Static Structure Factors of the XXZ-Model in the presence of a uniform field

M. Karbach, K.-H. Mütter and M. Schmidt

Physics Department, University of Wuppertal
42097 Wuppertal, Germany

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The static structure factors of the XXZ model in the presence of uniform field are determined from an exact computation of the groundstates at given total spin on rings with \( N = 4, 6, \ldots, 28 \) sites. In contrast to the naive expectation a weak uniform field strengthens the antiferromagnetic order in the transverse structure factor for the isotropic case.

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I. INTRODUCTION

The antiferromagnetic properties of the one-dimensional spin 1/2 XXZ-model with Hamiltonian:

\[
H = 2 \sum_{x=1}^{N} [S_1(x)S_1(x+1) + S_2(x)S_2(x+1) + \cos \gamma S_3(x)S_3(x+1)]
\] (1.1)

have been studied by analytical and numerical methods. The critical exponents \( \eta_j, j = 1, 3 \), which govern the large distance behavior of the spin-spin correlators in the groundstate:

\[
\langle 0| S_j(0)S_j(x)|0 \rangle \rightarrow \frac{(-1)^x}{x^{\eta_j}}, \quad j = 1, 3,
\]

are given by:

\[
\eta_1 = \eta_3^{-1} = 1 - \frac{\gamma}{\pi} \quad \text{for} \quad 0 < \gamma < \pi.
\]

At finite temperature \( T \) the spin-spin correlators decrease exponentially with a rate given by the inverse correlation length:

\[
\xi^{-1}(\gamma, T) \rightarrow \Phi(\gamma) \cdot T^\nu,
\]

with a critical exponent:

\[
\nu = 1,
\]

independent of \( \gamma \) and:

\[
\Phi(\gamma) = \frac{\gamma}{\sin \gamma} \left( 1 - \frac{\gamma}{\pi} \right).
\]

It has been shown in Ref. 3 that the structure factors:

\[
S_j(\gamma, p = 2\pi k/N, T, N) = 1 + (-1)^k 4 \langle 0| S_j(0)S_j(N/2)|0 \rangle + 8 \sum_{x=1}^{N/2-1} \langle 0| S_j(0)S_j(x)|0 \rangle \cdot \cos(px),
\]

1
are most suited to extract the critical behavior from finite systems. In Refs. [3,4] we have studied the static structure factors in the following three limits:

\[ p = \pi, \quad T = 0, \quad N \to \infty, \]

\[ p \to \pi, \quad T = 0, \quad N = \infty, \]

\[ p = \pi, \quad T \to 0, \quad N = \infty. \]

The transverse and longitudinal structure factors have a common form in each of these limits:

\[ S_j(\gamma, y_a) = r_j(\gamma) \frac{\eta_j(\gamma)}{\eta_j(\gamma)} - 1 \left(1 - y_a^{1-\eta_j(\gamma)}\right), \quad a = p, T, N, \tag{1.2} \]

where:

\[ y_N \equiv \frac{N}{N_j(\gamma)}, \quad y_p \equiv \frac{\pi - p_j(\gamma)}{\pi - p}, \quad y_T \equiv \frac{\xi(\gamma, T)}{\xi_j(\gamma)}, \]

are the “running variables”. The common form reflects the fact that the structure factors scale in the critical regime:

\[ p \to \pi, \quad T \to 0, \quad N \to \infty, \tag{1.3} \]

if we keep fixed:

\[ z_1 \equiv \left(1 - \frac{p}{\pi}\right) N, \quad z_2 \equiv \frac{N}{\xi(\gamma, T)}. \tag{1.4} \]

The antiferromagnetic properties of the model become visible in the singularities of the structure factors in the limit \( \xi \). The transverse structure factors are infinite in this limit; they develop a “hard” singularity. In contrast, the longitudinal structure factors stay finite. Their critical behavior is hidden in subleading terms which produce a “soft” singularity. Away from the critical regime \( \xi \) the antiferromagnetic properties are lost.

There are further possibilities to destroy antiferromagnetic ordering – e.g. by a uniform external field \( h \) or by frustration – i.e. by switching on a next-to-nearest neighbor interaction. In this paper we are going to study the effect of a uniform magnetic field on the zero temperature structure factors. For this purpose we have determined the static structure factors in the groundstates \( |S_3\rangle \) of the Hamiltonian \( (1.1) \) at given total spin \( S_3 \). The groundstates were computed with a Lanczos algorithm on rings with \( N = 4, 6, ..., 28 \) sites.

We will discuss the static structure factors as function of the magnetization \( M = S_3/N \). The known magnetization curve translates \( M \) into the fieldstrength \( h \). For convenience, we list in Table I the \( h \)-field values corresponding to our \( M \)-values:

| \( M \) \( h(\gamma = 0) \) | \( h(\gamma = 0.1\pi) \) | \( h(\gamma = 0.2\pi) \) | \( h(\gamma = 0.5\pi) \) |
|----------------|----------------|----------------|----------------|
| 0.96 | 0.93 | 0.83 | 0.38 |
| 1.20 | 1.17 | 1.06 | 0.50 |
| 1.59 | 1.54 | 1.41 | 0.71 |
| 1.83 | 1.78 | 1.64 | 0.87 |
| 1.91 | 1.86 | 1.72 | 0.92 |
| 2.00 | 1.95 | 1.81 | 1.00 |

The outline of the paper is as follows. In Sections II and III we discuss the characteristic features of the longitudinal structure factors as there are the \( p \) and \( M \) dependence and the finite-size effects. The same is done for the transverse structure factors in sections IV and V.
II. THE LONGITUDINAL STRUCTURE FACTORS AT FIXED MAGNETIZATION

The longitudinal structure factor of the XX-model ($\gamma = \pi/2$) is known from the exact solution obtained by Niemeijer in the fermion representation:

$$S_3(\gamma = \pi/2, p, M, N) = \frac{2}{\pi} \sum p \begin{cases} p & \text{for } 0 \leq p \leq p_3(M) \\ p_3(M) & \text{for } p_3(M) \leq p \leq \pi, \end{cases}$$

where

$$p_3(M) \equiv \pi(1 - 2M).$$

Though the result of Ref. 8 has been derived for the thermodynamical limit $N \to \infty$, (2.1) turns out to be correct for all system sizes with $N = 4, 6, 8, \ldots$. The linear behavior in $p$ has been found before for the case $M = 0$.

Let us next turn to the isotropic case $\gamma = 0$. Fig. 1 presents a panoramic view on the longitudinal structure factor with $N = 20, 22, \ldots, 28$. The emergence of the singularity at $p = \pi, M = 0$ is clearly visible. Along the momentum axis at $M = 0$ we see the logarithmic singularity:

$$S_3(\gamma = 0, p, M = 0) = r_3(0) \cdot \ln \left(1 - \frac{p}{\pi}\right),$$

discussed in Ref. 9. Along the magnetization axis:

$$p = p_0 \equiv \pi, \quad M = S_3/N \to 0,$$

we observe a logarithmic singularity in $M$. The same type of singularity is also found in the limit:

$$p = p_3(M), \quad M \to 0,$$

where $p_3(M)$ is given in (2.2). The longitudinal structure factor has its maximum at $p = p_3(M)$, $M$ fixed. With increasing strength of the uniform field the maximum position moves from $p = \pi$ to $p = 0$ – i.e. from antiferromagnetic to ferromagnetic order. Such a behavior has been conjectured by Müller et al.. Indications for this have been found also by Parkinson and Bonner and Ishimura and Shiba on small systems ($N \leq 14$). Johnson and Fowler were able to reformulate the isotropic Heisenberg model for large spins and magnetizations close to saturation in terms of a gas of magnons. By accident their prediction for the longitudinal structure factor in the limit $M \to 1/2$ is identical with the exact result (2.1) for the XX-model. In Fig. 2 we compare the longitudinal structure factors for $\gamma = 0$ and $\gamma = \pi/2$ at $M = 1/4$ and $M = 1/3$. For $M = 1/3$ the structure factors almost coincide. For smaller $M$ values, however, the isotropic structure factor deviates from (2.1). The cusp along the line (2.2) becomes more pronounced with decreasing values of $M$.

Looking at the finite-size effects which will be analyzed in the next section we find an $N^{-2}$ behavior away from the cusp and a slower decrease $N^{-\delta_3}$ with $\delta_3 \approx 0.5$ at the cusp $p = p_3(M)$. The change in the finite-size behavior signals the emergence of a nonanalytic behavior in the thermodynamical limit.

We have also determined the longitudinal structure factors for the anisotropies $\gamma/\pi = 0.1, 0.2$. The $p-M$ dependence of the longitudinal structure factor looks similar to the isotropic case. Instead of an infinity we find a peak at $p = \pi, M = 0$. In the limit $p \to \pi, M = 0$ the structure factor is adequately described by (1.2) with $a = p$. In the limit $M \to 0, p = \pi$ we find again a behavior of the form (1.2) with a running variable:

$$y_M = \frac{M}{M(\gamma)}.$$

The appearence of the cusp along the line $p = p_3(M)$ is indeed independent of the anisotropy parameter $\gamma$. For increasing values of $\gamma$ the cusp is less pronounced.

III. FINITE SIZE ANALYSIS OF THE LONGITUDINAL STRUCTURE FACTOR

In the critical regime

$$p \to \pi, \quad N \to \infty, \quad M = \frac{S_3}{N} \to 0, \quad T \to 0,$$
we expect the longitudinal structure factors to obey finite-size scaling:

\[
S_3(\gamma, p, M = S_3/N, T, N) = g_3(\gamma; z_1, z_2, z_3) \cdot S_3(\gamma, p, M, T, N = \infty)
\]  

In the combined limit \((3.1)\) we have to keep fixed \(z_1, z_2\) - defined in \((1.4)\) - and:

\[ z_3 \equiv M \cdot N = S_3. \]

In Ref. 4 we checked finite-size scaling in the combined limit:

It was found that finite-size scaling works for the transverse structure factors at all \(\gamma\) values. In contrast, finite-size scaling breaks down for the longitudinal structure factors, if \(\gamma > 0.3\pi\).

In this section we are going to study consequences of the ansatz \((3.2)\) in the limits \((2.4), (2.5)\) at zero-temperature. So far our estimates of the thermodynamical limit are restricted to magnetizations \(M \neq 0\), \(\pi\) (for \(M = 0\), \(\pi\)) and are linear in \(-p\) but rather large for \(p = \pi\). The extrapolations of the structure factors to the thermodynamical limit are represented by the solid dots in Fig. 3. Finite-size effects are small for \(p_0 = \pi\) but rather large for \(p_3 = \pi(1 - 2M)\). We have studied the finite-size effects in the differences:

\[
\Delta_j(\gamma, M, N) = S_3(\gamma = 0, p_j, M, N) + \ln(2M), \quad j = 0, 3,
\]

at fixed magnetizations:

\[
M = \begin{cases} 
\frac{1}{15}, \frac{2}{15} : & N = 8, 16, 24 \\
\frac{1}{15} : & N = 4, 8, 12, 16, 20, 24, 28 \\
\frac{1}{15}, \frac{2}{15} : & N = 6, 12, 18, 24, 
\end{cases}
\]

which can be realized on the systems with size \(N\). The \(N\)-dependence of the difference \((3.3)\) can be parametrized by:

\[
\Delta_0(\gamma, M, N) = \Delta_0(\gamma, M) + c_0(\gamma, M) \cdot N^{-2}, \quad \Delta_3(\gamma, M, N) = \Delta_3(\gamma, M) + c_3(\gamma, M) \cdot N^{-3}, \quad \delta_3 \approx 0.5.
\]

In our finite-size analysis we have included as well the magnetizations:

\[
M = \begin{cases} 
\frac{1}{10}, \frac{2}{10} : & N = 10, 20 \\
\frac{1}{10}, \frac{5}{12} : & N = 12, 24 \\
\frac{1}{10}, \frac{3}{11}, \frac{4}{11}, \frac{5}{11}, \frac{6}{11} : & N = 14, 28, 
\end{cases}
\]

which occur on two systems. Here we have assumed that the finite-size dependence is described correctly by \((3.4)\). The extrapolations of the structure factors to the thermodynamical limit are represented by the solid dots in Fig. 4.

So far our estimates of the thermodynamical limit are restricted to magnetizations \(M \geq 1/14\) due to the finiteness of our systems \(N \leq 28\). Additional information on the structure factors for \(M\)-values:

\[
M = \frac{1}{N}, \quad N = 14, 16, ..., 28,
\]

closer to the critical point \(M = 0\) can be obtained if finite-size scaling \((3.3)\) holds for the longitudinal structure factors in the limits \((2.4), (2.5)\) where we keep fixed \(z_3 = S_3\). This variable is just 1 for the sequence \((3.2)\), and we can compute the scaling function at this value from:

\[
g_j(\gamma, z_3) \bigg|_{z_3=1} = \frac{S_3(\gamma = 0, p = p_j, M = 1/14, N = 14)}{S_3(\gamma = 0, p = p_j, M = 1/14, N = \infty)}.
\]

In this way we get from the finite-size scaling ansatz \((3.1)\) in the limits \((2.4), (2.5)\) an estimate of the thermodynamical limit of the structure factors:

\[
\frac{S_3(\gamma = 0, p = p_j, M = 1/14, N = 14)}{S_3(\gamma = 0, p = p_j, M = 1/14, N = \infty)}.
\]
\[ S_3(\gamma = 0, p = p_j, M, N = \infty) = \frac{S_3(\gamma = 0, p = p_j, M = 1/N, N)}{g_j(\gamma, 1)}, \quad j = 0, 3, \quad (3.6) \]

for the sequence of \( M \) values in (3.3). The result for the differences (3.4) is marked by the open dots in Figs. 4(a),(b).

We have repeated the finite-size analysis – described above for the isotropic case – for: \( \gamma/\pi = 0.1, 0.2 \). The resulting estimate of the thermodynamical limit:

\[ \Delta_j(\gamma, M, N = \infty) = S_3(\gamma, p_j, M, N = \infty) - L_3(\gamma, M), \quad j = 0, 3, \]

versus the variable:

\[ L_3(\gamma, M) = -\frac{\eta_3(\gamma)}{\eta_3(\gamma) - 1} \left( 1 - (2M)^{1-\eta_3(\gamma)} \right), \]

is represented in Figs. 4(a),(b) by the triangles and squares, respectively.

**IV. THE TRANSVERSE STRUCTURE FACTORS AT FIXED MAGNETIZATION**

The most remarkable property of the transverse structure factor is its approximate constancy:

\[ S_1(\gamma, p, M, T = 0, N) \approx 2M, \quad \text{for} \quad 0 \leq p \leq 2\pi M, \quad (4.1) \]

which has been found by Müller et al. on small systems for the isotropic case \( \gamma = 0 \). For \( S_3 = MN = N^2/2 - 1 \) can be easily proven to be exact by means of the Bethe ansatz solution. For \( S_3 < N^2/2 - 1 \) and \( 0 < p \leq 2\pi M \), however, (4.1) is not exact. As an example we present in Figs. 5(a),(b) the momentum dependence of \( S_1 \) at \( M = 1/4, 1/3, 1/2 \), \( N = 8, 12, \ldots, 28 \) for \( \gamma = \pi/2 \) and \( \gamma = 0 \), respectively. The constancy in the regime \( p \leq 2\pi M \) is striking. Deviations from (4.1) can be seen on a scale magnified by a factor 100 in the inset of Figs. 5(a),(b). These deviations follow a single scaling curve which increases monotonically with momentum \( p \). On the scaling curve finite-size effects die out with \( N^{-2} \). At \( p = 2\pi M \), however, significant finite-size effects of the order \( N^{-\delta_1} \) with \( \delta_1 \approx 1.0 \) for \( \gamma = 0 \) and \( \delta_1 \approx 1.3 \) for \( \gamma = \pi/2 \) become apparent.

Beyond the regime (4.1) the transverse structure factor of the XX-model \( (\gamma = \pi/2) \) is linear in \((1 - p/\pi)^{-1/2}\), as can be seen from Fig. 5(a). Therefore we find the same type of singularity for \( p \to \pi \) at \( M = 0, 1/4, 1/3 \). In contrast to the naive expectation antiferromagnetic order is not destroyed in the transverse structure factors by an external field.

In the isotropic case \( (\gamma = 0) \) the transverse structure factor is approximately linear in \(-\ln(1 - p/\pi)\) for \( p > 2\pi M \), as can be seen from Fig. 5(b). This type of singularity was found for \( p \to \pi \) at \( M = 0 \). The slight curvature at \( M = 1/4 \) might indicate that the type of the singularity has changed here to a power behavior \((1 - p/\pi)^{-\alpha}\).

In the anisotropic case with \( \gamma/\pi = 0.1, 0.2 \) and \( M = 1/4 \) we find again the constant behavior (4.1) and a linear increase in \((1 - p/\pi)^{\eta_1-1}\). Again this type of singularity follows from (4.1) with \( a = p \) and \( M = 0 \).

**V. THE TRANSVERSE STRUCTURE FACTOR AT CRITICAL MOMENTUM**

Let us start with the XX-model \( (\gamma = \pi/2) \). Fig. 6(a) shows the transverse structure factor for \( p = \pi \) and \( N = 8, 10, \ldots, 28 \) as function of \( M \). In contrast to the longitudinal case we have no scaling in \( M \). At \( M = 0 \) we know from (4.1) with \( a = N \) that the transverse structure factors diverge as \( \sqrt{N} \). The same type of divergence appears at \( M = 1/4 \), as can be seen from Fig. 7(a). Here we compare the \( N \)-dependence of \( S_1(\gamma = \pi/2, p = \pi, M, N) \) for \( M = 0 \) and \( M = 1/4 \). In both cases there is a linear increase in \( \sqrt{N} \).

Let us now turn to the isotropic case \( (\gamma = 0) \). Here the longitudinal and transverse structure factors coincide provided that there is no external field. In the presence of a uniform field, however, they differ drastically. At \( p = \pi \), the longitudinal structure factor is infinite at \( M = 0 \), but becomes finite and monotonically decreasing for \( M > 0 \). In contrast the transverse structure factor stays at infinity for \( M > 0 \). Moreover, on finite systems, the longitudinal structure factor scales for \( M > 0 \) – as was demonstrated in Fig. 3 – whereas the corresponding transverse structure factor (at \( p = \pi \)) does not scale at all, as can be seen from Fig. 6(b). More surprising, at fixed \( M > 0 \) not too large, the transverse structure factors increase with the system size \( N \) stronger than at \( M = 0 \). A comparison of the \( N \)-dependence at \( M = 0 \) and \( M = 1/4 \) is shown in Fig. 7(b). At \( M = 1/4 \) the increase with \( \ln N \) is definitely steeper, which signals a strengthening of the singularity at \( p = \pi \). Note also that there are deviations from linearity in \( \ln N \),
which increase with $M$. This might indicate a change from a logarithmic behavior at $M = 0$ to a power behavior for $M > 0$.

In Ref. [9] Müller et al. reported on the transverse structure factor for $N = 10$; they found already that the dominant mode remains situated at $p = \pi$ independent of the field. Fig. 6(b) tells us that the strengthening of the singularity at $p = \pi$ becomes more and more pronounced with increasing system size $N$.

VI. CONCLUSIONS

In the presence of a uniform external field in $z$-direction the static structure factors of the XXZ-model show up the following features:

1. The longitudinal structure factors have a cusp along the line (2.2). In case of the XX-model ($\gamma = \pi/2$) there are no finite-size effects and the longitudinal structure factor is given by (2.1) for all system sizes with $N = 4, 6, ...$. For smaller values of $\gamma$ and $M$, the cusp becomes sharper. Finite-size effects decrease along the cusp with $N^{-\delta_3}$, $\delta_3 \approx 0.5$. Away from the cusp we find a more rapid decrease of the order $N^{-2}$.

2. The longitudinal structure factor is finite for $\gamma \neq 0$ and $p \to \pi$, $M \to 0$, but develops a logarithmic singularity in this limit for the isotropic case ($\gamma = 0$). This means: A uniform field weakens the antiferromagnetic order in the longitudinal structure factor for $\gamma = 0$.

3. The transverse structure factor is almost constant for $p \leq 2M\pi$ [cf.(4.1)]. Finite-size effects die out slowly with $N^{-\delta_1}$ with $\delta_1 \approx 1$ along the line $p = 2M\pi$, but rapidly with $N^{-2}$ away from this line.

4. In the limit $p \to \pi$, $M = 1/4$ fixed, we observe a singularity of the type $(1 - p/\pi)^{-1/2}$ in the transverse structure factor for $\gamma = \pi/2$. In the isotropic case ($\gamma = 0$) this singularity appears to be stronger than $-\ln(1 - p/\pi)$. This means: A weak uniform field strengthens the antiferromagnetic order in the transverse structure factor for $\gamma = 0$.

Therefore the effect of a uniform external field on the longitudinal and transverse structure factors for ($\gamma = 0$) is similar to the effect of switching on the anisotropy parameter $\gamma$. The logarithmic singularity found in the isotropic structure factor at $p = \pi$ changes with $\gamma$. It is strengthened in the transverse, but weakened in the longitudinal structure factor.
FIGURE CAPTIONS

FIG. 1 The longitudinal structure factor versus momentum $p$ and magnetization $M$ with a ridge along the line $p_3(M) = \pi(1 - 2M)$, for $N = 20, 22, \ldots, 28$.

FIG. 2 Comparison of the longitudinal structure factors at $\gamma = \pi/2$ [Eq. (2.1)] and $\gamma = 0$ for $M = 1/4$ ($\circ$), $1/3$ ($\bullet$), respectively.

FIG. 3 Scaling of the longitudinal structure factors $S_j(\gamma = 0, p, M, N)$, $j = 0, 3$ with $p_0 = \pi$ (open symbols), $p_3 = \pi(1 - 2M)$ (solid symbols), with the magnetization $M$.

FIG. 4(a) Estimate of the thermodynamical limit for the difference $\Delta_0(\gamma, M, N = \infty)$ [Eq. (3.3)] at momentum $p_0 = \pi$: Solid symbols represent results from the finite-size analysis (3.4), open symbols are results from finite-size scaling (3.6).

FIG. 4(b) Same as Fig. 4(a) for the difference $\Delta_3(\gamma, M, N = \infty)$ at the cusp $p_3(M) = \pi(1 - 2M)$.

FIG. 5(a) The momentum dependence of the transverse structure factor of the XX model ($\gamma = \pi/2$) at fixed magnetizations $M = 1/4$ ($\circ$), $M = 1/3$ ($\bullet$), respectively. The inset shows a magnification of the low momentum regime.

FIG. 5(b) Same as Fig. 5(a) for the transverse structure factor in the isotropic case ($\gamma = 0$). The inset shows a magnification of the low momentum regime.

FIG. 6(a) The transverse structure factor of the XX model ($\gamma = \pi/2$) versus magnetization $M$ at momentum $p = \pi$.

FIG. 6(b) Same as Fig. 6(a) for the isotropic model ($\gamma = 0$).

FIG. 7(a) Comparison of the size dependence of the transverse structure factors of the XX model ($\gamma = \pi/2$) at $p = \pi$: $M = 1/4$ ($\circ$), $M = 1/3$ ($\bullet$), respectively.

FIG. 7(b) Same as Fig. 7(a) for the isotropic model ($\gamma = 0$).
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FIG. 1

$S_3(\gamma=0,p,M,N)$

$-A \ln(1-p/\pi)$

$-A \ln(2M)$
$S_3(\gamma, p, M, N)$

- $p = \pi$
- $p = \pi(1-2M)$
\[ \Delta_3(\gamma, p = \pi, M, N = \infty) \]

- \( \gamma = 0 \)
- \( \gamma = 0.1\pi \)
- \( \gamma = 0.2\pi \)
$\Delta_3(\gamma, p = p_3(M), M, N = \infty)$

$\gamma = 0$

$\gamma = 0.1\pi$

$\gamma = 0.2\pi$
FIG. 5(a)

\[ S_{\gamma}(\gamma = \pi/2, p, M, N) \]

- M = 1/4
- M = 1/3

\[ (1-p/\pi)^{-1/2} \]
FIG. 5(b)

\[ S_f(\gamma = 0, p, M, N) \]

- \[ -\ln(1-p/\pi) \]

\( M = 1/4 \)
Figure 6(b) shows a graph with data points for \( N = 4 \) and \( N = 28 \). The graph plots \( S_f(\gamma = 0, p = \pi, M, N) \) against \( M \).
$S_j(\gamma=\pi/2, p=\pi, M, N)$

$M=0$

$M=1/4$
$S_f(q=0, p=\pi, M, N)$

FIG.