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# Density matrix elements and entanglement entropy for the spin-1/2 XXZ chain at $\Delta=1 / 2$ 

Jun Sato and Masahiro Shiroishi<br>Institute for Solid State Physics, University of Tokyo, Kashiwanoha 5-1-5, Kashiwa, Chiba 277-8581, Japan<br>E-mail: junji@issp.u-tokyo.ac.jp and siroisi@issp.u-tokyo.ac.jp

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#### Abstract

We have analytically obtained all the density matrix elements up to six lattice sites for the spin- $1 / 2$ Heisenberg XXZ chain at $\Delta=1 / 2$. We use the multiple integral formula of the correlation function for the massless XXZ chain derived by Jimbo and Miwa. As for the spin-spin correlation functions, we have newly obtained the fourth- and fifth-neighbour transverse correlation functions. We have calculated all the eigenvalues of the density matrix and analyse the eigenvalue distribution. Using these results the exact values of the entanglement entropy for the reduced density matrix up to six lattice sites have been obtained. We observe that our exact results agree quite well with the asymptotic formula predicted by the conformal field theory.


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(Some figures in this article are in colour only in the electronic version)

## 1. Introduction

The spin- $1 / 2$ antiferromagnetic Heisenberg XXZ chain is one of the most fundamental models for one-dimensional quantum magnetism, which is given by the Hamiltonian

$$
\begin{equation*}
\mathcal{H}=\sum_{j=-\infty}^{\infty}\left(S_{j}^{x} S_{j+1}^{x}+S_{j}^{y} S_{j+1}^{y}+\Delta S_{j}^{z} S_{j+1}^{z}\right) \tag{1.1}
\end{equation*}
$$

where $S_{j}^{\alpha}=\sigma_{j}^{\alpha} / 2$ with $\sigma_{j}^{\alpha}$ being the Pauli matrices acting on the $j$ th site and $\Delta$ is the anisotropy parameter. For $\Delta>1$, it is called the massive XXZ model where the system is gapful. Meanwhile for $-1<\Delta \leqslant 1$ case, the system is gapless and called the massless XXZ model. Especially we call it XXX model for the isotropic case $\Delta=1$.

The exact eigenvalues and eigenvectors of this model can be obtained by the Bethe ansatz method [1, 2]. Many physical quantities in the thermodynamic limit such as specific heat,
magnetic susceptibility, elementary excitations, etc. .. , can be exactly evaluated even at finite temperature by the Bethe ansatz method [2].

The exact calculation of the correlation functions, however, is still a difficult problem. The exceptional case is $\Delta=0$, where the system reduces to a lattice free-fermion model by the Jordan-Wigner transformation. In this case, we can calculate arbitrary correlation functions by means of Wick's theorem [3, 4]. Recently, however, there have been rapid developments in the exact evaluations of correlation functions for $\Delta \neq 0$ case also, since the Kyoto group (Jimbo, Miki, Miwa, Nakayashiki) derived a multiple integral representation for arbitrary correlation functions. Using the representation theory of the quantum affine algebra $U_{q}\left(s \hat{l}_{2}\right)$, they first derived a multiple integral representation for massive XXZ antiferromagnetic chain in 1992 [5, 6], which is before long extended to the XXX case [7, 8] and the massless XXZ case [9]. Later the same integral representations were reproduced by Kitanine et al [10] in the framework of quantum inverse scattering method. They have also succeeded in generalizing the integral representations to the XXZ model with an external magnetic field [10]. More recently the multiple integral formulae were extended to dynamical correlation functions as well as finite temperature correlation functions [11-14]. In this way it has been established now the correlation functions for XXZ model are represented by multiple integrals in general. However, these multiple integrals are difficult to evaluate both numerically and analytically.

For general anisotropy $\Delta$, it has been shown that the multiple integrals up to four dimension can be reduced to one-dimensional integrals [15-21]. As a result all the density matrix elements within four lattice sites have been obtained for general anisotropy [21]. Reducing the multiple integrals into one dimension, however, involves hard calculation, which makes difficult to obtain correlation functions on more than four lattice sites. On the other hand, at the isotropic point $\Delta=1$, an algebraic method based on the qKZ equation has been devised [22], and all the density matrix elements up to six lattice sites have been obtained [23, 24]. Moreover, as for the spin-spin correlation functions, up to seventh-neighbour correlation function $\left\langle S_{1}^{z} S_{8}^{z}\right\rangle$ for the XXX chain have been obtained from the generating functional approach [25, 26]. It is desirable that this algebraic method be generalized to the case with $\Delta \neq 1$. Actually, Boos et al have derived an exponential formula for the density matrix elements of the XXZ model, which does not contain multiple integrals [27-31]. It, however, seems still hard to evaluate the formula for general density matrix elements.

Among the general $\Delta \neq 0$, there is a special point $\Delta=1 / 2$, where some intriguing properties have been observed. Let us define a correlation function called emptiness formation probability (EFP) [8] which signifies the probability of finding a ferromagnetic string of length $n$ :

$$
\begin{equation*}
P(n) \equiv\left\langle\prod_{j=1}^{n}\left(\frac{1}{2}+S_{j}^{z}\right)\right\rangle . \tag{1.2}
\end{equation*}
$$

The explicit general formula for $P(n)$ at $\Delta=1 / 2$ was conjectured in [33]

$$
\begin{equation*}
P(n)=2^{-n^{2}} \prod_{k=0}^{n-1} \frac{(3 k+1)!}{(n+k)!}, \tag{1.3}
\end{equation*}
$$

which is proportional to the number of alternating sign matrices of size $n \times n$. Later this conjecture was proved by the explicit evaluation of the multiple integral representing the EFP [34]. Remarkably, one can also obtain the exact asymptotic behaviour as $n \rightarrow \infty$ from this formula, which is the unique valuable example except for the free fermion point $\Delta=0$. Note also that as for the longitudinal two-point correlation functions at $\Delta=1 / 2$, up to eighth-neighbour correlation function $\left\langle S_{1}^{z} S_{9}^{z}\right\rangle$ have been obtained in [32] by use of the multiple
integral representation for the generating function. Most outstanding is that all the results are represented by single rational numbers. These results motivated us to calculate other correlation functions at $\Delta=1 / 2$. Actually, we have obtained all the density matrix elements up to six lattice sites by the direct evaluation of the multiple integrals. All the results can be written by single rational numbers as expected. A direct evaluation of the multiple integrals is possible due to the particularity of the case for $\Delta=1 / 2$ as is explained below.

## 2. Analytical evaluation of multiple integral

Here we shall describe how we analytically obtain the density matrix elements at $\Delta=1 / 2$ from the multiple integral formula. Any correlation function can be expressed as a sum of density matrix elements $P_{\epsilon_{1}, \ldots, \epsilon_{n}}^{\epsilon_{1}^{\prime}, \ldots, \epsilon_{n}^{\prime}}$, which are defined by the ground state expectation value of the product of elementary matrices:

$$
\begin{equation*}
P_{\epsilon_{1}, \ldots, \epsilon_{n}}^{\epsilon_{1}^{\prime}, \ldots, \epsilon_{n}^{\prime}} \equiv\left\langle E_{1}^{\epsilon_{1}^{\prime} \epsilon_{1}} \cdots E_{n}^{\epsilon_{n}^{\prime} \epsilon_{n}}\right\rangle \tag{2.1}
\end{equation*}
$$

where $E_{j}^{\epsilon_{j}^{\prime} \epsilon_{j}}$ are $2 \times 2$ elementary matrices acting on the $j$ th site as
$E_{j}^{++}=\left(\begin{array}{ll}1 & 0 \\ 0 & 0\end{array}\right)_{[j]}=\frac{1}{2}+S_{j}^{z}, \quad E_{j}^{--}=\left(\begin{array}{ll}0 & 0 \\ 0 & 1\end{array}\right)_{[j]}=\frac{1}{2}-S_{j}^{z}$,
$E_{j}^{+-}=\left(\begin{array}{ll}0 & 1 \\ 0 & 0\end{array}\right)_{[j]}=S_{j}^{+}=S_{j}^{x}+\mathrm{i} S_{j}^{y}, \quad E_{j}^{-+}=\left(\begin{array}{ll}0 & 0 \\ 1 & 0\end{array}\right)_{[j]}=S_{j}^{-}=S_{j}^{x}-\mathrm{i} S_{j}^{y}$.
The multiple integral formula of the density matrix element for the massless XXZ chain reads [9]

$$
\begin{align*}
& P_{\epsilon_{1}, \ldots, \ldots, \epsilon_{n}}^{\epsilon_{1}^{\prime}, \ldots, \epsilon_{n}^{\prime}}=(-\nu)^{-n(n-1) / 2} \int_{-\infty}^{\infty} \frac{\mathrm{d} x_{1}}{2 \pi} \cdots \int_{-\infty}^{\infty} \frac{\mathrm{d} x_{n}}{2 \pi} \prod_{a>b} \frac{\sinh \left(x_{a}-x_{b}\right)}{\sinh \left[\left(x_{a}-x_{b}-\mathrm{i} f_{a b} \pi\right) \nu\right]} \\
& \times \prod_{k=1}^{n} \frac{\sinh ^{y_{k}-1}\left[\left(x_{k}+\mathrm{i} \pi / 2\right) \nu\right] \sinh ^{n-y_{k}}\left[\left(x_{k}-\mathrm{i} \pi / 2\right) \nu\right]}{\cosh ^{n} x_{k}} \tag{2.2}
\end{align*}
$$

where the parameter $v$ is related to the anisotropy as $\Delta=\cos \pi \nu$ and $f_{a b}$ and $y_{k}$ are determined as

$$
\begin{align*}
& f_{a b}=\left(1+\operatorname{sign}\left[\left(s^{\prime}-a+1 / 2\right)\left(s^{\prime}-b+1 / 2\right)\right]\right) / 2, \\
& y_{1}>y_{2}>\cdots>y_{s^{\prime}}, \quad \epsilon_{y_{i}}^{\prime}=+  \tag{2.3}\\
& y_{s^{\prime}+1}>\cdots>y_{n}, \quad \epsilon_{n+1-y_{i}}=-.
\end{align*}
$$

In the case of $\Delta=1 / 2$, namely $v=1 / 3$, the significant simplification occurs in the multiple integrals due to the trigonometric identity

$$
\begin{equation*}
\sinh \left(x_{a}-x_{b}\right)=4 \sinh \left[\left(x_{a}-x_{b}\right) / 3\right] \sinh \left[\left(x_{a}-x_{b}+\mathrm{i} \pi\right) / 3\right] \sinh \left[\left(x_{a}-x_{b}-\mathrm{i} \pi\right) / 3\right] \tag{2.4}
\end{equation*}
$$

Actually, if we note that the parameter $f_{a b}$ takes the value 0 or 1 , the first factor in the multiple integral at $v=1 / 3$ can be decomposed as

$$
\begin{align*}
& \frac{\sinh \left(x_{a}-x_{b}\right)}{\sinh \left[\left(x_{a}-x_{b}-\mathrm{i} \pi\right) / 3\right]}=4 \sinh \left(\frac{x_{a}-x_{b}}{3}\right) \sinh \left(\frac{x_{a}-x_{b}+\mathrm{i} \pi}{3}\right) \\
&=-1+\omega \mathrm{e}^{\frac{2}{3}\left(x_{a}-x_{b}\right)}+\omega^{-1} \mathrm{e}^{-\frac{2}{3}\left(x_{a}-x_{b}\right)},  \tag{2.5}\\
& \frac{\sinh \left(x_{a}-x_{b}\right)}{\sinh \left[\left(x_{a}-x_{b}\right) / 3\right]}=4 \sinh \left(\frac{x_{a}-x_{b}+\mathrm{i} \pi}{3}\right) \sinh \left(\frac{x_{a}-x_{b}-\mathrm{i} \pi}{3}\right) \\
&=1+\mathrm{e}^{\frac{2}{3}\left(x_{a}-x_{b}\right)}+\mathrm{e}^{-\frac{2}{3}\left(x_{a}-x_{b}\right)}, \tag{2.6}
\end{align*}
$$

where $\omega=\mathrm{e}^{\mathrm{i} \pi / 3}$. Expanding the trigonometric functions in the second factor into exponentials

$$
\begin{align*}
& \sinh ^{y-1}[(x+\mathrm{i} \pi / 2) / 3] \sinh ^{n-y}[(x-\mathrm{i} \pi / 2) / 3] \\
& \quad=2^{1-n}\left(\omega^{1 / 2} \mathrm{e}^{x / 3}-\omega^{-1 / 2} \mathrm{e}^{-x / 3}\right)^{y-1}\left(\omega^{-1 / 2} \mathrm{e}^{x / 3}-\omega^{1 / 2} \mathrm{e}^{-x / 3}\right)^{n-y} \\
& \quad=2^{1-n} \sum_{l=0}^{y-1} \sum_{m=0}^{n-y}(-1)^{l+m}\binom{y-1}{l}\binom{n-y}{m} \omega^{y-l+m-(n+1) / 2} \mathrm{e}^{\frac{1}{3}(n-2 l-2 m-1) x}, \tag{2.7}
\end{align*}
$$

we can explicitly evaluate the multiple integral by use of the formula
$\int_{-\infty}^{\infty} \frac{\mathrm{e}^{\alpha x} \mathrm{~d} x}{\cosh ^{n} x}=2^{n-1} B\left(\frac{n+\alpha}{2}, \frac{n-\alpha}{2}\right), \quad \operatorname{Re}(n \pm \alpha)>0$,
where $B(p, q)$ is the beta function defined by

$$
\begin{equation*}
B(p, q)=\int_{0}^{1} t^{p-1}(1-t)^{q-1} \mathrm{~d} t, \quad \operatorname{Re}(p), \operatorname{Re}(q)>0 \tag{2.9}
\end{equation*}
$$

Below we shall explicitly describe the procedure for simple cases. The $n=1$ case is rather trivial

$$
\begin{equation*}
P_{+}^{+}=P_{-}^{-}=\int_{-\infty}^{\infty} \frac{\mathrm{d} x}{2 \pi} \frac{1}{\cosh x}=\frac{1}{2} . \tag{2.10}
\end{equation*}
$$

Note that $P_{-}^{+}=P_{+}^{-}=0$ due to the condition $P_{\epsilon_{1}, \ldots, \epsilon_{n}}^{\epsilon_{1}^{\prime}, \ldots, \epsilon_{n}^{\prime}}=0$ if $\sum_{j=1}^{n} \epsilon_{j} \neq \sum_{j=1}^{n} \epsilon_{j}^{\prime}$.
Next let us calculate $P_{++}^{++}$as an example. From equation (2.3), we have in this case $s^{\prime}=2, y_{1}=2, y_{2}=1, f_{21}=1$. Substituting these parameters into the integral formula (2.2), we have

$$
\begin{align*}
P_{++}^{++}= & (-3) \int_{-\infty}^{\infty} \frac{\mathrm{d} x_{1}}{2 \pi} \int_{-\infty}^{\infty} \frac{\mathrm{d} x_{2}}{2 \pi} \frac{\sinh \left(x_{2}-x_{1}\right)}{\sinh \left[\left(x_{2}-x_{1}-\mathrm{i} \pi\right) / 3\right]} \\
& \times \frac{\sinh \left[\left(x_{1}+\mathrm{i} \pi / 2\right) / 3\right]}{\cosh ^{2} x_{1}} \frac{\sinh \left[\left(x_{2}-\mathrm{i} \pi / 2\right) / 3\right]}{\cosh ^{2} x_{2}} \\
= & (-3) \int_{-\infty}^{\infty} \frac{\mathrm{d} x_{1}}{2 \pi \cosh ^{2} x_{1}} \int_{-\infty}^{\infty} \frac{\mathrm{d} x_{2}}{2 \pi \cosh ^{2} x_{2}}\left(-1+\omega \mathrm{e}^{\frac{2}{3}\left(x_{2}-x_{1}\right)}+\omega^{-1} \mathrm{e}^{-\frac{2}{3}\left(x_{2}-x_{1}\right)}\right) \\
& \times \frac{1}{4}\left(\omega^{1 / 2} \mathrm{e}^{x_{1} / 3}-\omega^{-1 / 2} \mathrm{e}^{-x_{1} / 3}\right)\left(\omega^{-1 / 2} \mathrm{e}^{x_{2} / 3}-\omega^{1 / 2} \mathrm{e}^{-x_{2} / 3}\right) \\
= & \left(-\frac{3}{4}\right)\left[(-2)\left(I_{1 / 3} I_{1 / 3}+I_{1} I_{1}\right)+2\left(\omega+\omega^{-1}\right)\left(I_{1 / 3} I_{1 / 3}+I_{1 / 3} I_{1}\right)\right] \\
= & \frac{1}{8} \tag{2.11}
\end{align*}
$$

where
$I_{\alpha}=\int_{-\infty}^{\infty} \frac{\mathrm{e}^{\alpha x} \mathrm{~d} x}{2 \pi \cosh ^{2} x}=\frac{1}{\pi} B(1+\alpha / 2,1-\alpha / 2), \quad$ for $\quad|\alpha|<2$,
and we have used the fact that $I_{1 / 3}=1 / 3, I_{1}=1 / 2, \omega+\omega^{-1}=1$.
In this way we have succeeded in calculating all the density matrix elements up to six lattice sites. All the results are represented by single rational numbers, which are presented in appendix A.

Any spin correlation function can be expressed as a linear combination of density matrix elements. For example longitudinal and transverse two-point correlation functions can be written in terms of density matrices as
$\left\langle S_{1}^{z} S_{n}^{z}\right\rangle=\frac{1}{4} \sum_{\epsilon_{1}, \ldots, \epsilon_{n}} \epsilon_{1} \epsilon_{n} P_{\epsilon_{1}, \ldots, \epsilon_{n}}^{\epsilon_{1}, \ldots, \epsilon_{n}}, \quad\left\langle S_{1}^{x} S_{n}^{x}\right\rangle=\frac{1}{4} \sum_{\epsilon_{1}, \ldots, \epsilon_{n}} P_{-\epsilon_{1}, \epsilon_{2}, \ldots, \epsilon_{n-1},-\epsilon_{n}}^{\epsilon_{1}, \epsilon_{2}, \ldots, \epsilon_{n-1}, \epsilon_{n}}$

Table 1. Comparison with the asymptotic formula of the transverse correlation function

|  | $\left\langle S_{1}^{x} S_{2}^{x}\right\rangle$ | $\left\langle S_{1}^{x} S_{3}^{x}\right\rangle$ | $\left\langle S_{1}^{x} S_{4}^{x}\right\rangle$ | $\left\langle S_{1}^{x} S_{5}^{x}\right\rangle$ | $\left\langle S_{1}^{x} S_{6}^{x}\right\rangle$ |
| :--- | :---: | :--- | :---: | :--- | :---: |
| Exact | -0.156250 | 0.0800781 | -0.0671234 | 0.0521997 | -0.0467664 |
| Asymptotics | -0.159522 | 0.0787307 | -0.0667821 | 0.0519121 | -0.0466083 |

Especially as for the transverse correlation functions, we have newly obtained the fourth- and fifth-neighbour correlation functions from our results of density matrix elements on six lattice sites as
$\left\langle S_{1}^{x} S_{2}^{x}\right\rangle=-\frac{5}{32}=-0.15625$,
$\left\langle S_{1}^{x} S_{3}^{x}\right\rangle=\frac{41}{512}=0.080078125$,
$\left\langle S_{1}^{x} S_{4}^{x}\right\rangle=-\frac{4399}{65536}=-0.0671234130859375$,
$\left\langle S_{1}^{x} S_{5}^{x}\right\rangle=\frac{1751531}{33554432}=0.0521996915340423583984375$,
$\left\langle S_{1}^{x} S_{6}^{x}\right\rangle=-\frac{3213760345}{68719476736}=-0.046766368104727007448673248291015625$.
The asymptotic formula of the transverse two-point correlation function for the massless XXZ chain is established in $[35,36]$
$\left\langle S_{1}^{x} S_{1+n}^{x}\right\rangle \sim A_{x}(\eta) \frac{(-1)^{n}}{n^{\eta}}-\tilde{A}_{x}(\eta) \frac{1}{n^{\eta+\frac{1}{\eta}}}+\cdots, \quad \eta=1-v$,
$A_{x}(\eta)=\frac{1}{8(1-\eta)^{2}}\left[\frac{\Gamma\left(\frac{\eta}{2-2 \eta}\right)}{2 \sqrt{\pi} \Gamma\left(\frac{1}{2-2 \eta}\right)}\right]^{\eta} \exp \left[-\int_{0}^{\infty}\left(\frac{\sinh (\eta t)}{\sinh (t) \cosh [(1-\eta) t]}-\eta \mathrm{e}^{-2 t}\right) \frac{\mathrm{d} t}{t}\right]$,
$\tilde{A}_{x}(\eta)=\frac{1}{2 \eta(1-\eta)}\left[\frac{\Gamma\left(\frac{\eta}{2-2 \eta}\right)}{2 \sqrt{\pi} \Gamma\left(\frac{1}{2-2 \eta}\right)}\right]^{\eta+\frac{1}{\eta}} \exp \left[-\int_{0}^{\infty}\left(\frac{\cosh (2 \eta t) \mathrm{e}^{-2 t}-1}{2 \sinh (\eta t) \sinh (t) \cosh [(1-\eta) t]}\right.\right.$
$\left.\left.+\frac{1}{\sinh (\eta t)}-\frac{\eta^{2}+1}{\eta} \mathrm{e}^{-2 t}\right) \frac{\mathrm{d} t}{t}\right]$,
where $\Gamma(s)$ is the Gamma function defined by $\Gamma(s)=\int_{0}^{\infty} t^{s-1} \mathrm{e}^{-t} \mathrm{~d} t$. This asymptotic formula produces a good numerical value even for small $n$ as is shown in table 1. Note that the longitudinal correlation function was obtained up to eighth-neighbour correlation $\left\langle S_{1}^{z} S_{9}^{z}\right\rangle$ from the multiple integral representation for the generating function [32]. Note also that up to third-neighbour both longitudinal and transverse correlation functions for general anisotropy $\Delta$ were obtained in [21].

## 3. Reduced density matrix and entanglement entropy

Below let us discuss the reduced density matrix for a finite sub-chain and its entanglement entropy. The density matrix for the infinite system at zero temperature has the form

$$
\begin{equation*}
\rho_{\mathrm{T}} \equiv|\mathrm{GS}\rangle\langle\mathrm{GS}|, \tag{3.1}
\end{equation*}
$$

where $|\mathrm{GS}\rangle$ denotes the ground state of the total system. We consider a finite sub-chain consisting of sites $1, \ldots, n$, the rest of which is regarded as an environment. We define the


Figure 1. Eigenvalue-distribution of density matrices.

Table 2. Entanglement entropy $S(n)$ of a finite sub-chain of length $n$.

| $S(1)$ | $S(2)$ | $S(3)$ | $S(4)$ |
| :--- | :--- | :--- | :--- |
| 1 | 1.3716407621868583 | 1.5766810784924767 | 1.7179079372711414 |
|  |  | $S(5)$ | $S(6)$ |
|  |  | 1.8262818282012363 | 1.9144714710902746 |

reduced density matrix for this sub-chain by tracing out the environment from the infinite chain

$$
\begin{equation*}
\rho_{n} \equiv \rho_{1,2, \ldots, n}=\operatorname{tr}_{-\infty, \ldots, 0, n+1, \ldots, \infty} \rho_{\mathrm{T}}=\left[P_{\epsilon_{1}, \ldots, \epsilon_{n}}^{\epsilon_{1}^{\prime}, \ldots, \epsilon_{n}^{\prime}}\right]_{\epsilon_{j}, \epsilon_{j}^{\prime}= \pm} \tag{3.2}
\end{equation*}
$$

where $\operatorname{tr}_{n_{1}, n_{2}}, \ldots$ means the trace over the sites $n_{1}, n_{2}, \ldots$. We have numerically evaluated all the eigenvalues $\omega_{\alpha}\left(\alpha=1,2, \ldots, 2^{n}\right)$ of the reduced density matrix $\rho_{n}$ up to $n=6$. We show the distribution of the eigenvalues in figure 1. The distribution is less degenerate compared with the isotropic case $\Delta=1$ shown in [24]. In the odd $n$ case, all the eigenvalues are two-fold degenerate due to the spin-reverse symmetry.

Subsequently, we exactly evaluate the von Neumann entropy (Entanglement entropy) defined as

$$
\begin{equation*}
S(n) \equiv-\operatorname{tr} \rho_{n} \log _{2} \rho_{n}=-\sum_{\alpha=1}^{2^{n}} \omega_{\alpha} \log _{2} \omega_{\alpha} \tag{3.3}
\end{equation*}
$$

The exact numerical values of $S(n)$ up to $n=6$ are shown in table 2. By analysing the behaviour of the entanglement $S(n)$ for large $n$, we can see how long quantum correlations reach [37]. In the massive region $\Delta>1$, the entanglement entropy will be saturated as $n$ grows due to the finite correlation length. This means that the ground state is well approximated by a subsystem of a finite length corresponding to the large eigenvalues of the reduced density matrix. On the other hand, in the massless case $-1<\Delta \leqslant 1$, the conformal field theory predict that the entanglement entropy shows a logarithmic divergence as $n \rightarrow \infty$ [38]

$$
\begin{equation*}
S(n) \sim \frac{1}{3} \log _{2} n+k_{\Delta}, \tag{3.4}
\end{equation*}
$$

where $k_{\Delta}$ represents a constant term depending on the anisotropy $\Delta$. Our exact results up to $n=6$ agree quite well with the asymptotic formula as shown in figure 2 . We estimate the numerical value of the constant term $k_{\Delta=1 / 2}$ as $k_{\Delta=1 / 2} \sim S(6)-\frac{1}{3} \log _{2} 6=1.0528$. This numerical value is slightly smaller than the isotropic case $\Delta=1$, where the constant $k_{\Delta=1}$ is estimated as $k_{\Delta=1} \sim 1.0607$ from the exact data for $S(n)$ up to $n=6$ [24]. At free fermion


Figure 2. Entanglement entropy $S(n)$ of a finite sub-chain of length $n$.
point $\Delta=0$, the exact asymptotic formula has been obtained in [39]

$$
\begin{align*}
& S(n) \sim \frac{1}{3} \log _{2} n+k_{\Delta=0}, \\
& k_{\Delta=0}=1 / 3-\int_{0}^{\infty} \mathrm{d} t\left\{\frac{\mathrm{e}^{-t}}{3 t}+\frac{1}{t \sinh ^{2}(t / 2)}-\frac{\cosh (t / 2)}{2 \sinh ^{3}(t / 2)}\right\} / \ln 2 \tag{3.5}
\end{align*}
$$

In this case the numerical value for the constant term is given by $k_{\Delta=0}=1.0474932144 \cdots$.

## 4. Summary and discussion

We have succeeded in obtaining all the density matrix elements on six lattice sites for XXZ chain at $\Delta=1 / 2$. Especially, we have newly obtained the fourth- and fifth-neighbour transverse spin-spin correlation functions. Our exact results for the transverse correlations show good agreement with the asymptotic formula established in [35, 36]. Subsequently we have calculated all the eigenvalues of the reduced density matrix $\rho_{n}$ up to $n=6$. From these results we have exactly evaluated the entanglement entropy, which shows a good agreement with the asymptotic formula derived via the conformal field theory. Finally, we remark that similar procedures to evaluate the multiple integrals are also possible at $v=1 / n$ for $n=4,5,6, \ldots$, since there are similar trigonometric identities as (2.4). We will report the calculation of correlation functions for these cases in subsequent papers.

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## Appendix. Density matrix elements up to $n=6$

In this appendix we present all the independent-density matrix elements defined in equation (2.1) up to $n=6$. Other elements can be computed from the relations

$$
\begin{equation*}
P_{\epsilon_{1}, \ldots, \epsilon_{n}}^{\epsilon_{1}^{\prime}, \ldots, \epsilon_{n}^{\prime}}=0 \quad \text { if } \quad \sum_{j=1}^{n} \epsilon_{j} \neq \sum_{j=1}^{n} \epsilon_{j}^{\prime}, \tag{A.1}
\end{equation*}
$$

$$
\begin{align*}
& P_{\epsilon_{1}, \ldots, \epsilon_{n}}^{\epsilon_{1}^{\prime}, \ldots, \epsilon_{n}^{\prime}}=P_{\epsilon_{1}^{\prime}, \ldots, \epsilon_{n}^{\prime}}^{\epsilon_{1}, \ldots, \epsilon_{n}}=P_{-\epsilon_{1}, \ldots,-\epsilon_{n}^{\prime}}^{-\epsilon_{1}^{\prime}, \ldots,-\epsilon_{n}^{\prime}}=P_{\epsilon_{n}, \ldots, \epsilon_{1}}^{\epsilon_{n}^{\prime}, \ldots, \epsilon_{1}^{\prime}},  \tag{A.2}\\
& P_{+, \epsilon_{1}, \ldots, \epsilon_{n}}^{+,+\epsilon_{1}^{\prime}, \ldots, \epsilon_{n}^{\prime}}+P_{-, \epsilon_{1}, \ldots, \epsilon_{n}}^{-,, \epsilon_{1}^{\prime}, \ldots, \epsilon_{n}^{\prime}}=P_{\epsilon_{1}, \ldots, \epsilon_{n},+}^{\epsilon_{1}^{\prime}, \ldots, \epsilon_{n}^{\prime},+}+P_{\epsilon_{1}, \ldots, \epsilon_{n},--}^{\epsilon_{1}^{\prime}, \ldots, \epsilon_{n}^{\prime},-}=P_{\epsilon_{1}, \ldots, \epsilon_{n}}^{\epsilon_{1}^{\prime}, \ldots, \epsilon_{n}^{\prime}}, \tag{A.3}
\end{align*}
$$

and the formula for the EFP $[33,34]$,

$$
\begin{equation*}
P(n)=P_{+, \ldots,+}^{+, \ldots,+}=2^{-n^{2}} \prod_{k=0}^{n-1} \frac{(3 k+1)!}{(n+k)!} . \tag{A.4}
\end{equation*}
$$

A.1. $n \leqslant 4$
$P_{+-}^{-+}=-\frac{5}{16}=-0.3125, \quad P_{++-}^{-++}=\frac{41}{512}=0.0800781$,
$P_{+-++}^{-+++}=-\frac{221}{8192}=-0.0269775, \quad P_{++-+}^{-+++}=\frac{1579}{65536}=0.0240936$,
$P_{+++-}^{-+++}=-\frac{289}{32768}=-0.00881958, \quad P_{+-++}^{+-++}=\frac{1037}{16384}=0.0632935$,
$P_{++-+}^{+++}=-\frac{2005}{32768}=-0.0611877, \quad P_{+-+-}^{--++}=-\frac{3821}{65536}=-0.0583038$,
$P_{++--}^{--+}=\frac{1393}{65536}=0.0212555, \quad P_{+-+-}^{-+-+}=\frac{4883}{32768}=0.149017$,
$P_{+--+}^{-++-}=\frac{3091}{32768}=0.0943298$.
A.2. $n=5$
$P_{+-++}^{-++++}=-\frac{14721}{8388608}=-0.00175488, \quad P_{++-++}^{-++++}=\frac{37335}{16777216}=0.00222534$,
$P_{+++++}^{-++++}=-\frac{48987}{33554432}=-0.00145993, \quad P_{++++-}^{-++++}=\frac{13911}{33554432}=0.00041458$,
$P_{+-+++}^{+-++}=\frac{179699}{33554432}=0.00535545, \quad P_{++-++}^{+++++}=-\frac{120337}{16777216}=-0.00717264$,
$P_{+++-+}^{+-+++}=\frac{165155}{33554432}=0.004922, \quad P_{++-++}^{++++}=\frac{168313}{16777216}=0.0100322$,
$P_{+--++}^{--+++}=\frac{31069}{2097152}=0.0148149, \quad P_{+-+++}^{--++}=-\frac{411583}{16777216}=-0.0245323$,
$P_{+-++-}^{--+++}=\frac{196569}{16777216}=0.0117164, \quad P_{++-+-}^{--+++}=-\frac{281271}{33554432}=-0.00838253$,
$P_{+++--}^{--++}=\frac{79673}{33554432}=0.00237444, \quad P_{+--++}^{-+-++}=-\frac{1441787}{33554432}=-0.0429686$,
$P_{+-++}^{-+-++}=-\frac{1261655}{33554432}=-0.0376002, \quad P_{++-+}^{-+++}=\frac{59459}{2097152}=0.0283523$,
$P_{+-+-}^{-++-+}=\frac{1575515}{33554432}=0.046954, \quad P_{+-++}^{-+++-}=-\frac{696151}{33554432}=-0.0207469$,
$P_{+-+-}^{-+++-}=\frac{1366619}{33554432}=0.0407284$.
A.3. $n=6$

$$
\begin{aligned}
& P_{++++++}^{-+++++}=-\frac{1546981}{34359738368}=-0.0000450231, \quad P_{++++++}^{-++++}=\frac{5095899}{68719476736}=0.0000741551, \\
& P_{+++++}^{-++++}=-\frac{2366275}{34359738368}=-0.0000688677, \quad P_{+++++}^{-++++}=\frac{2455833}{68719476736}=0.0000357371, \\
& P_{+++++-}^{-++++}=-\frac{284577}{34359738368}=-8.28228 \times 10^{-6} \text {, } \\
& P_{++-+++}^{+-+++}=-\frac{20086627}{68719476736}=-0.000292299, \\
& P_{+++++}^{+++++}=-\frac{10295153}{68719476736}=-0.000149814, \\
& P_{+++-++}^{+++++}=-\frac{35087523}{68719476736}=-0.000510591, \\
& P_{+-+++}^{--++++}=-\frac{214080091}{68719476736}=-0.00311528, \\
& P_{+-+++-}^{--++++}=-\frac{57522267}{68719476736}=-0.000837059, \\
& P_{+++++}^{--++++}=-\frac{154538459}{68719476736}=-0.00224883 \text {, } \\
& P_{+++-+}^{--++++}=\frac{6708473}{8589934592}=0.000780969 \text {, } \\
& P_{++++--}^{--+++}=\frac{3860673}{34359738368}=0.00011236 \text {, } \\
& P_{+++-++}^{-++++}=\frac{12211375}{1073741824}=0.0113727 \text {, } \\
& P_{+++++}^{-++++}=\frac{56183761}{17179869184}=0.00327033 \text {, } \\
& P_{++-+-+}^{-++++}=\frac{606065059}{68719476736}=0.00881941 \text {, } \\
& P_{+++-+}^{-+-+++}=-\frac{108202041}{34359738368}=-0.00314909, \\
& P_{+-+++}^{-++++}=\frac{7860495}{1073741824}=0.00732066 \text {, } \\
& P_{+-+++}^{-++++}=\frac{1044016671}{68719476736}=0.0151924 \text {, } \\
& P_{++--++}^{-++-+}=\frac{676957849}{68719476736}=0.00985103 \text {, } \\
& P_{++++-}^{-++++}=\frac{6581795}{1073741824}=0.00612977 \text {, } \\
& P_{+-+++}^{-++++}=-\frac{185522333}{34359738368}=-0.00539941 \text {, } \\
& P_{+-+++}^{-++++}=-\frac{103539423}{8589934592}=-0.0120536 \text {, } \\
& P_{++-++}^{-++++}=-\frac{267901987}{34359738368}=-0.00779697 \text {, } \\
& P_{+++--+}^{-++++}=-\frac{309855965}{68719476736}=-0.004509 \text {, } \\
& P_{+-+-++}^{-++++}=-\frac{296882461}{68719476736}=-0.00432021, \\
& P_{++-+++}^{-++++}=\frac{5095899}{68719476736}=0.0000741551, \\
& P_{+++++}^{-++++}=\frac{2455833}{68719476736}=0.0000357371 \text {, } \\
& P_{+-++++}^{+++++}=\frac{2927709}{17179869184}=0.000170415 \text {, } \\
& P_{+++-++}^{+-+++}=\frac{19268565}{68719476736}=0.000280395 \text {, } \\
& P_{++-+++}^{++-++}=\frac{17781349}{34359738368}=0.000517505 \text {, } \\
& P_{+--++}^{--++++}=\frac{48421023}{34359738368}=0.00140924 \text {, } \\
& P_{+-+++}^{--++++}=\frac{88171589}{34359738368}=0.00256613 \text {, } \\
& P_{++-++}^{--++++}=\frac{56776545}{34359738368}=0.00165241 \text {, } \\
& P_{++++-}^{--++++}=\frac{60809571}{68719476736}=0.000884896 \text {, } \\
& P_{+++-+-}^{--++++}=-\frac{33366621}{68719476736}=-0.000485548 \text {, } \\
& P_{+--+++}^{-+-+++}=-\frac{85706851}{17179869184}=-0.0049888 \text {, } \\
& P_{+-++-+}^{-+-+++}=-\frac{332557469}{34359738368}=-0.0096787, \\
& P_{++-++}^{-+-+++}=-\frac{430452959}{68719476736}=-0.00626391, \\
& P_{++-++}^{-++++}=-\frac{123612511}{34359738368}=-0.0035976 \text {, } \\
& P_{+++++-}^{-+-++}=\frac{70061315}{34359738368}=0.00203905 \text {, } \\
& P_{++-+++}^{-++-+}=-\frac{591759525}{34359738368}=-0.0172225 \text {, } \\
& P_{+-++-}^{-++++}=-\frac{367905053}{68719476736}=-0.00535372 \text {, } \\
& P_{++-++}^{-++-+}=-\frac{988973861}{68719476736}=-0.0143915 \text {, } \\
& P_{+++-+}^{-++-++}=\frac{363618785}{68719476736}=0.00529135 \text {, } \\
& P_{+-+++}^{-+++-+}=\frac{901633567}{68719476736}=0.0131205 \text {, } \\
& P_{+-+++-}^{-+++-+}=\frac{38524625}{8589934592}=0.00448486 \text {, } \\
& P_{++-++}^{-++-+}=\frac{12750645}{1073741824}=0.011875 \text {, } \\
& P_{+-+++}^{-++++}=\frac{29410257}{17179869184}=0.0017119 \text {, } \\
& P_{+-+++}^{-++++}=\frac{35985105}{8589934592}=0.00418922 \text {, }
\end{aligned}
$$

$$
\begin{aligned}
& P_{++--++}^{-++++}=\frac{92176287}{34359738368}=0.00268268, \quad P_{+--++}^{+--+++}=\frac{202646807}{34359738368}=0.0058978, \\
& P_{+-+-++}^{+--++}=-\frac{972245985}{68719476736}=-0.014148 \text {, } \\
& P_{++-+++}^{+--++}=-\frac{211696415}{17179869184}=-0.0123224 \text {, } \\
& P_{+-++-+}^{+--+++}=\frac{217687057}{17179869184}=0.0126711 \text {, } \\
& P_{+++--+}^{+--++}=\frac{78922695}{17179869184}=0.00459391 \text {, } \\
& P_{+-+-++}^{+-+++}=\frac{1196499417}{34359738368}=0.0348227 \text {, } \\
& P_{+-++-+}^{+-+-++}=-\frac{2209522727}{68719476736}=-0.0321528, \\
& P_{++-++}^{+++++}=\frac{1108384987}{34359738368}=0.0322582 \text {, } \\
& P_{+-++-+}^{+++++}=\frac{530683585}{17179869184}=0.0308899 \text {, } \\
& P_{++--++}^{+++++}=\frac{347202525}{17179869184}=0.0202098 \text {, } \\
& P_{+--++-}^{---++}=-\frac{268623007}{68719476736}=-0.00390898 \text {, } \\
& P_{+-+-+-}^{---++}=\frac{46285135}{8589934592}=0.0053883 \text {, } \\
& P_{+-++-+}^{---++}=-\frac{136974885}{68719476736}=-0.00199325 \text {, } \\
& P_{++-+--}^{---+++}=\frac{19939391}{17179869184}=0.00116063 \text {, } \\
& P_{+++---}^{---++}=-\frac{18442085}{68719476736}=-0.000268368 \text {, } \\
& P_{+--++-}^{--+-++}=\frac{1018463205}{68719476736}=0.0148206 \text {, } \\
& P_{+-+-+-}^{--+-+}=-\frac{1454513249}{68719476736}=-0.021166 \text {, } \\
& P_{+-++--}^{--+-++}=\frac{277721503}{34359738368}=0.00808276 \text {, } \\
& P_{++-+--}^{--+++}=-\frac{335265249}{68719476736}=-0.00487875 \text {, } \\
& P_{+-+++}^{--+++}=-\frac{369408975}{17179869184}=-0.0215024 \text {, } \\
& P_{+-+-+-}^{--+++}=\frac{1104236607}{34359738368}=0.0321375 \text {, } \\
& P_{+-++-+}^{--+++}=-\frac{880560357}{68719476736}=-0.0128138 \text {, } \\
& P_{++-++-}^{--++-+}=-\frac{876924641}{68719476736}=-0.0127609 \text {, } \\
& P_{+---++}^{--+++}=\frac{113631201}{17179869184}=0.00661421 \text {, } \\
& P_{+-+++}^{--+++}=-\frac{292857807}{17179869184}=-0.0170466, \\
& P_{+-+-++}^{--+++}=\frac{548645951}{34359738368}=0.0159677 \text {, } \\
& P_{++--++}^{--++-}=-\frac{377925345}{68719476736}=-0.00549954 \text {, } \\
& P_{+--++-}^{-+-++}=\frac{1719255909}{34359738368}=0.0500369 \text {, } \\
& P_{+-+-+-}^{-+-+-+}=-\frac{5350158879}{68719476736}=-0.0778551 \text {, } \\
& P_{+--+-+}^{-+-++}=\frac{1565770597}{34359738368}=0.0455699 \text {, } \\
& P_{+-+-++}^{-+-++}=-\frac{3059753503}{68719476736}=-0.0445253, \\
& P_{+-++-}^{-++-+}=-\frac{2117554719}{68719476736}=-0.0308145 \text {. }
\end{aligned}
$$

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