The exact two-spinon longitudinal dynamical structure factor of the anisotropic XXZ model

Isaac Pérez Castillo
Department of Quantum Physics and Photonics, Institute of Physics,
UNAM, P.O. Box 20-364, 01000 Mexico City, Mexico and
London Mathematical Laboratory, 18 Margravine Gardens, London W6 8RH, United Kingdom

Inelastic neutron scattering experiments are commonly used to unveil how excitations on Heisenberg spin models play a role in dynamical correlations functions. For a certain class of materials, like CsCoCl$_3$ or CsCoBr$_3$ salts, it turns out that their magnetic properties are fairly well approximated by quasi-one dimensional XXZ models, which enjoy the property of quantum integrability. In these instances, one can in principle use their underlying algebraic structure to describe very precisely how excitations, the so-called spinons, participate in dynamical correlations functions. Even though the available theories (either algebraic Bethe ansatz or quantum group approach) provide all the needed physical quantities such as form factors, complete set of eigenstates and spectrum, it is typically a rather daunting task, however, to obtain sufficiently simple analytical expressions for computing Dynamical Structure Factors (DSFs), valuable, e.g., for parameters estimation based on experimental data. This is particularly the case for the longitudinal DSF of the XXZ model, which has eluded a formal mathematical treatment thus far. Using the quantum group approach, we present here an exact and simple expression of the 2-spinon longitudinal DSF and show our results to be consistent with the expected sum rules and the isotropic and Ising antiferromagnet limiting cases.

Heisenberg spin chains [1] represent a long-standing arena to introduce, test, and deeply understand seminal concepts in strongly correlated quantum systems. While the eigenstates and eigenvectors of the one-dimensional quantum spin chain with spin $S = 1/2$ have been known ever since Hans Bethe’s original work [2], it took around 60 years to get a handle on the properties of its ground state and its excitations, the so-called spinons [3]. It turned out along the way that spin $S = 1/2$ Heisenberg chains with nearest neighbor interactions and other similar models have the very attractive property of quantum integrability [4, 5]. This allows one to understand and, in principle, to control very precisely the nature of these excitations and their impact in dynamical correlation functions. While all the mathematical ingredients to obtain dynamical correlation functions such as eigenstates, eigenvalues and form factors, etc. are readily available, it turned out that correlations involving the $z$ component of the spin operator posed a very difficult task. This situation has been ignored for a while due to the fact that inelastic neutron scattering measurements of experimentally available quasi-1D Heisenberg antiferromagnets, as for instance the Ising-type materials CsCoCl$_3$ [6, 7] and CsCoBr$_3$ [8, 9], do not require the knowledge of the longitudinal DSF of the spin operator. However, recent experiments performed on Yb$_2$Pt$_2$Pb do need those formulas since, due to a strong anisotropy of the Landé $g$-factor, only the longitudinal correlation can be measured by neutron scattering [10].

The main goal of the present Letter is to present an exact and compact expression for the two-spinon contribution to the longitudinal DSF using quantum group approach and assess the correctness of our analytical findings with some expected sum rules. Our formulas are very simple and compact and may be used to draw some conclusions on whether emergent Hamiltonians for newly studied materials, such as Yb$_2$Pt$_2$Pb, are correctly captured by the XXZ model with only nearest-neighbour interactions.

As we will be using the results from the quantum group approach [11], we will directly tackle the spin $S = 1/2$ XXZ antiferromagnetic chain of infinite length given by the Hamiltonian:

$$H_{XXZ} = -J \sum_{n=-\infty}^{\infty} \left( S_n^x S_{n+1}^x + S_n^y S_{n+1}^y + \Delta S_n^z S_{n+1}^z \right),$$

where $S_n^x, S_n^y, S_n^z$ are the spin-$1/2$ operators acting on site $n$, and $\Delta$ is the anisotropy parameter. We will focus on the massive regime with $-\infty < \Delta < -1$. The limit $\Delta \to -\infty$ corresponds to the Ising antiferromagnet, around which, most of its properties can be easily calculated using perturbation theory. In particular, the excitations above the doubly degenerate ground states (Néel states) correspond to domain walls [12], i.e., spinons, which can be envisaged as solitons of unit length in the lattice space. Moreover, in the vicinity of the Ising antiferromagnetic point, domain-wall pair states are the excitations that mainly contribute to neutron scattering amplitudes [8, 13].

Within the algebraic approach of the celebrated Kyoto school [11], it is known that multi-spinon excitations, denoted as $|\{\xi\}_m\{\epsilon\}_n;i\rangle$ with $|\{\xi\}_m = \{\xi_1, \ldots, \xi_m\}$ and $|\epsilon\}_n = \{\epsilon_1, \ldots, \epsilon_m\}$, can be generated starting from the doubly degenerate ground state $|\text{vac}\rangle_{(i)}$ for given $\Delta < -1$ with $i = 0, 1$. Each spinon indexed by $j = 1, \ldots, m$ is characterised by a pair $(\xi_j, \epsilon_j)$, where the spectral parameter $\xi_j \in \mathbb{C}: |\xi_j| = 1$ lives on the complex unit circle while $\epsilon_j \in \{-, +\}$ labels the spinon’s spin orientation. The $m$ spinon excitations are exact eigenstates of the Hamiltonian, and as such also translationally invariant,

$$H_{XXZ} |\{\xi\}_m\{\epsilon\}_n;i\rangle = E(|\{\xi\}_m\{\xi\}_m;i\rangle, |\{\xi\}_m\{\epsilon\}_n;i\rangle ,$$

$$T |\{\xi\}_m\{\epsilon\}_n;i\rangle = e^{iP(|\xi\}_m\{\xi\}_m;i\rangle, |\{\xi\}_m\{\epsilon\}_n;i\rangle (1-i)\text{.}$$

Here $T$ denotes the translation operator by one lattice site, $E(|\{\xi\}_m\rangle = \sum_{j=1}^{m} \epsilon(\xi_j)$ and $P(|\{\xi\}_m\rangle = \sum_{j=1}^{m} p(\xi_j)$. Hence-

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forth, we will use an elliptic parametrization to represent spinons. We choose \( \xi = i e^{i \pi \beta / 2 K} \) with \(-K \leq \beta < K \), where \( K \equiv K(k) \) is the complete elliptic integral of the first kind. The anisotropy parameter becomes \( \Delta = - \cosh \left( \frac{\pi K'}{K} \right) \), where \( K' \equiv K(k') \), and \( k' \equiv \sqrt{1 - k^2} \) begins the complementary elliptic modulus. The spinon’s energy and momentum take the simple form:

\[
e(\beta) = I \text{dn}(\beta), \quad p(\beta) = am(\beta) + \frac{2}{\kappa} \quad (3)
\]

with \( \text{dn}(x) \equiv \text{dn}(x, k) \) and \( \text{am}(x) \equiv \text{am}(x, k) \) the usual Jacobi elliptic functions with elliptic modulus \( k \) and \( I \equiv \frac{1}{\kappa} \sinh \left( \frac{\pi K'}{K} \right) \) is the energy scale of the spinon.

The role that spinons play in dynamical spin-spin correlations can be measured experimentally by neutron scattering. We focus on the longitudinal DSF at zero temperature, which takes the following form for the infinite chain:

\[
S_{zz}^{zz}(Q, \omega) = \sum_{m = -\infty}^{\infty} \int_{-\infty}^{\infty} dt e^{i(\omega t - Q n)} \langle S_{zz}^{zz}(t) S_{zz}^{zz}(0) \rangle, \quad (4)
\]

where the bracket \( \langle \cdots \rangle \) corresponds to averaging with respect to the two ground state vacua [14]. Using the results of quantum group approach, \( S_{zz}^{zz}(Q, \omega) \) can be rewritten as a series Lehmann representation that emphasizes the physical role that the multispinon excitations play into this two-point correlation function:

\[
S_{zz}^{zz}(Q, \omega) = \sum_{m \text{ even } \geq 0} S_{zz}^{zz}_{(m)}(Q, \omega), \quad (5)
\]

where \( S_{zz}^{zz}_{(m)}(Q, \omega) \) is the contribution from transitions between the two ground states and the m-spinon states. These transitions naturally involved the form factors \( \langle \text{vac} | S_{zz}^{zz}_{(m)}(\xi) | \text{vac} \rangle \), connecting the two vacua with the m-spinon states via the \( z \) component of the spin operator. From the whole sum in Eq. (4), we will focus on the contributions \( m = 0 \) and \( m = 2 \), as they carry most of the weight of \( S_{zz}^{zz}(Q, \omega) \) for a wide range of values of the anisotropy parameter \( \Delta \), as we will see below by inspecting several sum rules.

The zeroth contribution \( S_{zz}^{zz}_{(0)}(Q, \omega) \) can be easily derived [15]. Unlike the transverse case, it is non-zero and directly related to the squared staggered static background magnetization, thus contributing at \( \omega = 0 \):

\[
S_{zz}^{zz}_{(0)}(Q, \omega) = \pi^2 \left( \frac{q_0^2 q_{\infty}^2}{q_0^2 q_{\infty}^2} \right)^4 \delta_{Q,0} \delta(\omega) \quad (6)
\]

where \( q_0 = e^{-\pi K'/K} \) is the so-called elliptic nome and the notation \( \langle \alpha; q \rangle_{\infty} \) corresponds to the \( q \)-Pochhammer symbol.

The next contribution, \( S_{zz}^{zz}_{(2)}(Q, \omega) \), comes from non-trivial transitions from the two ground states to the two-spinon continuum band. Mathematical progress in the evaluation of this term has been hindered due to the inability of evaluating an essential singularity [16] of the two-spinon form factor formula provided by [11]. Luckily, there are recent alternatives to obtain this form factor [16–19]. Thus, resolving the two-spinon continuum dispersion relation correctly [20], and after lengthy and tedious mathematical manipulations [14], we are able to obtain the following simple exact expression of the two-spinon longitudinal DSF:

\[
S_{zz}^{zz}_{(2)}(Q, \omega) = \sqrt{q_0 k} \frac{\omega^2 + \kappa \omega_B^2 + B}{\omega_B} \sum_{\sigma = \pm 1} \frac{1 + \sigma \cos(Q)}{W_{\omega}} \times \quad (7)
\]

\[
\frac{\sigma_2^2(\beta^{(\sigma)})}{\sigma_2^2(\beta^{(\sigma)})} \frac{\omega^2 - \sigma(B - \kappa \omega_B^2)}{|\Delta| - \sigma \cos \left( \frac{\pi K'}{2} \right)} \left[ 1 - \kappa \delta_{\sigma, +} + \delta_{\sigma, -} \right] \tilde{I}_{Q}(\omega) \in C_{\sigma}(Q, \omega). \]

The expression provided by Eq. (7) is the main result of the present Letter. Here, the support of the DSF is given by the indicator function \( \tilde{I}_Q(\omega) \in C_{\sigma}(Q, \omega) \), equal to 1 if the point \( (Q, \omega) \) lies within the continuum sheet \( C_{\sigma}(Q, \omega) \), and 0 otherwise. These two sheets for \( \sigma \in \{-1, +1\} \) result from the overlapping of a two-spinon dispersion relation band with another one shifted by \( \pi \), everything modulus \( 2\pi \). As a result, the lower and upper boundaries of the sheet \( C_{\sigma}(Q, \omega) \) are given by [20, 21]:

\[
\Omega_{lo}(Q) = \left\{ \begin{array}{ll} 0 & Q \in [Q_\kappa, \pi - Q_\kappa], \\ \omega_+(Q) & Q \in [\pi - Q_\kappa, \pi], \end{array} \right. \quad (8)
\]

\[
\Omega_{up}(Q) = \omega_-(Q), \quad Q \in [Q_\kappa, \pi], \quad (9)
\]

respectively, with the definitions [using Eq. (3)]:

\[
\kappa = \frac{1 - k'}{1 + k'}, \quad Q_\kappa = a \cos(\kappa),
\]

\[
\omega_\pm(Q) = \frac{\pi K'}{4 + \kappa^2} \left( 1 \mp 2 \kappa \cos(Q) \right), \quad (10)
\]

\[
\omega_0(Q) = \frac{2\pi}{4 + \kappa^2} \sin(Q). \quad \]

The continuum sheet \( C_{-}(Q, \omega) \) is simply the sheet \( C_{\sigma}(Q, \omega) \) reflected around \( \pi/2 \). The expression for \( \beta^{(\sigma)}_\omega \) in Eq. (7) comes from solving the two-spinon dispersion relation and takes the following form [14, 20, 21]:

\[
\beta^{(\sigma)}_\omega(Q, \omega) = \text{dn}^{-1} \left( \frac{1 + \sigma \cos(Q)}{|\sin(Q)|} \sqrt{\omega^2 - \kappa^2 \omega_B^2(Q) + B \omega^2 \omega_B^2(Q) - B}, k \right), \quad (11)
\]

while the functions \( B \equiv B(Q, \omega) \) and \( W_{\sigma} \equiv W_{\sigma}(Q, \omega) \) also appearing in Eq. (7) read

\[
B(Q, \omega) = \sqrt{\omega^2 - \kappa^2 \omega_B^2(Q)} \sqrt{\omega^2 - \omega_0^2(Q)} \quad (12)
\]

\[
W_{\sigma}(Q, \omega) = \frac{\kappa^2 \omega_0(Q)}{\omega} - \left( \frac{B(Q, \omega)}{\omega} + \sigma \cos(Q) \right)^2,
\]

respectively. Finally, \( \vartheta_\Delta(\beta^{(\sigma)}_\omega) \) refers to Neville’s theta function while the function \( \vartheta_2^2(\beta) \) reads

\[
\vartheta_2^2(\beta) \equiv \exp \left[ - \sum_{k = 1}^{\infty} \frac{e^{2\kappa_0 k / \kappa}}{\kappa_0} \cosh(2\kappa_0 k / \kappa) \cos(2\kappa_0 k / \kappa) - 1 \right], \quad (13)
\]

with \( \epsilon = \frac{\pi K'}{K} \).
To make sure that formula (7) is correct, we have carried out a number of checks. First of all, one can show that the asymptotic expansion of Eq. (7) close to the Ising antiferromagnetic point are consistent with the perturbation theory results provided in [13]. Similarly, one can perform the isotropic limit $\Delta \to -1$ to recover the previously known result [22] for the isotropic case. Alternatively, one can use the results of [23] for the massless regime and take the isotropic limit.

Secondly, to further assess the correctness of our formula we have analysed several well-known sum rules for dynamical spin-spin correlation functions [24, 25]. For simplicity, we will solely focus on the total integrated intensity and the first frequency moment sum rules, which are given by:

$$a(\Delta) \equiv \int_0^\infty d\omega \int_0^{2\pi} dQ Q S^{zz}(Q,\omega) = \frac{1}{3},$$

$$g(Q, \Delta) \equiv \int_0^\infty d\omega \omega S^{zz}(Q,\omega) = -2J F_x (1 + \cos Q),$$

respectively. Here $F_x = \langle S^x_{i} S^x_{i+1} \rangle$ is the nearest neighbor static correlation function for which an exact formula is known [26]. Let us denote as $a_{(m)}(\Delta)$ and $g_{(m)}(Q, \Delta)$ the $m$-spinon contribution to each of the above two sum rules.

Let us start discussing the total integrated intensity sum rule $a(\Delta)$. This comparison is shown in Fig. 2, where we plot the various contributions of the total integrated intensity as a function of $-\Delta$. More precisely, the blue solid line corresponds to the zeroth contribution $a_{(0)}(\Delta)$, which is Baxter’s formula for the contribution to the staggered magnetization. Similarly, the solid orange line shows $a_{(2)}(\Delta)$ coming from the theory, while the solid green line represents the sum of both contributions. We can conclude that the two-spinon contribution carries most of the weight of the DSF for values of $\Delta \lesssim -2$, as they saturated to the value 1/4 (shown in the figure by a solid red line) of this sum rule, while when approaching the isotropic case for $-2 \lesssim \Delta \leq -1$ higher spinon excitations start contributing. This comparison with the sum rule demonstrates the correctness of our formula.

Next, we compare the first frequency moment sum rule $g(Q, \Delta)$ between theory and the exact formula in Fig. 3 as a function of the total momentum $Q$ and for three values of the anisotropy parameter $\Delta$. The dashed line shows the exact complete result for $g(Q, \Delta)$ [Eq. (15)], while the solid lines with matching colors correspond to the analytical result for $g_{(2)}(Q, \Delta)$. Similar to Fig. 2, they agree fairly well for $\Delta \lesssim -2$ where the zeroth and two-spinon contribution dominates the DSF. Note, in particular, that the value of $g_{(2)}(Q, \Delta)$ tends to zero as we approach the Ising antiferromagnetic point. This is expected since, at this point, there is no dynamics associated to the $z$-component of the spin operator.
since Heisenberg’s introduction of the model, to obtain a correct formula for the two-spinon contribution to the transverse DSF [20] and an extra 12 years to obtain a similar formula for its longitudinal counterpart. Hopefully, with the methods developed here more rapid advancement can be achieved on other interesting observables in order to arrive to a more complete description of this fascinating model.

IPC thanks hospitality of Brookhaven National Laboratory and acknowledges discussions, interests and help with the manuscript to Andreas Weichselbaum, Igor Zalykniak and J.S Caux. He also acknowledges partial financial support from funding UNAM-DGAPA-PAPIIT-IN106219.

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