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LETTER TO THE EDITOR

Next-nearest-neighbour correlation functions of the spin-$\frac{1}{2}$ *XXZ* chain at the critical region

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Abstract

The correlation functions of the spin-$\frac{1}{2}$ *XXZ* chain in the ground state are expressed in the form of multiple integrals. For $-1 < \Delta < 1$, they were obtained by Jimbo and Miwa in 1996. In particular, the next-nearest-neighbour correlation functions are given as certain three-dimensional integrals. We show that these can be reduced to one-dimensional integrals and thereby we evaluate the values of the next-nearest-neighbour correlation functions. We have also found that the remaining one-dimensional integrals can be evaluated analytically, when $\nu = \cos^{-1}(\Delta)/\pi$ is a rational number.

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The spin-$\frac{1}{2}$ *XXZ* chain is one of the fundamental models in the study of low-dimensional magnetism. The Hamiltonian is given by

$$H = \sum_{j=-\infty}^{\infty} \left\{ S_j^x S_{j+1}^x + S_j^y S_{j+1}^y + \Delta S_j^z S_{j+1}^z \right\} \tag{1}$$

where $S = \sigma/2$ and σ are Pauli matrices. The model can be solved by Bethe ansatz method and diverse physical properties have been investigated by varying the anisotropy parameter Δ [1–4]. In particular, in the region $-1 < \Delta \leqslant 1$, the ground state is critically disordered and the excitation spectrum is gapless. Then the long-distance asymptotics of the two-point correlation functions such as $\left\langle S_j^\alpha S_{j+k}^\alpha \right\rangle_{k \gg 1}$ $\alpha = x, y, z$ are shown to decay as a power law via a field theoretical approach; see, for example, [5] and references therein. However, if possible, it is more desirable

(1) to calculate $\langle S_j^\alpha S_{j+k}^\alpha \rangle$ for finite k first; and
(2) to derive its asymptotic behaviour exactly.

Unfortunately such a programme has not been achieved except for the $\Delta = 0$ case [6, 7].

In 1996, Jimbo and Miwa [8] obtained the multiple integral representation for the arbitrary correlation functions of the XXZ chain for $-1 < \Delta < 1$. For example, the emptiness formation probability (EFP) [9] defined by

$$P(n) = \left\langle \prod_{j=1}^{n} \left(S_j^z + \frac{1}{2} \right) \right\rangle \tag{2}$$

has the integral representation

$$\begin{aligned} P(n) = (-\nu)^{-\frac{n(n-1)}{2}} \int_{-\infty}^{\infty} \frac{\mathrm{d}x_1}{2\pi} \cdots \int_{-\infty}^{\infty} \frac{\mathrm{d}x_n}{2\pi} \prod_{a>b} \frac{\sinh(x_a - x_b)}{\sinh((x_a - x_b - \mathrm{i}\pi)\nu)} \\ \times \prod_{k=1}^{n} \frac{\sinh^{n-k}((x_k + \mathrm{i}\pi/2)\nu) \sinh^{k-1}((x_k - \mathrm{i}\pi/2)\nu)}{\cosh^n x_k} \end{aligned} \tag{3}$$

where the parameter ν is related to the anisotropy Δ as

$$\nu = \frac{1}{\pi} \cos^{-1}(\Delta). \tag{4}$$

Recently, there has been an increasing amount of research concerning the properties of the EFP [9–22]. Particularly, in the isotropic limit $\Delta \to 1 (\nu \to 0)$, the general method to evaluate the multiple integral has recently been developed by Boos and Korepin [16–18].

It is of some importance to note that $P(2)$ and $P(3)$ are related to the nearest-neighbour and next-nearest-neighbour correlation functions:

$$\langle S_j^z S_{j+1}^z \rangle = P(2) - \tfrac{1}{4} \tag{5}$$

$$\langle S_j^z S_{j+2}^z \rangle = 2\left(P(3) - P(2) + \tfrac{1}{8}\right). \tag{6}$$

One of our purposes in this letter is to evaluate $\langle S_j^z S_{j+2}^z \rangle$ through the integral representations of $P(3)$ and $P(2)$. Similarly, the nearest-neighbour and the next-nearest-neighbour transverse correlation functions, respectively, have the integral representations:

$$\langle S_j^x S_{j+1}^x \rangle = -\frac{1}{2\nu} \int_{-\infty}^{\infty} \frac{\mathrm{d}x_1}{2\pi} \int_{-\infty}^{\infty} \frac{\mathrm{d}x_2}{2\pi} \frac{\sinh(x_2 - x_1)}{\sinh((x_2 - x_1)\nu)} \frac{\sinh((x_1 + \mathrm{i}\pi/2)\nu) \sinh((x_2 - \mathrm{i}\pi/2)\nu)}{\cosh^2 x_1 \cosh^2 x_2} \tag{7}$$

and

$$\begin{aligned} \langle S_j^x S_{j+2}^x \rangle = -\frac{1}{\nu^3} \prod_{k=1}^{3} \int_{-\infty}^{\infty} \frac{\mathrm{d}x_k}{2\pi} \frac{\sinh^{3-k}((x_k + \mathrm{i}\pi/2)\nu) \sinh^{k-1}(x_k - \mathrm{i}\pi/2)\nu)}{\cosh^3 x_k} \\ \times \frac{\sinh(x_2 - x_1)}{\sinh((x_2 - x_1)\nu)} \frac{\sinh(x_3 - x_1)}{\sinh((x_3 - x_1)\nu)} \frac{\sinh(x_3 - x_2)}{\sinh((x_3 - x_2 - \mathrm{i}\pi)\nu)}. \end{aligned} \tag{8}$$

It has already been shown by Jimbo and Miwa that the two-dimensional integral for $P(2)$ reduces to the one-dimensional integral for arbitrary ν as

$$P(2) = \frac{1}{2} + \frac{1}{2\pi^2 \sin \pi\nu} \frac{\partial}{\partial\nu} \left\{ \sin \pi\nu \int_{-\infty}^{\infty} \frac{\sinh(1-\nu)w}{\sinh w \cosh \nu w} \mathrm{d}w \right\} \tag{9}$$

which leads to the one-dimensional integral representation of $\langle S_j^z S_{j+1}^z \rangle$ via the relation (5). The result coincides with a different derivation of $\langle S_j^z S_{j+1}^z \rangle$ from the ground-state energy per site e_0

$$\begin{aligned}\langle S_j^z S_{j+1}^z \rangle &= \frac{\partial e_0}{\partial \Delta} = -\frac{1}{\pi \sin \pi\nu} \frac{\partial e_0}{\partial \nu} \\ &= \frac{1}{4} + \frac{\cot \pi\nu}{2\pi} \int_{-\infty}^{\infty} \frac{\mathrm{d}w}{\sinh w} \frac{\sinh(1-\nu)w}{\cosh \nu w} - \frac{1}{2\pi^2} \int_{-\infty}^{\infty} \frac{\mathrm{d}w}{\sinh w} \frac{w \cosh w}{(\cosh \nu w)^2}\end{aligned} \tag{10}$$

where

$$e_0 = \frac{\Delta}{4} - \frac{\sin \pi\nu}{2\pi} \int_{-\infty}^{\infty} \frac{\sinh(1-\nu)w}{\sinh w \cosh \nu w} \mathrm{d}w. \tag{11}$$

Similarly we can obtain the one-dimensional integral representation for $\langle S_j^x S_{j+1}^x \rangle$ as

$$\begin{aligned}\langle S_j^x S_{j+1}^x \rangle &= \frac{1}{2}\left(e_0 - \Delta \langle S_j^z S_{j+1}^z \rangle\right) \\ &= -\frac{1}{4\pi \sin \pi\nu} \int_{-\infty}^{\infty} \frac{\mathrm{d}w}{\sinh w} \frac{\sinh(1-\nu)w}{\cosh \nu w} + \frac{\cos \pi\nu}{4\pi^2} \int_{-\infty}^{\infty} \frac{\mathrm{d}w}{\sinh w} \frac{w \cosh w}{(\cosh \nu w)^2}.\end{aligned} \tag{12}$$

Thus, for the nearest-neighbour correlation functions, we know that the two-dimensional integrals given for the Jimbo–Miwa formula can be reduced to one-dimensional integrals. The main result of this letter is that three-dimensional integrals for $P(3)$ and $\langle S_j^x S_{j+2}^x \rangle$ can also be reduced to one-dimensional integrals. In other words, we have succeeded in performing the integrals for $P(3)$ and $\langle S_j^x S_{j+2}^x \rangle$ twice. Our results are

$$\begin{aligned}P(3) = \frac{1}{2} + \int_{-\infty-\mathrm{i}\delta}^{\infty-\mathrm{i}\delta} \frac{\mathrm{d}x}{\sinh x} \bigg[&\frac{1-\cos 2\pi\nu}{16\pi^2} \frac{\partial}{\partial \nu} \left\{ \frac{\cosh 3\nu x}{(\sinh \nu x)^3} \right\} + \frac{3 \tan \pi\nu}{8\pi} \frac{\cosh 3\nu x}{(\sinh \nu x)^3} \\ &- \frac{4-\cos 2\pi\nu}{4\pi^2} \frac{\partial(\coth \nu x)}{\partial \nu} - \frac{(4-\cos 2\pi\nu)\coth \nu x}{2\pi \sin 2\pi\nu} \bigg]\end{aligned} \tag{13}$$

and

$$\begin{aligned}\langle S_j^x S_{j+2}^x \rangle = \int_{-\infty-\mathrm{i}\delta}^{\infty-\mathrm{i}\delta} \frac{\mathrm{d}x}{\sinh x} \bigg[&-\frac{(\sin \pi\nu)^2}{8\pi^2} \frac{\partial}{\partial \nu} \left\{ \frac{\cosh 3\nu x}{(\sinh \nu x)^3} \right\} \\ &- \frac{3 \cos 2\pi\nu (1-\cos 2\pi\nu)}{8\pi \sin 2\pi\nu} \frac{\cosh 3\nu x}{(\sinh \nu x)^3} + \frac{1}{4\pi^2} \frac{\partial(\coth \nu x)}{\partial \nu} \\ &+ \frac{\{1 + 3\cos 2\pi\nu - 3(\cos 2\pi\nu)^2\} \coth \nu x}{2\pi \sin 2\pi\nu} \bigg].\end{aligned} \tag{14}$$

Here, δ $(0 < |\delta| < \pi)$ should take some non-zero real value, which is introduced to avoid the singularity at the origin. We, however, note that the singular term may be subtracted from the integrand in principle, as its residue vanishes. Or alternatively, by applying the Fourier transform, we can express the one-dimensional representations (13) and (14) as

$$\begin{aligned}P(3) = \frac{1}{2} &+ \int_{-\infty}^{\infty} \frac{\mathrm{d}w}{\sinh w} \frac{\sinh(1-\nu)w}{\cosh \nu w} \left[\frac{1 + 2\cos 2\pi\nu}{2\pi \sin 2\pi\nu} + \frac{3 \tan \pi\nu}{4\pi^3} w^2 \right] \\ &- \int_{-\infty}^{\infty} \frac{\mathrm{d}w}{\sinh w} \frac{\cosh w}{(\cosh \nu w)^2} \left[\frac{3}{4\pi^2} w + \frac{(\sin \pi\nu)^2}{4\pi^4} w^3 \right]\end{aligned} \tag{15}$$

and

$$\begin{aligned}\langle S_j^x S_{j+2}^x \rangle = &-\int_{-\infty}^{\infty} \frac{\mathrm{d}w}{\sinh w} \frac{\sinh(1-\nu)w}{\cosh \nu w} \left[\frac{1}{2\pi \sin 2\pi\nu} + \frac{3 \cos 2\pi\nu \tan \pi\nu}{4\pi^3} w^2 \right] \\ &+ \int_{-\infty}^{\infty} \frac{\mathrm{d}w}{\sinh w} \frac{\cosh w}{(\cosh \nu w)^2} \left[\frac{\cos 2\pi\nu}{4\pi^2} w + \frac{(\sin \pi\nu)^2}{4\pi^4} w^3 \right].\end{aligned} \tag{16}$$

Table 1. Some analytical values of the correlation functions when ν takes rational values.

ν	$\left\langle S_j^x S_{j+1}^x \right\rangle$	$\left\langle S_j^z S_{j+1}^z \right\rangle$	$\left\langle S_j^x S_{j+2}^x \right\rangle$	$\left\langle S_j^z S_{j+2}^z \right\rangle$
0	$\frac{1}{12} - \frac{\ln 2}{3}$	$\frac{1}{12} - \frac{\ln 2}{3}$	$\frac{1}{12} - \frac{4\ln 2}{3} + \frac{3\zeta(3)}{4}$	$\frac{1}{12} - \frac{4\ln 2}{3} + \frac{3\zeta(3)}{4}$
$\frac{1}{2}$	$-\frac{1}{2\pi}$	$-\frac{1}{\pi^2}$	$\frac{1}{\pi^2}$	0
$\frac{1}{3}$	$-\frac{5}{32}$	$-\frac{1}{8}$	$\frac{41}{512}$	$\frac{7}{256}$
$\frac{1}{4}$	$-\frac{\sqrt{2}}{2\pi} + \frac{\sqrt{2}}{2\pi^2}$	$-\frac{1}{4} + \frac{1}{\pi} - \frac{2}{\pi^2}$	$\frac{3}{16} - \frac{1}{\pi} + \frac{2}{\pi^2}$	$-\frac{5}{8} + \frac{4}{\pi} - \frac{6}{\pi^2}$
$\frac{1}{5}$	$-\frac{3}{64} - \frac{3\sqrt{5}}{64}$	$-\frac{19}{8} + \sqrt{5}$	$\frac{7737}{1024} - \frac{3429\sqrt{5}}{1024}$	$-\frac{3529}{512} + \frac{1589\sqrt{5}}{512}$
$\frac{1}{6}$	$\frac{\sqrt{3}}{48} - \frac{1}{\pi} + \frac{3\sqrt{3}}{4\pi^2}$	$-\frac{7}{18} + \frac{\sqrt{3}}{\pi} - \frac{3}{\pi^2}$	$\frac{247}{576} - \frac{17\sqrt{3}}{12\pi} + \frac{33}{8\pi^2}$	$-\frac{283}{288} + \frac{11\sqrt{3}}{3\pi} - \frac{39}{4\pi^2}$
$\frac{2}{3}$	$\frac{47}{128} - \frac{\sqrt{3}}{4} - \frac{9}{32\pi}$	$\frac{23}{32} - \frac{\sqrt{3}}{4} - \frac{9}{8\pi}$	$-\frac{2719}{8192} + \frac{47\sqrt{3}}{256} + \frac{441}{1024\pi}$	$\frac{8671}{4096} - \frac{49\sqrt{3}}{64} - \frac{1305}{512\pi}$
$\frac{3}{4}$	$-\frac{4\sqrt{6}}{27} + \frac{64\sqrt{2}}{243} - \frac{\sqrt{2}}{6\pi} - \frac{8\sqrt{6}}{81\pi} - \frac{\sqrt{2}}{18\pi^2}$	$\frac{781}{972} - \frac{8\sqrt{3}}{27} - \frac{1}{3\pi} - \frac{32\sqrt{3}}{81\pi} - \frac{2}{9\pi^2}$	$-\frac{22111}{34992} + \frac{8\sqrt{3}}{27} + \frac{1}{3\pi} + \frac{160\sqrt{3}}{729\pi} + \frac{2}{9\pi^2}$	$\frac{36169}{17496} - \frac{160\sqrt{3}}{243} - \frac{4}{3\pi} - \frac{608\sqrt{3}}{729\pi} - \frac{\sqrt{2}}{3\pi^2}$
1	$-\frac{1}{8}$	0	$\frac{1}{8}$	0

Note that in the representations (15) and (16), there are no singularities at the origin. This is a similar situation to equations (10) and (12). Combining equations (9) and (15), we can also write the one-dimensional integral representation for $\left\langle S_j^z S_{j+2}^z \right\rangle$ through the relation (6):

$$\left\langle S_j^z S_{j+2}^z \right\rangle = \frac{1}{4} + \int_{-\infty}^{\infty} \frac{\mathrm{d}w}{\sinh w} \frac{\sinh(1-\nu)w}{\cosh \nu w} \left[\frac{\cot 2\pi\nu}{\pi} + \frac{3\tan\pi\nu}{2\pi^3} w^2 \right] - \int_{-\infty}^{\infty} \frac{\mathrm{d}w}{\sinh w} \frac{\cosh w}{(\cosh \nu w)^2} \left[\frac{1}{2\pi^2} w + \frac{(\sin \pi\nu)^2}{2\pi^4} w^3 \right]. \tag{17}$$

Now let us discuss some properties of the obtained one-dimensional representations (16) and (17). At first glance, some integrands in equations (16) and (17) are divergent at $\nu = 1/2$ and also in the limit $\nu \to 0$ and $\nu \to 1$, due to the the factor $1/\sin 2\pi\nu$. However, by investigating the integrands carefully, we have found that these singular terms cancel each other out, therefore yielding definite finite values for the correlation functions:

- $\nu = 1/2$

$$\left\langle S_j^x S_{j+2}^x \right\rangle = \frac{1}{\pi^2} \qquad \left\langle S_j^z S_{j+2}^z \right\rangle = 0 \tag{18}$$

- $\nu \to 0$

$$\left\langle S_j^x S_{j+2}^x \right\rangle \qquad \left\langle S_j^z S_{j+2}^z \right\rangle \to \tfrac{1}{12} - \tfrac{4}{3}\ln 2 + \tfrac{3}{4}\zeta(3) \tag{19}$$

- $\nu \to 1$

$$\left\langle S_j^x S_{j+2}^x \right\rangle \to \tfrac{1}{8} \qquad \left\langle S_j^z S_{j+2}^z \right\rangle \to 0. \tag{20}$$

It is especially intriguing to observe that the $\nu \to 0$ limit (19) reproduces the known result by one of the authors in [23].

More generally, we have found that, when ν takes a rational value, the one-dimensional integrals can be evaluated analytically. Some of our explicit results are summarized in table 1. We can see that the correlation functions are, in general, a polynomial of $1/\pi$. Particularly, when $\nu = 1/3$, we expect all the correlation functions to be given solely as a single rational number (cf [13, 14]). Figures 1 and 2 plot the numerical values of the nearest-neighbour and the next-nearest-neighbour correlation functions calculated from the one-dimensional integral

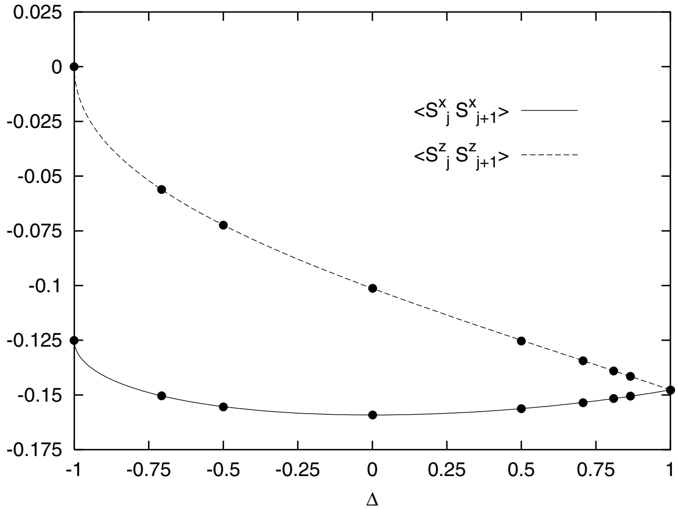

Figure 1. Nearest-neighbour correlation functions for the *XXZ* chain.

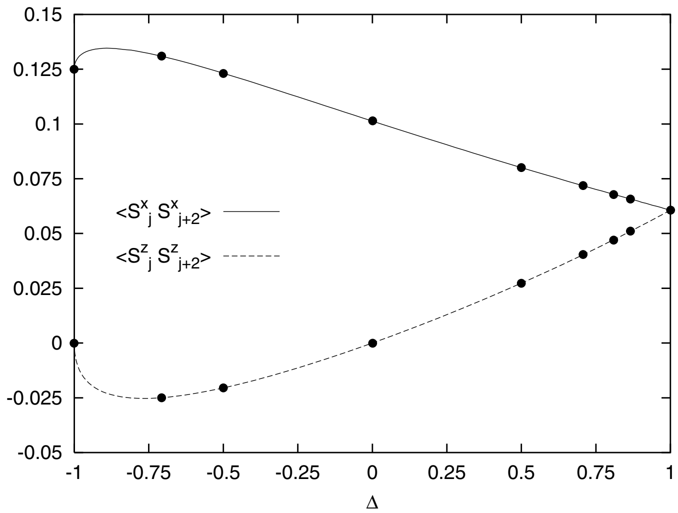

Figure 2. Next-nearest-neighbour correlation functions for the *XXZ* chain.

representations. For comparison, the analytical values in table 1 are represented by filled circles.

We have obtained equations (13) and (14) by generalizing the method developed by Boos and Korepin [16, 17], which allows us to calculate the multiple integrals for the correlation functions of the *XXX* model ($\Delta = 1$). Below we briefly outline the derivation of equations (13) and (14). The details of the calculations will be published in a separate paper [24]. First we introduce the following convenient notation for $P(3)$:

$$P(3) = \prod_{k=1}^{3} \int_{-\infty-i/2}^{\infty-i/2} \frac{\mathrm{d}\lambda_k}{2\pi\mathrm{i}} U_3(\lambda_1, \lambda_2, \lambda_3) T_3(\lambda_1, \lambda_2, \lambda_3). \tag{21}$$

Here

$$U_3(\lambda_1, \lambda_2, \lambda_3) = \frac{\pi^3 \prod_{1\leqslant k<j\leqslant 3} \sinh \pi(\lambda_j - \lambda_k)}{\nu^3 \prod_{j=1}^{3} \sinh^3 \pi\lambda_j} \tag{22}$$

and

$$T_3(\lambda_1, \lambda_2, \lambda_3) = \frac{(qz_1 - 1)^2(qz_2 - 1)(z_2 - 1)(z_3 - 1)^2}{8(z_2 - qz_1)(z_3 - qz_1)(z_3 - qz_2)} \tag{23}$$

with $q \equiv \mathrm{e}^{2\pi i\nu}$, $z_i \equiv \mathrm{e}^{2\pi\nu\lambda_i}$ $(i = 1, 2, 3)$. Then, after a similar but more complicated calculation of Boos and Korepin [17], we can transform the integrand $T_3(\lambda_1, \lambda_2, \lambda_3)$ into a certain *canonical form* without changing the value of the integral as

$$T_\mathrm{c} = P_0 + \frac{P_1}{z_2 - z_1} \tag{24}$$

where

$$P_0 = \frac{(1+q)^2}{8q}\frac{z_1}{z_3} \tag{25}$$

$$\begin{aligned} P_1 = {} & \frac{3(1+q)}{2q} - \frac{(1+10q+q^2)z_1}{8q} - \frac{3(1+q)^2}{8q^2 z_1} \\ & + z_3\left\{-\frac{1+10q+q^2}{8q} + \frac{3(1+q)z_1}{8} + \frac{3(1+q)}{8qz_1}\right\} \\ & + \frac{1}{z_3}\left\{-\frac{3(1+q)^2}{8q^2} + \frac{3(1+q)z_1}{8q} + \frac{(1+q)(1+q+q^2)}{8q^3 z_1}\right\}. \end{aligned} \tag{26}$$

We find that the first part of T_c, namely P_0, can be integrated easily

$$\prod_{k=1}^{3}\int_{-\infty-i/2}^{\infty-i/2} \frac{\mathrm{d}\lambda_k}{2\pi \mathrm{i}} U_3(\lambda_1, \lambda_2, \lambda_3)\frac{(1+q)^2\,\mathrm{e}^{2\pi\nu(\lambda_1-\lambda_3)}}{8q} = \frac{1}{2}. \tag{27}$$

The second part $P_1/(z_2 - z_1)$ can be integrated twice, namely with respect to λ_3 and $a \equiv (\lambda_2 + \lambda_1)/2$. Finally, the remaining one-dimensional integration with respect to $d \equiv (\lambda_2 - \lambda_1)/2$ together with equation (27) gives the expression (13).

Similarly, for $\langle S_j^x S_{j+2}^x\rangle$, $T_3(\lambda_1, \lambda_2, \lambda_3)$ in equation (21) is replaced by

$$T_3(\lambda_1, \lambda_2, \lambda_3) = \frac{(qz_1 - 1)^2(qz_2 - 1)(z_2 - 1)(z_3 - 1)^2}{8q(z_2 - z_1)(z_3 - z_1)(z_3 - qz_2)}. \tag{28}$$

As a corresponding canonical form, we have found

$$T_\mathrm{c} = \frac{P_1}{z_2 - z_1} \tag{29}$$

with

$$\begin{aligned} P_1 = {} & -\frac{(1+q)(3+q^2)}{8q^2} + \frac{(3-2q+3q^2)z_1}{8q} + \frac{(1+q)^2}{8q^3 z_1} \\ & + z_3\left\{\frac{3-q}{4q} - \frac{(1+q)z_1}{8q} + \frac{(1+q)(-2+q)}{8q^2 z_1}\right\} \\ & + \frac{1}{z_3}\left\{\frac{1+q}{2q} - \frac{(1+q)z_1}{8} - \frac{1+q}{8q^2 z_1}\right\}. \end{aligned} \tag{30}$$

Again, after integrating with respect to λ_3 and $a \equiv (\lambda_2 + \lambda_1)/2$, we arrive at the one-dimensional integral representation (14).

In conclusion, we have shown that the multiple integrals for the correlation functions of the *XXZ* chain at the critical region $-1 < \Delta < 1$ can be reduced to one-dimensional integrals in the case of next-nearest-neighbour correlation functions. This property will be generalized to other higher-neighbour correlations as well as the correlations in the massive region ($\Delta > 1$) [25, 26]. In this respect, we would like to refer to the recent work by Boos, Korepin and Smirnov [27], which has shown the reducibility of the multiple integrals in the case of the *XXX* chain.

In our future work, we are particularly interested in calculating the third-neighbour correlation functions $\langle S_j^x S_{j+3}^x \rangle$ and $\langle S_j^z S_{j+3}^z \rangle$ for general Δ. For $\Delta = 1$, these were recently calculated in [28] from the multiple integrals [9, 29] using the Boos–Korepin method.

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