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1995 J. Phys.: Condens. Matter 7 2829

(http://iopscience.iop.org/0953-8984/7/14/020)

J. Phys.: Condens. Matter 7 (1995) 2829–2841. Printed in the UK

Static structure factors of the *XXZ*-model in the presence of a uniform field

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Received 1 November 1994

Abstract. The static structure factors of the XXZ-model in the presence of a uniform field are determined from an exact computation of the ground states at given total spin on rings with $N = 4, 6, \ldots, 28$ sites. Against the naive expectation, a weak uniform field strengthens the antiferromagnetic order in the transverse structure factor for the isotropic case.

1. Introduction

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

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

have been studied by analytical [1] and numerical [2, 3, 4] methods. The critical exponents η_j, $j = 1, 3$, which govern the large-distance behaviour of the spin–spin correlators in the ground state:

$$\langle 0|S_j(0)S_j(x)|0\rangle \longrightarrow \frac{(-1)^x}{x^{\eta_j}} \qquad j = 1, 3$$

are given by [5]

$$\eta_1 = \eta_3^{-1} = 1 - \frac{\gamma}{\pi} \qquad \text{for } 0 \leqslant \gamma \leqslant \frac{\pi}{2}.$$

At finite temperature T the spin–spin correlators decrease exponentially with a rate given by the inverse correlation length [6]:

$$\xi^{-1}(\gamma, T) \longrightarrow \Phi(\gamma)T^{\nu}$$

with the critical exponent

$$\nu = 1$$

independent of γ and

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

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0953-8984/95/142829+13$19.50

It has been shown in [3] that the structure factors

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

are most suited for extracting the critical behaviour from finite systems. In [3, 4] we have studied the static structure factors in the following three limits:

$$\begin{array}{lll} p = \pi & T = 0 & N \to \infty \\ p \to \pi & T = 0 & N = \infty \\ p = \pi & T \to 0 & N = \infty. \end{array}$$

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

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

where

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

are the 'running variables'. The common form reflects the fact that the structure factors scale in the critical regime as

$$p \longrightarrow \pi \qquad T \longrightarrow 0 \qquad N \longrightarrow \infty \tag{1.3}$$

if we keep

$$z_1 \equiv \left(1 - \frac{p}{\pi}\right) N \qquad z_2 \equiv \frac{N}{\xi(\gamma, T)} \tag{1.4}$$

fixed. The antiferromagnetic properties of the model are manifested in the singularities of the structure factors in the limit (1.3). The transverse structure factors are infinite in this limit; they develop a 'hard' singularity. In contrast, the longitudinal structure factors stay finite. Their critical behaviour is hidden in sub-leading terms which produce a 'soft' singularity. Away from the critical regime (1.3) the antiferromagnetic properties are lost.

Table 1. Magnetization and the corresponding h-fields.

M	1/8	1/6	1/4	1/3	3/8	1/2
$h(\gamma = 0)$	0.96	1.20	1.59	1.83	1.91	2.00
$h(\gamma = 0.1\pi)$	0.93	1.17	1.54	1.78	1.86	1.95
$h(\gamma = 0.2\pi)$	0.83	1.06	1.41	1.64	1.72	1.81
$h(\gamma = 0.5\pi)$	0.38	0.50	0.71	0.87	0.92	1.00

There are further possibilities for destroying antiferromagnetic ordering—e.g. by applying a uniform external field h or by frustration—i.e. by switching on a next-to-nearest neighbour 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 ground states $|S_3\rangle$ of the Hamiltonian (1.1) at given total spin S_3. The ground states were computed with a Lánczos algorithm on rings with $N = 4, 6, \ldots, 28$ sites.

We will discuss the static structure factors as functions of the magnetization $M = S_3/N$. The known [1, 7] magnetization curve translates M into the field strength h. For convenience, we list in table 1 the h-field values corresponding to our M-values.

The outline of the paper is as follows. In sections 2 and 3 we discuss the characteristic features of the longitudinal structure factors, such as the p- and M-dependence and the finite-size effects. The same is done for the transverse structure factors in sections 4 and 5.

2. 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 [8] in the fermion representation:

$$S_3(\gamma = \pi/2, p, M, N) = \frac{2}{\pi}\begin{cases} p & \text{for } 0 \leqslant p \leqslant p_3(M) \\ p_3(M) & \text{for } p_3(M) \leqslant p \leqslant \pi \end{cases} \tag{2.1}$$

where

$$p_3(M) \equiv \pi(1 - 2M). \tag{2.2}$$

Though the result of [8] has been derived for the thermodynamical limit $N \to \infty$, equation (2.1) turns out to be correct for all system sizes with $N = 4, 6, 8 \ldots$. The linear behaviour in p has been found before [3] for the case where $M = 0$.

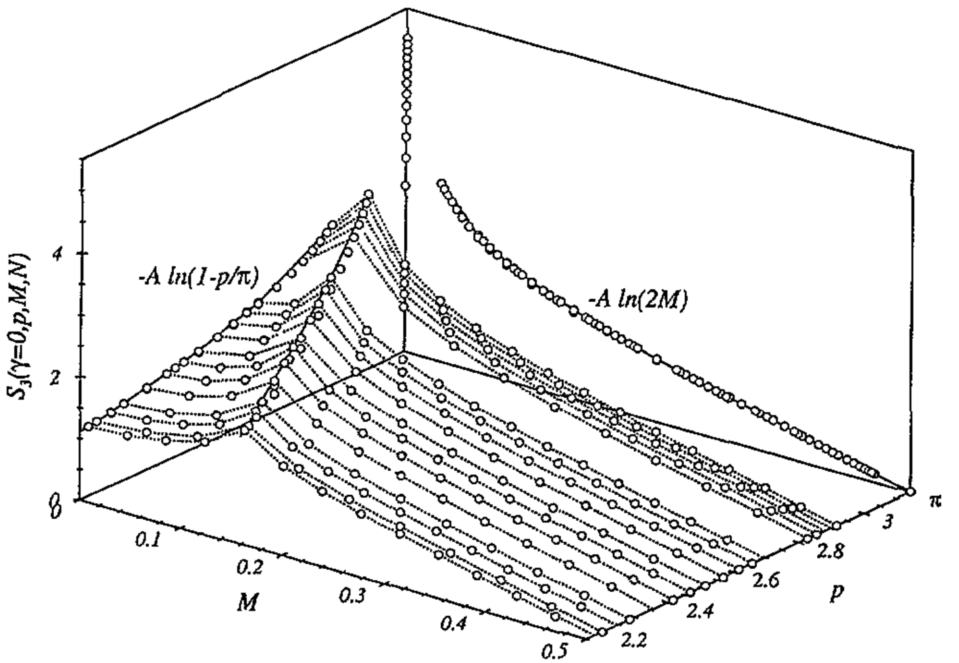


Figure 1. The longitudinal structure factor versus momentum p and magnetization M with a ridge along the line $p_3(M) = \pi(1 - 2M)$, for $N = 20, 22, \ldots, 28$.

Let us next turn to the isotropic case where $\gamma = 0$. Figure 1 presents a panoramic view of 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 for $M = 0$ we

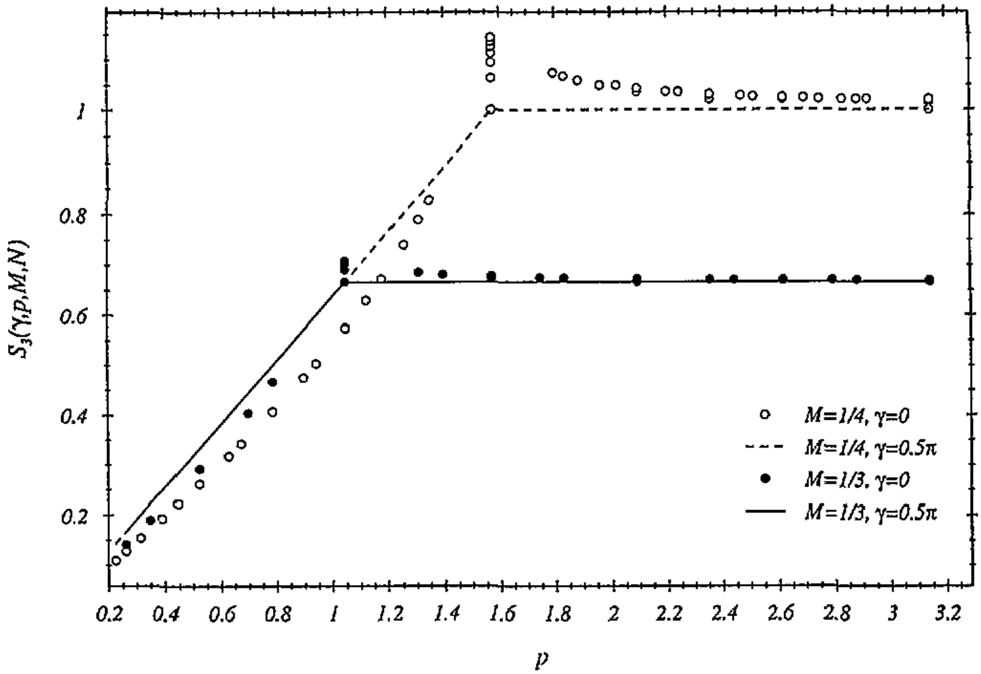


Figure 2. A comparison of the longitudinal structure factors for $\gamma = \pi/2$ (equation (2.1)) and $\gamma = 0$ for $M = 1/4$ (○), $1/3$ (•), respectively.

see the logarithmic singularity

$$S_3(\gamma = 0, p, M = 0) = r_3(0) \ln\left(1 - \frac{p}{\pi}\right) \tag{2.3}$$

discussed in [3]. Along the magnetization axis where

$$p = p_0 \equiv \pi \qquad M = S_3/N \longrightarrow 0 \tag{2.4}$$

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

$$p = p_3(M) \qquad M \longrightarrow 0 \tag{2.5}$$

where $p_3(M)$ is given in (2.2). The longitudinal structure factor has its maximum at $p = p_3(M)$, with 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 behaviour has been conjectured by Müller [9] *et al.* Indications for this have been found also by Parkinson and Bonner [10] and Ishimura and Shiba [11] for small systems ($N \leqslant 14$). Johnson and Fowler [12] were able to reformulate the isotropic Heisenberg model for large spins and magnetizations close to saturation in terms of a gas of magnons. Fortuitously 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 figure 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 analysed in the next section we find an N^{-2} behaviour away from the cusp and a slower decrease, $N^{-\delta_3}$ with $\delta_3 \approx 0.5$, at the cusp

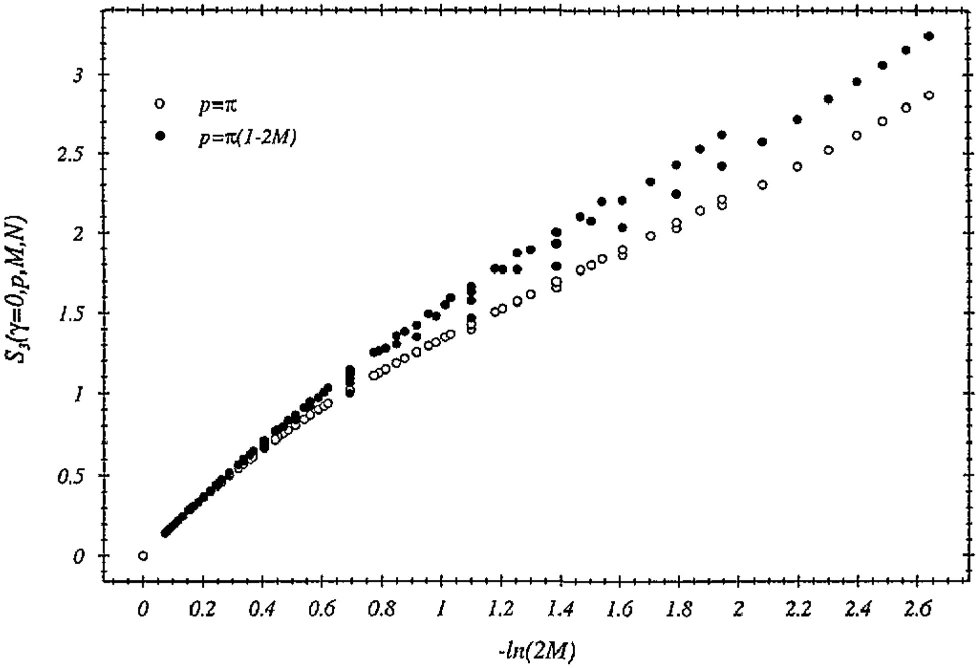


Figure 3. The scaling of the longitudinal structure factors $S_3(\gamma = 0, p, M, N)$, $j = 0, 3$ with $p_0 = \pi$ (open symbols), $p_3 = \pi(1 - 2M)$ (solid symbols), with the magnetization M.

$p = p_3(M)$. The change in the finite-size behaviour signals the emergence of a non-analytic behaviour 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 that in 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 behaviour of the form (1.2) with a running variable

$$y_M = \frac{M(\gamma)}{M}. \tag{2.6}$$

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

3. Finite-size analysis of the longitudinal structure factor

In the critical regime

$$p \longrightarrow \pi \qquad N \longrightarrow \infty \qquad M = \frac{S_3}{N} \longrightarrow 0 \qquad T \longrightarrow 0 \tag{3.1}$$

we expect the longitudinal structure factors to obey finite-size scaling:

$$S_3(\gamma, p, M = S_3/N, T, N) = g_3(\gamma; z_1, z_2, z_3) S_3(\gamma, p, M, T, N = \infty). \tag{3.2}$$

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

$$z_3 \equiv MN = S_3.$$

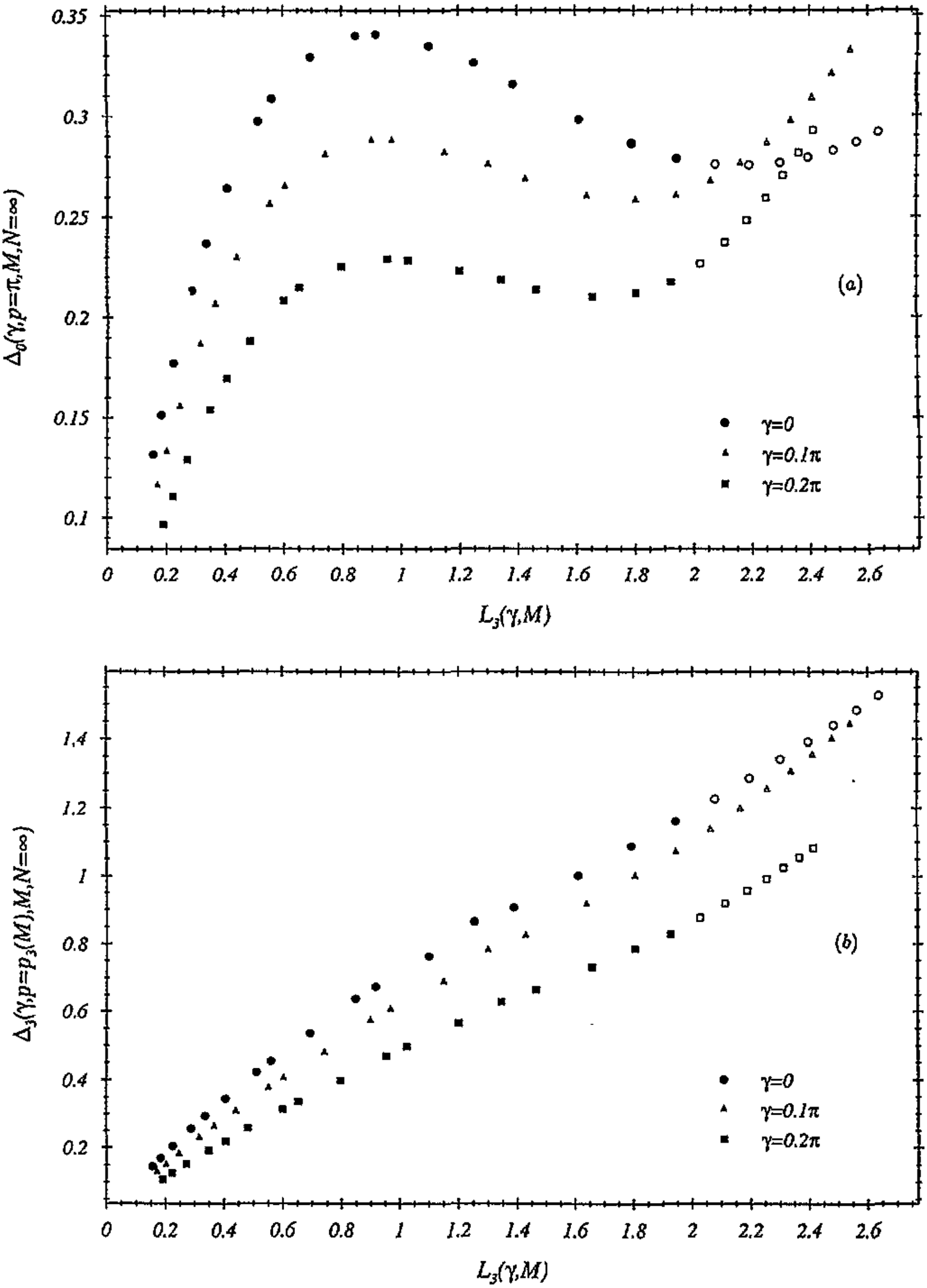
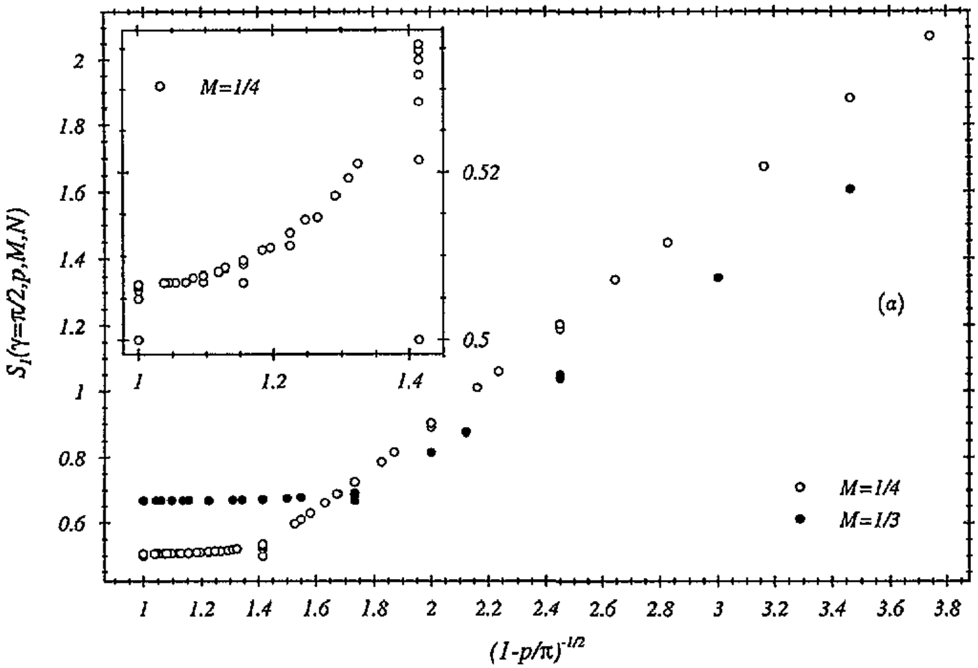


Figure 4. (*a*) An estimate of the thermodynamical limit for the difference $\Delta_0(\gamma, M, N=\infty)$ (equation (3.3)) for momentum $p_0=\pi$: solid symbols represent results from the finite-size analysis (3.4); open symbols are results from finite-size scaling (3.6). (*b*) As figure (*a*) but for the difference $\Delta_3(\gamma, M, N=\infty)$ at the cusp $p_3(M)=\pi(1-2M)$.



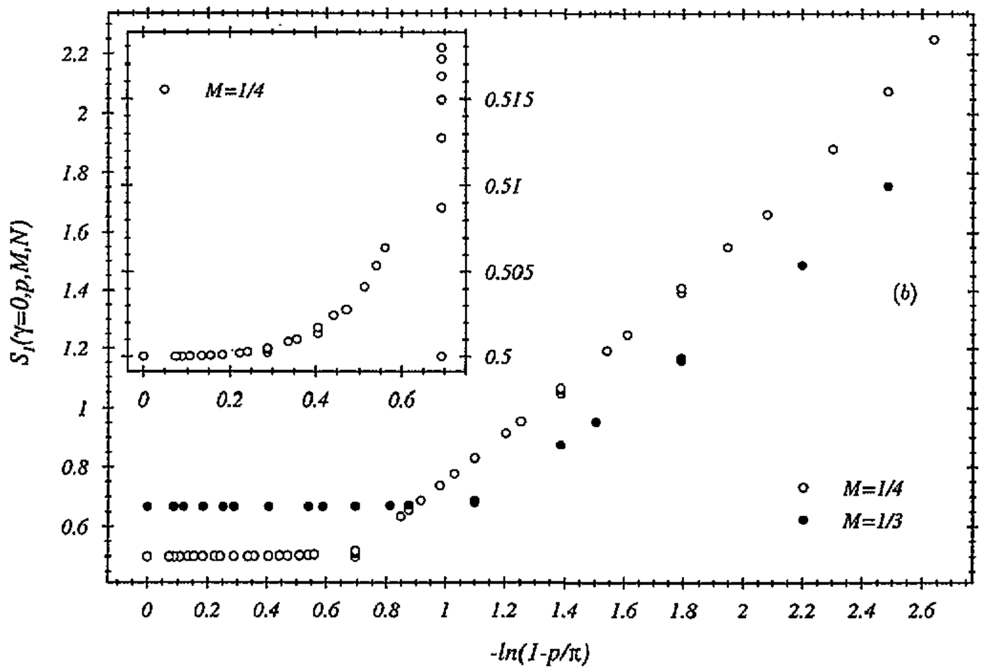
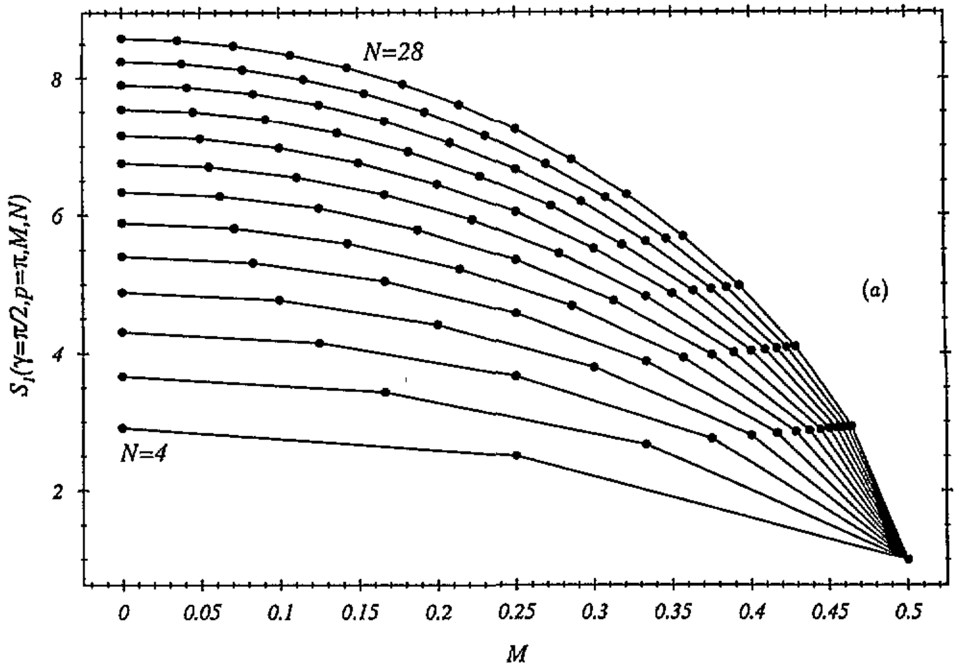


Figure 5. (*a*) The momentum dependence of the transverse structure factor of the XX-model ($\gamma = \pi/2$) for fixed magnetizations $M = 1/4$ (∘), $M = 1/3$ (•), respectively. The inset shows a magnification of the low-momentum regime. (*b*) As figure 5(*a*) but for the transverse structure factor in the isotropic case ($\gamma = 0$). The inset shows a magnification of the low-momentum regime.



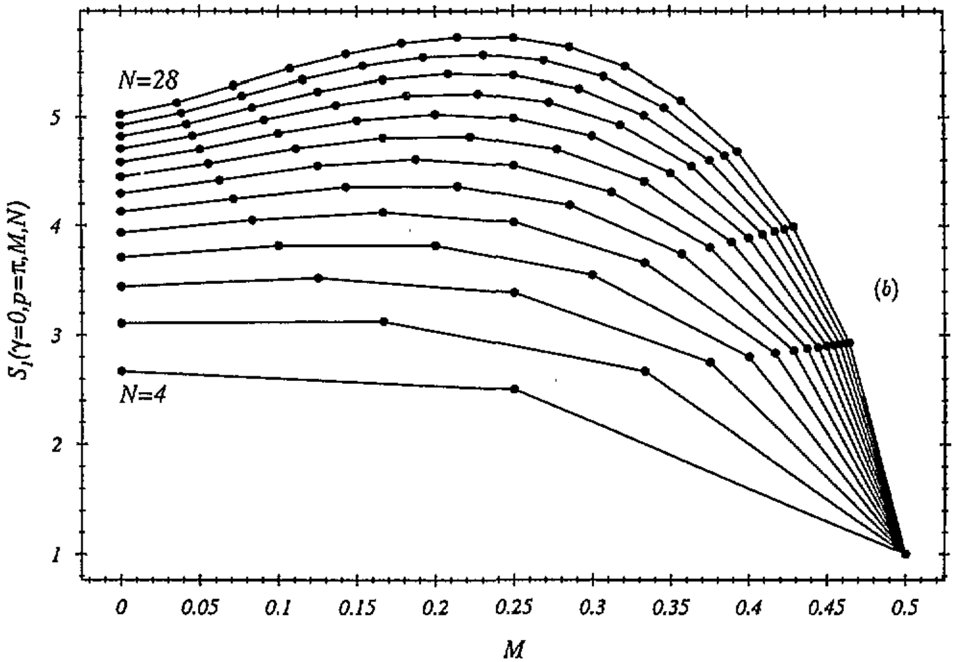
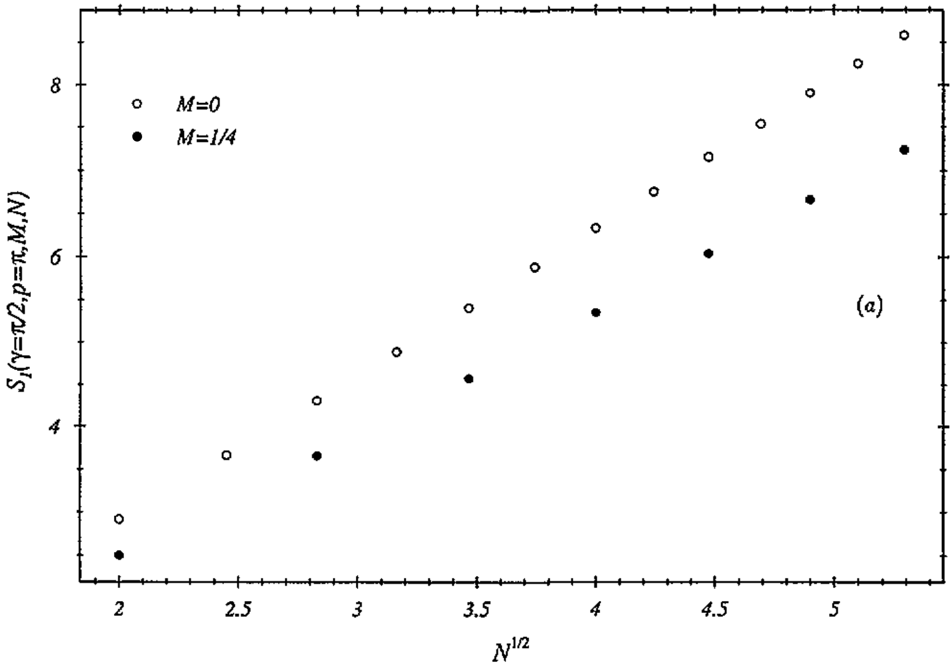


Figure 6. (*a*) The transverse structure factor of the XX-model ($\gamma = \pi/2$) versus magnetization M for momentum $p = \pi$. (*b*) As (*a*) but for the isotropic model ($\gamma = 0$).



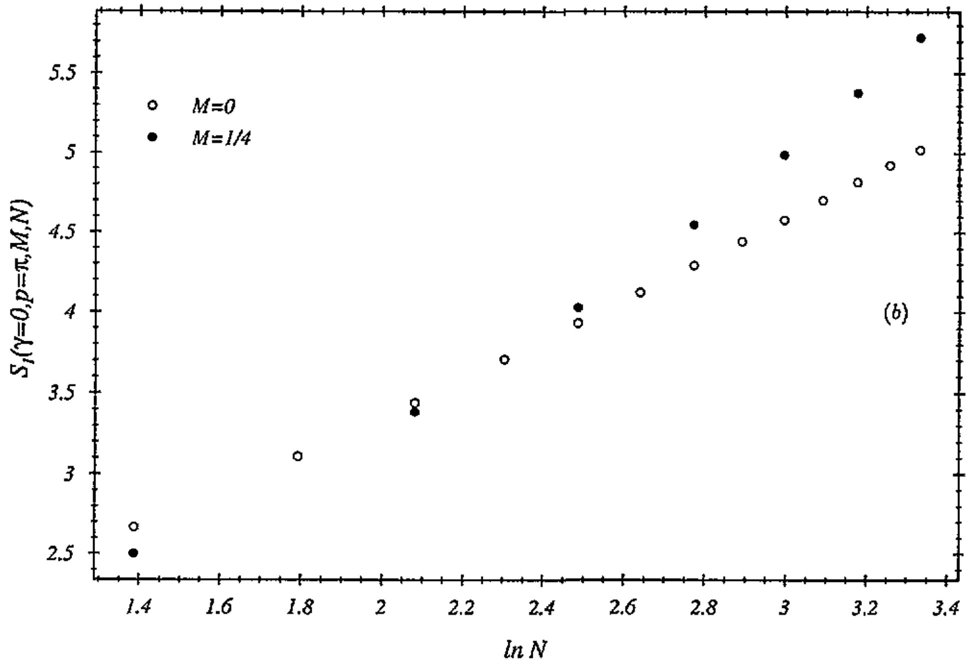


Figure 7. (*a*) A comparison of the size dependence of the transverse structure factors of the XX-model ($\gamma = \pi/2$) for $p = \pi$: $M = 1/4$ (○), $M = 1/3$ (•), respectively. (*b*) As (*a*) but for the isotropic model ($\gamma = 0$).

In [4] we checked finite-size scaling in the combined limit

$$T \longrightarrow 0 \qquad N \longrightarrow \infty \qquad z_2 \text{ fixed}$$

and

$$p = \pi \qquad M = 0.$$

It was found that finite-size scaling works for the transverse structure factors for all γ-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) and (2.5) at zero temperature. The behaviour of the isotropic structure factor can be read from (1.2):

$$S_3(\gamma = 0, p = \pi, M, N = \infty) \stackrel{M\to 0}{\longrightarrow} r_3(0) \ln \frac{M}{M_i}$$

where $i = 0, 3$ stands for the two limits (2.4), (2.5). The isotropic structure factors for finite systems with N sites scale with M (for $M \neq 0$) and are linear in $-\ln M$ in the limit $M \to 0$, as can be seen from figure 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

$$\Delta_j(\gamma = 0, M, N) = S_3(\gamma = 0, p_j, M, N) + \ln(2M) \qquad j = 0, 3 \tag{3.3}$$

for fixed magnetizations:

$$M = \begin{cases} \frac{1}{8}, \frac{3}{8}: & N = 8, 16, 24 \\ \frac{1}{4}: & N = 4, 8, 12, 16, 20, 24, 28 \\ \frac{1}{6}, \frac{2}{6}: & N = 6, 12, 18, 24 \end{cases}$$

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

$$\begin{aligned} \Delta_0(\gamma, M, N) &= \Delta_0(\gamma, M) + c_0(\gamma, M)N^{-2} \\ \Delta_3(\gamma, M, N) &= \Delta_3(\gamma, M) + c_3(\gamma, M)N^{-\delta_3} \qquad \delta_3 \approx 0.5. \end{aligned} \tag{3.4}$$

In our finite-size analysis we have also included the magnetizations

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

which occur for 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 the solid dots in figure 4.

So far our estimates of the thermodynamical limit are restricted to magnetizations $M \geqslant 1/14$ due to the finiteness of our systems $N \leqslant 28$. Additional information on the structure factors for the M-values

$$M = \frac{1}{N} \qquad N = 14, 16, \ldots, 28 \tag{3.5}$$

closer to the critical point $M = 0$ can be obtained if finite-size scaling (3.2) holds for the longitudinal structure factors in the limits (2.4), (2.5) where we keep $z_3 = S_3$ fixed. This variable is just 1 for the sequence (3.5), and we can compute the scaling function at this value from

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

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:

$$S_3(\gamma = 0, p = p_j, M, N = \infty) = \frac{S_3(\gamma = 0, p = p_j, M = 1/N, N)}{g_j(\gamma, 1)} \qquad j = 0, 3 \qquad (3.6)$$

for the sequence of M-values in (3.5). The result for the differences (3.4) is marked by the open dots in figures 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

$$\Delta_j(\gamma, M, N = \infty) = S_3(\gamma, p_j, M, N = \infty) - L_3(\gamma, M) \qquad j = 0, 3$$

versus the variable

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

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

4. The transverse structure factors at fixed magnetization

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

$$S_1(\gamma, p, M, T = 0, N) \approx 2M \qquad \text{for } 0 \leqslant p \leqslant 2\pi M \qquad (4.1)$$

which has been found by Müller *et al* [9] for small systems for the isotropic case $\gamma = 0$. For $S_3 = MN = N/2 - 1$ equation (4.1) can be easily proven to be exact by means of the Bethe *ansatz* solution. For $S_3 < N/2 - 1$ and $0 < p \leqslant 2M\pi$, however, equation (4.1) is not exact. As an example we present in figures 5(a), (b) the momentum dependence of S_1 at $M = 1/4, 1/3$, $N = 4, 6, \ldots, 28$ for $\gamma = \pi/2$ and $\gamma = 0$, respectively. The constancy in the regime where $p \leqslant 2\pi M$ is striking. Deviations from (4.1) can be seen on a scale magnified by a factor 100 in the inset of figures 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 as N^{-2}. At $p = 2M\pi$, 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 figure 5(a). Therefore we find the same type of singularity for $p \to \pi$ for $M = 0, 1/4, 1/3$. Against naive expectation, antiferromagnetic order in the transverse structure factors is not destroyed by an external field.

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

In the anisotropic case with $\gamma/\pi = 0.1, 0.2$ and $M = 1/4$ we find again the constant behaviour (4.1) and a linear increase in $(1 - p/\pi)^{\eta_1 - 1}$. Again this type of singularity follows from (1.2) with $a = p$ and $M = 0$.

5. The transverse structure factor at critical momentum

Let us start with the XX-model ($\gamma = \pi/2$). Figure 6(a) shows the transverse structure factor for $p = \pi$ and $N = 4, 6, \ldots, 28$ as function of M. In contrast to what occurs in the longitudinal case we have no scaling in M. At $M = 0$ we know from (1.2) 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 figure 7(a). Here we compare the N-dependence of $S_\mathrm{l}(\gamma = \pi/2, p = \pi, M, N)$ 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 figure 3—whereas the corresponding transverse structure factor (at $p = \pi$) does not scale at all, as can be seen from figure 6(b). More surprising, for fixed $M > 0$ not too large, the transverse structure factors increase with the system size N more strongly than for $M = 0$. A comparison of the N-dependence for $M = 0$ and that for $M = 1/4$ is shown in figure 7(b). For $M = 1/4$ 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 behaviour at $M = 0$ to a power behaviour for $M > 0$.

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

6. 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.

(i) 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 $N = 4, 6, \ldots$. For smaller values of γ 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 of N^{-2}.

(ii) 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 that a uniform field *weakens* the antiferromagnetic order in the *longitudinal* structure factor for $\gamma = 0$.

(iii) The transverse structure factor is almost constant for $p \leqslant 2M\pi$ (see (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.

(iv) In the limit $p \to \pi$, with $M = 1/4$ 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 that a weak uniform field *strengthens* the antiferromagnetic order in the *transverse* strucure factor for $\gamma = 0$.

Such a surprising behaviour is implicitly predicted in [13].

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 γ. The logarithmic singularity found in the isotropic structure factor at $p = \pi$ changes with γ. It is strengthened in the transverse structure factor, but weakened in the longitudinal structure factor.

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