Computation of Dynamical Correlation Functions of Heisenberg Chains in a Magnetic Field

Jean-Sébastien Caux[1] and Jean Michel Maillet[2]
[1]Institute for Theoretical Physics, University of Amsterdam, 1018 XE Amsterdam, The Netherlands
[2]Laboratoire de Physique, École Normale Supérieure de Lyon, 69364 Lyon, France
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We compute the momentum- and frequency-dependent longitudinal spin structure factor for the spin-1/2 *XXZ* Heisenberg spin chain in a magnetic field, using exact determinant representations for form factors on the lattice. Multiparticle (i.e., multispinon) contributions are computed numerically throughout the Brillouin zone, yielding saturation of the sum rule to high precision.

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Exact solutions of quantum models, either on the lattice or in the continuum, are invaluable in the study of nonperturbative aspects of low-dimensional physics. Bethe's construction of the full set of eigenstates of Heisenberg's spin exchange model [1], by the method today known as the Bethe ansatz [2], has ultimately led to a wide variety of exact results on the thermodynamics of integrable models, with a broad spectrum of applications [3,4].

A long-standing limitation of the Bethe ansatz was that the dynamics of such models was not directly accessible. In recent years, however, enormous progress has been made for correlation functions of the Heisenberg spin chain [5–7]. In particular, matrix elements of any local operator between two Bethe states can now be written as matrix determinants [6]. Combined with formulas for eigenstate norms [8], this yields exact expressions for form factors on the lattice, thereby opening the door to the computation of dynamical correlation functions.

In this Letter, we implement this program for one of the cornerstones of the theory of integrable models, the anisotropic Heisenberg chain in a magnetic field:

$$H = J\sum_{j=1}^{N}\left[S_j^xS_{j+1}^x + S_j^yS_{j+1}^y + \Delta\left(S_j^zS_{j+1}^z - \frac{1}{4}\right) - hS_j^z\right] \tag{1}$$

with periodic boundary conditions. The anisotropy parameter Δ will be chosen to lie in the gapless regime $-1 < \Delta \leq 1$, and therefore the model provides a well-controlled realization of quantum critical behavior.

Our interest lies in space- and time-dependent spin correlation functions. We numerically compute the longitudinal dynamical spin structure factor, defined as the Fourier transform of the spin-spin correlation function:

$$S^{zz}(q,\omega) = \frac{1}{N}\sum_{j,j'=1}^{N} e^{iq(j-j')}\int_{-\infty}^{\infty} dt e^{i\omega t}\langle S_j^z(t)S_{j'}^z(0)\rangle_c, \tag{2}$$

where the subscript c means that we take the connected part $\langle S^zS^z\rangle - \langle S^z\rangle^2$. This quantity has broad applicability, from the quantitative description of neutron scattering data [9–12] to the theory of entanglement [13].

Two-particle contributions to correlators for the isotropic Heisenberg chain in a field were studied at fixed momentum q in [14], and for *XXZ* at zero field at $q = \pi$ in [15], and at $q = \pi/2$ in [16]. In particular, this allowed (at low energies) for a numerical check of conformal scaling exponents [2] to an impressive degree of accuracy. Here, we present results for all momenta, including multiparticle contributions. This yields data beyond the reach of field theory, allows us to quantify the accuracy of our results via the sum rule, and also opens the door to computing space- and time-dependent correlators. Such multiparticle contributions should also allow better fits to neutron scattering data for the continua and intensities (e.g., in [10]) than presently existing fits.

The exact solution through the Bethe ansatz for model (1) is well known [2]. The reference state is taken to be the state with all spins up, $|0\rangle = \otimes_{i=1}^N|\uparrow\rangle_i$. The Hilbert space separates into subspaces of fixed magnetization, determined from the number of reversed spins M. We take the number of sites N and of reversed spins M to both be even. Eigenstates in each subspace are completely determined for $2M \leq N$ by a set of rapidities $\{\lambda_j\}$, $j = 1,\ldots,M$, solution to the Bethe equations

$$\arctan\left[\frac{\tanh(\lambda)}{\tan(\zeta/2)}\right] - \frac{1}{N}\sum_{k=1}^{M}\arctan\left[\frac{\tanh(\lambda-\lambda_k)}{\tan\zeta}\right] = \pi\frac{I_j}{N}, \tag{3}$$

where $\Delta = \cos\zeta$. Each choice of a set of distinct half-integers $\{I_j\}$, $j = 1,\ldots,M$ [with I_j defined mod(N)] uniquely specifies a set of rapidities, and therefore an eigenstate. The energy and momentum of a state are

$$\begin{aligned} E &= J\sum_{i=1}^{M}\frac{-\sin^2\zeta}{\cosh 2\lambda_i - \cos\zeta} - h\left(\frac{N}{2} - M\right), \\ q &= \pi M + \frac{2\pi}{N}\sum_{i=1}^{M} I_i \bmod 2\pi. \end{aligned} \tag{4}$$

The ground state is given by $I_j^0 = -\frac{M+1}{2} + j$, $j = 1,\ldots,M$.

In terms of form factors, the structure factor can be written as a sum over matrix elements of the Fourier transform of the spin operators, $S_q^z = \frac{1}{\sqrt{N}}\sum_j e^{iqj}S_j^z$:

$$S^{zz}(q,\omega) = 2\pi \sum_{\alpha\neq 0} |\langle 0|S_q^z|\alpha\rangle|^2 \delta(\omega - \omega_\alpha) \qquad (5)$$

over the whole set of eigenstates (distinct from the ground state) in the fixed M subspace. Each term in (5) can be obtained [6] as a product of determinants of M-dimensional matrices, fully determined for a given eigenstate by a knowledge of the corresponding set of rapidities. For the sake of brevity we do not reproduce the expressions for these matrices here.

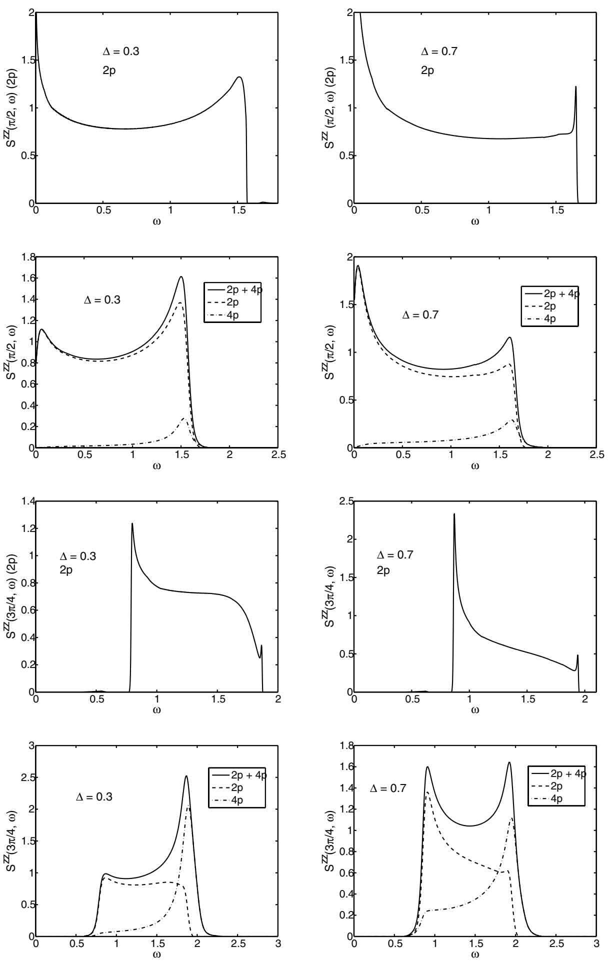

FIG. 1. Constant momentum q slices of the structure factor as a function of frequency ω, at $q = \pi/2$ and $3\pi/4$, for XXZ with $\Delta = 0.3$ and $\Delta = 0.7$ at $M = N/4$. $2p$ denotes two-particle contributions, while $4p$ denotes four-particle contributions. Resulting curves are extrapolations to infinite size from $N = 4096$ ($2p$) and 384 ($2p + 4p$) (note that since the δ functions in Eq. (5) are broadened to width $\log N/N$, the two-particle peaks appear sharper in the $2p$-only graphs than in the $2p + 4p$ ones). $2p$ contributions carry most of the weight at $q = \pi/2$, but $4p$ ones become comparable at $q = 3\pi/4$.

Obtaining the spin structure factor involves three steps: scanning through the eigenstates, solving the Bethe equations, and computing the determinants. Since the contributions are rapidly decreasing functions of the number of particles (spinons) involved, one can attain a high degree of precision. Leading contributions to the structure factor come from even numbers of one-particle excitations, for which there is one hole in the distribution of I's in the interval corresponding to the ground state. Four- and six-particle contributions are those with two and three holes in the distribution of the I's. It is well known that the Bethe equations (3) can also yield complex rapidities in the form of strings (bound states). This leads to reductions in the determinants (we will publish the formulas elsewhere). Such contributions are found to be strongly suppressed.

We present results for two cases: $\Delta = 0.3$, and $\Delta = 0.7$, both with $M = N/4$. We give two slices of $S^{zz}(q,\omega)$ at $q = \pi/2, 3\pi/4$ as a function of ω in Fig. 1, including contributions from up to four particles (six-particle and bound-state contributions are too small). We give density plots for the whole region $q \in [0, \pi]$ in Fig. 2, including up to six-particle contributions. In all cases, we use Eq. (5) where we broaden the δ functions to width $\log N/N$ to obtain smooth curves. The gapped regime $|\Delta| > 1$, relevant to experiments on $CsCoCl_3$ [17], and the isotropic case $\Delta = 1$ are

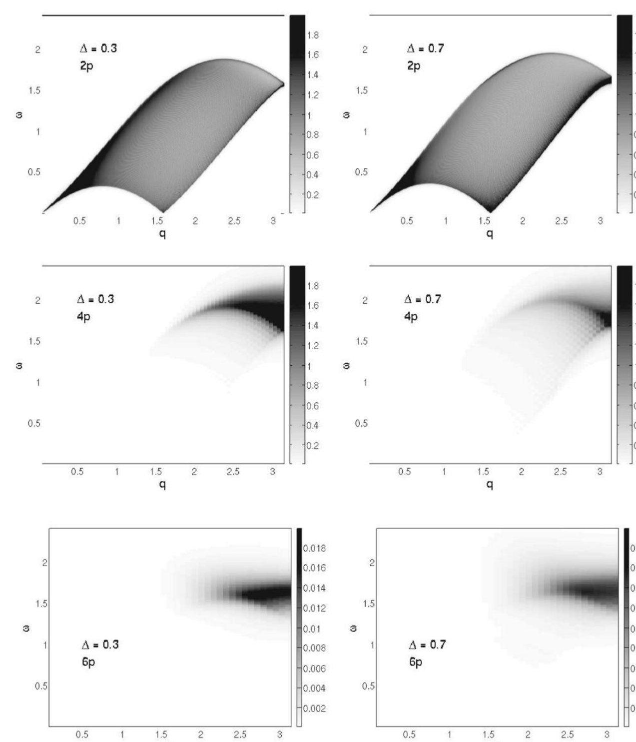

FIG. 2. Longitudinal structure factor as a function of momentum q and frequency ω, for $\Delta = 0.3$, and $\Delta = 0.7$ at $M = N/4$. Two-, four-, and six-particle contributions (labeled $2p$, $4p$, and $6p$) are plotted for system sizes $N = 768$, 128, and 80, respectively.

TABLE I. Contributions of two-, four-, and six-particle sectors to the sum rule for $\Delta = 0.3$ (%).

N	$2p$	$4p$	$6p$	Total
768	70.29			70.3
128	78.86	20.25		99.11
80	82.17	17.52	0.23	99.92

TABLE II. Contributions of two-, four-, and six-particle sectors to the sum rule for $\Delta = 0.7$ (%).

N	$2p$	$4p$	$6p$	Total
768	69.85			69.85
128	81.43	17.17		98.60
80	85.19	14.02	0.28	99.49

also accessible with this method. We will present all these results elsewhere.

Computing the structure factor for all momenta allows us to check the saturation of the sum rule

$$\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{1}{N} \sum_q S^{zz}(q, \omega) = \frac{1}{4}\left[1 - \left(1 - \frac{2M}{N}\right)^2\right] \equiv C. \quad (6)$$

For $M = N/4$, the sum rule requires $C = 0.1875$.

We compute two-particle contributions up to $N = 768$, and four- and six-particle ones up to 128 and 80, respectively. Two-particle contributions monotonically decrease with system size, while four- and six-particle ones first increase, then decrease, due to interplay between the finite-size gap and state counting. The contribution to the sum rule from states with one 2-string and two holes is computed up to $N = 256$, and yields only $4.4 \times 10^{-7}\%$ for $\Delta = 0.3$, and $3.0 \times 10^{-7}\%$ for $\Delta = 0.7$. Results are presented in Tables I and II. Two-particle terms account for about 70% of the sum rule, similar to the 72.89% result computed for the thermodynamic limit of the isotropic chain in zero field using quantum affine symmetry [18,19]. Including four-particle states gives around 99% of the sum rule for 128 sites, and including up to six-particle states goes well over 99% for 80 sites. We can estimate the relative contributions for infinite size: for example, for $\Delta = 0.3$, and extrapolating from $N = 256, 512, 768$, two-particle contributions should yield $66\% \pm 1\%$ of the sum rule. Four-particle contributions, from data for $N = 64, 96, 128$, should yield $37\% \pm 7\%$ while six-particle ones should yield $0.8\% \pm 0.2\%$ from data for $N = 48, 64, 80$.

In summary, we have numerically obtained dynamical correlation functions of integrable models on the lattice using determinant representations for form factors, in the fundamental case of the anisotropic Heisenberg chain in a field. We have shown that by including multiparticle contributions, the sum rule can be saturated to very high precision.

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