 2\eta)}{\sinh(v_b - u_j)} - \frac{\sinh(2\eta)}{\sinh^2(u_a - v_b)} \prod_{j=1 \neq a}^N \frac{\sinh(u_j - v_b + 2\eta)}{\sinh(u_j - v_b)}, \quad (\text{C36})$$

$$K_{ab}^{(x)} = T_{ab} + \frac{(-1)^b \sinh^3(2\eta) \operatorname{sgn}(x - b)}{\cosh(v_a - \eta) \cosh(v_a + \eta)} \prod_{l=1 \neq x, b}^N \frac{\sinh(u_l - u_b + 2\eta)}{\sinh(u_l - u_b)} \frac{\cosh(u_b + \eta) \cosh(u_x - \eta)}{\prod_i^N \sinh(u_b - v_i) \prod_{i < j \neq x, b} \sinh(u_i - u_j)} \\ \times \left(\frac{\cosh(u_b - \eta)}{\cosh(u_b + \eta)} - \frac{\sinh(u_x - u_b + 2\eta)}{\sinh(u_x - u_b - 2\eta)} + \frac{\sinh 2\eta \cosh(u_b - 2\eta) \sinh u_x}{\cosh(u_x - \eta) \cosh(u_b + \eta)} \right), \quad (\text{C37})$$

when $b \neq x$,

$$K_{ax}^{(x)} = \frac{\sinh(2\eta) \sinh(2v_a)}{\cosh^2(v_a - \eta) \cosh^2(v_a + \eta)} \quad (\text{C38})$$

when $b = x$, $G_{ab}^{(x)} = T_{ab}$ when $b \neq x$, and $G_{ax}^{(x)} = K_{ax}^{(x)}$ when $b = x$. The result in Eq. (C34) was checked numerically for $N = 2, 3$ using the direct summation over the spacial coordinates. Equations (C34)–(C37) are Eqs. (13)–(16).

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