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Finite-size effects in the integrable *XXZ* Heisenberg model with arbitrary spin

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Abstract. The finite-size effects in the spectrum of the integrable *XXZ* Heisenberg chain with arbitrary spin-S are studied analytically on the basis of the string hypothesis for bound states and numerically by solving the associated Bethe ansatz equations. The finite-size corrections to the spectrum and to the low-temperature behaviour of the free energy are found to be similar to the universal predictions for conformally invariant theories, although the model is, in general, not Lorentz invariant, since it can have an arbitrary number of branches for low-energy excitations with different Fermi velocities depending on the value of S and the anisotropy parameter γ.

1. Introduction

In recent years there has been a significant advance in the understanding of the critical properties of two-dimensional statistical systems and, equivalently, $(1+1)$-dimensional quantum systems as a consequence of the application of the concept of conformal invariance. This concept provides a simple means for the classification of universality classes in terms of a single dimensionless number, namely the central charge c of the underlying Virasoro algebra. Integrable lattice models in their continuum limit (both two-dimensional vertex models [1] and the related quantum spin chains [2-4]) have been widely used to obtain realisations of conformal field theories. The identification of the critical continuum theory corresponding to a given lattice model is easily achieved by using the predictions of conformal field theory. The central charge c as well as the conformal dimensions $\bar{\Delta}_i$, Δ_i of the primary fields of the continuum theory determine the scaling of the spectra of finite systems. While the spectrum of low-lying excitations is gapless at criticality the energy levels of systems of finite length N (we measure lengths in units of the lattice spacing) are separated by gaps of order $1/N$. Conformal invariance relates the size of these gaps to the central charge and the scaling dimensions $X_i = \Delta_i + \bar{\Delta}_i$ and spins $s_i = \Delta_i - \bar{\Delta}_i$ of the conformal fields [5-7]. The energy $E_0(N)$ of the finite-N ground state and energy E_i and momentum P_i of low-lying excited states scale like

$$E_0(N) - N\varepsilon_\infty = -\frac{\pi v}{6N}\,c + o\left(\frac{1}{N}\right) \tag{1.1a}$$

$$E_i(N, I^+, I^-) - E_0(N) = \frac{2\pi v}{N}(X_i + I^+ + I^-) + o\left(\frac{1}{N}\right) \tag{1.1b}$$

$$P_i(N, I^+, I^-) - P_0 = 2d\mathcal{P}_F + \frac{2\pi}{N}(s + I^+ - I^-). \tag{1.1c}$$

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In (1.1) ε_∞ is the energy density in the ground state of the infinite system, v and $\mathscr{P}_F$ are the Fermi velocity and momentum, respectively, d and $I^\pm \geqslant 0$ are integers. Another prediction from conformal invariance that has been used to identify the central charge for a given continuum theory is the occurrence of a universal term in the low-temperature expansion of the free energy [7]:

$$F(T) = F_0 - \frac{\pi T^2}{6} \frac{c}{v} + o(T^2). \tag{1.2}$$

In addition to the vanishing of mass terms (which leads to scale invariance) a conformally invariant field theory has to be Lorentz invariant, i.e. all low-energy excitations must have linear dispersion with the same Fermi velocity v in the vicinity of the Fermi level. This is manifest in the predictions (1.1) and (1.2). However, there exist systems that have linear excitations with different velocities at criticality. One such model that has been studied recently [8] is the Hubbard chain away from half filling; another large class of such models can be found among the integrable spin-S generalisations of the anisotropic XXZ Heisenberg chain [4, 9–11]. The Hamiltonian of these systems is a polynomial of degree $2S$ in local SU(2) spin operators, the leading term given by the familiar $S = \frac{1}{2}$ expression

$$H = \sum_{n=1}^{N} (S_n^x S_{n+1}^x + S_n^y S_{n+1}^y + \Delta S_n^z S_{n+1}^z). \tag{1.3}$$

For $0 \leqslant \Delta \leqslant 1$ the system is antiferromagnetic and has massless excitations only. In this phase the anisotropy is conveniently parametrised by the real number γ with

$$\Delta = \cos \gamma. \tag{1.4}$$

The standard approach for the construction of the integrable XXZ chain for given spin-S is the quantum inverse scattering method. A physical (i.e. Hermitian) Hamiltonian is obtained if the anisotropy parameter γ is in either one of the allowed regions characterised by the following inequalities [4]:

$$\begin{aligned} &\cos \gamma(2S+1) > \cos \gamma n \qquad \text{for } n = 2S-1, 2S-3, \ldots, -2S+1 \\ &\cos \gamma(2S+1) < \cos \gamma n \qquad \text{for } n = 2S-1, 2S-3, \ldots, -2S+1. \end{aligned} \tag{1.5}$$

(These conditions are equivalent to the existence of certain bound states, namely strings of length $(2S+1)$, see section 2 below).

Kirillov and Reshetikhin have solved this model for arbitrary spin in the allowed regions (1.5) for the anisotropy. Using standard Bethe ansatz techniques they found for the leading term in a low-temperature expansion of the bulk free energy [11]

$$F(T) = F_0 - \frac{\pi T^2}{6} \sum_i \frac{c_i}{v_i} + o(T^2). \tag{1.6}$$

Here the v_i are the Fermi velocities for the different branches of low-energy excitations and $c_i = 3k_i/(k_i + 2)$ with certain positive integers k_i related to the continued fraction expansion of the parameter γ. While the Fermi velocities v_i are continuous functions of the anisotropy the set of numbers $\{c_i\}$ does not change in any of the regions allowed by (1.5).

For anisotropies in one of the intervals

$$k < \frac{\pi}{\gamma} < k + \frac{k}{2S-k} \tag{1.7}$$

with k and $2S/k$ integer there exists a single Fermi velocity only and the sum in (1.6) reduces to one term [4]. In this case the theory is conformally invariant, from (1.2) the central charge is found to be $c=3k/(k+2)$. Finite-size scaling methods have been applied [3, 4] to identify the corresponding continuum field theory as a semidirect product of a Gaussian [12] and a $Z(k)$ parafermion model [13]. For $S \leqslant 3$ all the regions allowed by the inequalities (1.5) are of the form (1.7). For larger S, however, there exist allowed intervals of anisotropy where more than one Fermi velocity exists. In these intervals the expression (1.6) for the free energy can be thought of as a generalisation of the conformal result (1.2) to the case of not Lorentz invariant critical theories. The question arises whether similar generalisations of (1.1), i.e. a universal tower structure in the spectra of finite systems similar to the one existing in conformally invariant theories, can be found in the higher-spin XXZ chains with more than one Fermi velocity.

In the present work we address this question by investigating the finite-size scaling properties of these models both analytically and numerically. Our paper is organised as follows. In the next section we review the Bethe ansatz analysis and the construction of the ground state for the infinite chain [4, 9–10]. In section 3 we use the techniques introduced by Woynarovich *et al* [14] (for earlier work using similar methods see also [15]) to obtain analytical expressions for the finite-size corrections to the energies of the ground state and low-lying excitations. The results do indeed indicate how (1.1) have to be generalised to describe the spectra of finite, not Lorentz invariant theories: just as with the low-temperature behaviour of the free energy, the scaling of the ground state energy is determined by a set of γ-independent numbers $\tilde{c}_i$, which seems to indicate a composite continuum theory made up of several independent fields. The scaling of excited states, however, shows that this is not true: the generalisation of the X_i in (1.1b) contains contributions with different velocities v_i.

A drawback in this approach is that the $\tilde{c}_i$ determining the scaling of the ground-state energy are all found to be unity which, in general, does not agree with the c_i obtained from the low-temperature expansion of the free energy (equation (1.6)). In the Lorentz invariant, and hence conformal, regions (1.7) the scaling dimensions X_i derived here are the contributions of the Gaussian constituent of the continuum field theory only, the contributions from the parafermionic $Z(k)$ sector are missing. This is a well known shortcoming of this method for the analytical calculation of spectra of finite chains [3]: it is based on the string hypothesis which assumes a certain structure for the bound states (see below). This hypothesis does give the right results in the thermodynamic limit $N \to \infty$ (in which (1.6) has been derived), but is known to neglect certain finite-size effects [16, 17]—hence the prediction for the $\tilde{c}_i$ and the energies of excited states in the finite chain is only of limited value. Nevertheless, the analytical results obtained this way can be used as a basis for our analysis of numerical finite-size data in section 4 where we investigate the simplest system in this class of spin chains with more than one branch of low-energy excitations, namely the $S=\frac{7}{2}$ chain with anisotropies in the interval $\frac{5}{2} < (\pi/\gamma) < 3$. As in the conformally invariant cases (1.7) we find that the discrepancy between the exact numerical results and the analytical prediction based on the string assumption can be understood in terms of contributions of $Z(k_i)$ parafermion operators.

In fact, it appears that if one formally sets all the Fermi velocities v_i to a common value v—such that the theory is conformally invariant in spite of the existence of different branches of low-energy excitations—the continuum theory corresponding to the spin-S XXZ chain with free energy (1.6) can be interpreted as a multicomponent model with constituents being products of Gaussian and $Z(k_i)$ parafermion models. Similar multicomponent conformal field theories with purely Gaussian constituents have been found before in the investigation of q-state vertex models [18] and nested Bethe ansatz models [19, 20].

2. The ground state of the infinite chain

Eigenstates of the spin-S XXZ chain with anisotropy parameter γ are characterised by the solutions $\{\lambda_j\}$ of the Bethe ansatz equations [4, 9–10]:

$$\left(\frac{\sinh[\frac{1}{2}\gamma(\lambda_j+\mathrm{i}2S)]}{\sinh[\frac{1}{2}\gamma(\lambda_j-\mathrm{i}2S)]}\right)^N=\prod_{k\neq j}\left(\frac{\sinh[\frac{1}{2}\gamma(\lambda_j-\lambda_k+2\mathrm{i})]}{\sinh[\frac{1}{2}\gamma(\lambda_j-\lambda_k-2\mathrm{i})]}\right). \tag{2.1}$$

A given eigenstate $|\lambda_1,\ldots,\lambda_M\rangle$ has total magnetisation $\langle\Sigma_n S_n^z\rangle=(SN-M)$. The energy and momentum of a state corresponding to a solution $\{\lambda_k\}$ of (2.1) are

$$E=\sum_k\frac{-\sin(2S\gamma)}{\sinh[\frac{1}{2}\gamma(\lambda_k+2\mathrm{i}S)]\sinh[\frac{1}{2}\gamma(\lambda_k-2\mathrm{i}S)]} \tag{2.2}$$

$$P=-i\ln(t_N^{(S)}(-\mathrm{i}\gamma)/[a_0(-\mathrm{i}\gamma)]^N)=2\sum_k\tan^{-1}(\tanh(\tfrac{1}{2}\gamma\lambda_k)\cot(\gamma S)). \tag{2.3}$$

In the thermodynamic limit we consider state characterised by M roots λ_k with M/N fixed, $0\leqslant M/N\leqslant S$ and $N\to\infty$. In this limit the solutions of the Bethe ansatz equations (2.1) are known to be arranged in bound states, characterised by uniformly spaced sets of complex λ_j, so-called *strings*. For large but finite N a string of length n and parity $\nu_n=\pm1$ is a group of n roots λ_j arranged like $(1\leqslant k\leqslant n)$:

$$\lambda_{i,k}^n=\lambda_i^n+\mathrm{i}\left(n+1-2k+\frac{\pi}{2\gamma}(1-\nu_\sigma\nu_n)\right)+\delta_k. \tag{2.4}$$

Here the real number λ_i^n is the string's centre, $\delta_k=(\delta_{n-k})^*$ are corrections that vanish for the infinite system, and $\nu_\sigma=\exp(\mathrm{i}\pi[2S\gamma/\pi])$ is the spin parity ($[x]$ denotes the integer part of x).

The possible values of the string length and the corresponding parity depend on the value of the anisotropy γ. A construction of the allowed values of n and ν_n was given by Takahashi and Suzuki [21]. For a given value of γ they introduced the following sequences of real numbers p_i and integers b_i, y_i, m_i:

$$p_0=\frac{\pi}{\gamma}\qquad p_1=1\qquad b_i=\left[\frac{p}{p_{i+1}}\right]\qquad p_{i+1}=p_{i-1}-b_{i-1}p_i \tag{2.5a}$$

$$y_{-1}=0\qquad y_0=1\qquad y_1=b_0\qquad y_{i+1}=y_{i-1}+b_iy_i \tag{2.5b}$$

$$m_0=0\qquad m_1=b_0\qquad m_{i+1}=m_i+b_i. \tag{2.5c}$$

In (2.5) the b_i are related to the continued fraction expansion of p_0:

$$p_0=[b_0,b_1,b_2,\ldots]=b_0+\cfrac{1}{b_1+\cfrac{1}{b_2+\ldots}} \tag{2.6a}$$

$$\frac{p_i}{p_{i+1}}=[b_i,b_{i+1},\ldots]. \tag{2.6b}$$

With these definitions they found that the lengths and parities of the bound states (2.4) are given by the Takahashi numbers and related parities:

$$n_j = y_{i-1} + (j - m_i) y_i \qquad m_i \leqslant j < m_{i+1} \tag{2.7a}$$

$$\nu_j \equiv \nu_{n_j} = \exp\left(i\pi \left[\frac{n_j - 1}{p_0} \right] \right) \qquad j \neq m_1, \ \nu_{m_1} = -1. \tag{2.7b}$$

It can be shown that the set of inequalities (1.5) is equivalent to the statement that $2S+1$ is one of the Takahashi numbers (2.7).

In the regions of anisotropy allowed by (1.5) all the roots of the Bethe ansatz equations (2.1) are arranged in string configurations (2.4). Neglecting the finite-size corrections δ_k, this allows us to write down equations for the centres $\lambda_i^{(j)}$ of the n_j-strings:

$$N t_{j,2S}(\lambda_i^{(j)}) = 2\pi J_i^{(j)} + \sum_k \sum_{n=1}^{M_k} \Theta_{jk}(\lambda_i^{(j)} - \lambda_n^{(k)}). \tag{2.8}$$

Here M_k is the number of n_k-strings, the $J_i^{(j)}$ are integers (or half-odd integers), and the functions $t_{j,2S}$ and Θ_{jk} are given by

$$t_{j,2S}(\lambda) = \sum_{l=1}^{\min(n_j, 2S)} f(\lambda : |n_j - 2S| + 2l - 1, \ \nu_j \nu_\sigma) \tag{2.9a}$$

$$\Theta_{jk}(\lambda) = f(\lambda : |n_j - n_k|, \ \nu_j\nu_k) + f(\lambda : n_j + n_k, \ \nu_j \nu_k)$$
$$+ 2 \sum_{l=1}^{\min(n_j, n_k)-1} f(\lambda ; |n_j - n_k| + 2l, \ \nu_j \nu_k) \tag{2.9b}$$

where

$$f(\lambda : n, \nu) = \begin{cases} 2\nu \tan^{-1}[(\cot(n\gamma/2))^\nu \tanh(\gamma\lambda/2)] & \text{if } n/p_0 \notin \mathbb{Z} \\ 0 & \text{if } n/p_0 \in \mathbb{Z} \end{cases}. \tag{2.9c}$$

The energy of a given solution of the string equations (2.8) can be obtained from (2.2) to be

$$E = \sum_j \sum_{i=1}^{M_k} \varepsilon_j^{(0)}(\lambda_i^{(j)}) \tag{2.10}$$

where

$$\varepsilon_j^{(0)}(\lambda) = -4p_0 a_{j,2S}(\lambda) \equiv \frac{2}{\gamma} t'_{j,2S}(\lambda) \tag{2.11}$$

is the bare energy of the n_j-strings. The momentum of the state $\{\lambda_i^{(j)}\}$ is found to be

$$P = \frac{2\pi}{N} \sum_j \sum_{i=1}^{M_k} J_i^{(j)}. \tag{2.12}$$

In the thermodynamic limit $N \to \infty$ one introduces particle and hole densities $\rho_j(\lambda)$, $\rho_j^{\text{h}}(\lambda)$ of n_j-strings [22]. These densities are determined by the integral equations

$$a_{j,2S}(\lambda) = (-1)^{r(j)}(\rho_j^{\text{h}}(\lambda) + \rho_j(\lambda)) + \sum T_{jk} * \rho_k(\lambda) \tag{2.13}$$

where the integer $r(j)$ is the Takahashi sector corresponding to the n_j-string, namely $m_{r(j)} \leqslant j < m_{r(j)+1}$ in (2.7a), $a_{j,2S}(\lambda)$ is defined in (2.11) and

$$T_{jk}(\lambda) = \frac{1}{2\pi} \frac{\mathrm{d}}{\mathrm{d}\lambda} \Theta_{jk}(\lambda). \tag{2.14}$$

The symbol $a^*b(\lambda)$ denotes the convolution

$$a^*b(\lambda) = \int_{-\infty}^{+\infty} \mathrm{d}\mu \, a(\lambda-\mu) b(\mu). \tag{2.15}$$

The ground state of the model is defined in terms of the solution of the integral equation for the *dressed energies* ε_j of the n_j-strings:

$$4p_0 a_{j,2S}(\lambda) + \varepsilon_j^+(\lambda) + \varepsilon_j^-(\lambda) + \sum (-1)^{r(k)} T_{jk} * \varepsilon_k^-(\lambda) = 0. \tag{2.16}$$

Here $\varepsilon_j^{\mp}(\lambda)$ are the positive and negative parts of the functions $\varepsilon_j(\lambda)$. The lowest-energy state is obtained by filling all the negative energy levels, i.e. it corresponds to a filled Dirac sea (the Dirac sea consists of all strings for which $\varepsilon_j^-(\lambda) \neq 0$). For zero magnetic field the $\varepsilon_j(\lambda)$ are either strictly negative ($r(j)$ has to be even for the sea strings) or strictly positive (for which $r(j)$ has to be odd), or they vanish identically [4, 11].

Kirillov and Reshetikhin [11] have solved the set of integral equations (2.16) for any γ such that (1.5) are satisfied. Their solution depends non-trivially on the Takahashi sector in which the Takahashi number $(2S+1)$ is found (the existence of a Takahashi number $(2S+1)$ is guaranteed in the allowed regions (1.5)), i.e. the integer r in

$$n_\sigma = 2S+1 \qquad \text{for } m_r \leqslant \sigma < m_{r+1}. \tag{2.17}$$

Note that r is a function of both the spin-S and the anisotropy $\gamma = \pi/p_0$. The ground-state configuration consists of filled negative energy bands of j_0-strings where [4]

$$\{j_0\} = \begin{cases} \{m_2, m_4, \ldots, m_{r-1}\}(\cup\{m_{r+1}\} \quad \text{if } \sigma > m_r) & \text{if } r \text{ odd} \\ \{m_2, m_4, \ldots, m_{r-2}\} \cup \begin{Bmatrix} \{m_{r-1}-1\} & \text{if } \sigma = m_r \\ \{m_r, \sigma-1\} & \text{if } \sigma > m_r \end{Bmatrix} & \text{if } r \text{ even.} \end{cases} \tag{2.18}$$

The bands with positive energy (labelled by Kirillov and Reshetikhin as 'breathers' in analogy to the sine-Gordon system) are:

$$\{j_1\} = \begin{cases} \{j\colon m_{2i-1} \leqslant j < m_{2i};\, 2i \leqslant r\} & \text{if } \sigma = m_r \\ \{j\colon m_{2i-1} \leqslant j < m_{2i};\, 2i \leqslant r+1\} & \text{if } \sigma > m_r \end{cases}. \tag{2.19}$$

All other strings have zero energy. Despite this apparently very complicated dependence of the ground-state configuration on the anisotropy it can be shown that the set of string *lengths* $\{n_0 \equiv n_j | j \in \{j_0\}\}$ does not change within any of the intervals of anisotropy allowed by (1.5) [4].

There are no massive excitations, the low-lying excitations have linear dispersion with velocities given by the Fermi velocities of the filled bands:

$$v_{j_0} = \frac{1}{2\pi\rho_{j_0}(\lambda)} \frac{\partial}{\partial\lambda} \varepsilon_{j_0}^-(\lambda) \bigg|_{\lambda=\infty}. \tag{2.20}$$

3. The energy of the finite chain

To obtain finite-size corrections to the low-lying states of the XXZ spin chain in a given allowed region of the anisotropy we start by considering Dirac seas of the strings which are present in the infinite-N ground state (2.18) only. For such a state we choose the quantum numbers $J_i^{(j)}$ in the string equations (2.8) as follows: for $j \in \{j_0\}$ let $J_j^{\pm} = \frac{1}{2}M_j \bmod 1$ such that

$$J_j^+ - J_j^- = M_j \qquad J_j^+ + J_j^- = -2D_j \tag{3.1}$$

and further let $J_i^{(j)}$ take on all values $\frac{1}{2}(M_j+1) \bmod 1$ between J_j^+ and J_j^-. This corresponds to a Dirac sea of n_j-strings with M_j particles, D_j of them moved from the left Fermi point to the right one. The effect of holes in these seas near the Fermi points and of excitations of strings not present in the ground state can be easily included later.

Following Woynarovich *et al* [14], we introduce functions

$$z_{j,N}(\lambda) = \frac{1}{2\pi}\left\{ t_{j,2S}(\lambda) - \frac{1}{N}\sum_k \sum_{n=1}^{M_k} \Theta_{jk}(\lambda - \lambda_n^{(k)})\right\} \tag{3.2a}$$

$$\rho_{j,N}(\lambda) = \frac{\partial}{\partial\lambda} z_{j,N}(\lambda). \tag{3.2b}$$

By definition, $z_{j,N}$ fulfils

$$z_{j,N}(\lambda_i^{(k)}) = \frac{J_i^{(j)}}{N}. \tag{3.3}$$

To obtain an integral equation for the $\rho_{j,N}$ we make use of the Euler-Maclaurin summation formula:

$$\frac{1}{N}\sum_i f(\lambda_i^{(j)}) = \int_j \mathrm{d}\lambda\, f(\lambda)\rho_{j,N}(\lambda) - \frac{1}{24N^2}\left(\frac{f'(\Lambda_j^+)}{\rho_{j,N}(\Lambda_j^+)} - \frac{f'(\Lambda_j^-)}{\rho_{j,N}(\Lambda_j^-)}\right) \tag{3.4}$$

where $\int_k$ stands for an integral with boundaries $\Lambda_k^{\pm}$. These boundaries are defined by $z_{j,N}(\Lambda_j^{\pm}) = J_j^{\pm}/N$. Application of this formula to (3.2) yields an integral equation for $\rho_{j,N}(\lambda)$:

$$\begin{aligned}\rho_{j,N}(\lambda) = a_{j,2S}(\lambda) &- \frac{1}{24N^2}\sum_k\left(\frac{T'_{jk}(\lambda-\Lambda_k^+)}{\rho_{k,N}(\Lambda_k^+)} - \frac{T'_{jk}(\lambda-\Lambda_k^-)}{\rho_{k,N}(\Lambda_k^-)}\right)\\ &- \sum_k \int_k \mathrm{d}\mu\, T_{jk}(\lambda-\mu)\rho_{k,N}(\mu).\end{aligned} \tag{3.5}$$

Here $\Lambda^{\pm}$ are determined by

$$\int_j \mathrm{d}\lambda\, \rho_{j,N}(\lambda) = \frac{1}{N}M_j \tag{3.6a}$$

$$\frac{1}{2}\left(\int_{\Lambda_j^+}^{\infty} - \int_{-\infty}^{\Lambda_j^-}\right)\mathrm{d}\lambda\, \rho_{j,N}(\lambda) = \frac{1}{N}D_j. \tag{3.6b}$$

The solution of the integral equation (3.5) can be written formally as

$$\rho_{j,N}(\lambda) = \rho_j(\lambda|\Lambda^{\pm}) - \frac{1}{24N^2}\sum_k\left(\frac{f_{jk}^+(\lambda)}{\rho_{k,N}(\Lambda_k^+)} - \frac{f_{jk}^-(\lambda)}{\rho_{k,N}(\Lambda_k^-)}\right) \tag{3.7}$$

where $\rho_j(\lambda|\Lambda^{\pm})$ and $f^{\pm}_{jk}(\lambda)$ are defined by

$$\rho_j(\lambda|\Lambda^{\pm}) = a_{j,2S}(\lambda) - \sum_k \int_k \mathrm{d}\mu\ T_{jk}(\lambda-\mu)\rho_k(\lambda|\Lambda^{\pm}) \tag{3.8a}$$

$$f^{\pm}_{jk}(\lambda) = \pm T'_{jk}(\lambda - \Lambda^{\pm}_k) - \sum_m \int_m \mathrm{d}\mu\ T_{jm}(\lambda-\mu) f^{\pm}_{mk}(\mu). \tag{3.8b}$$

(Note that $\rho_j(\lambda|\Lambda^{\pm})$ is actually the density of the infinite chain as defined by (2.13) for given values of $\Lambda^{\pm}$.)

Application of the Euler–Maclaurin summation formula (3.4) to the expression (2.10) for the energy gives

$$E = N\varepsilon(M_j/N, D_j/N) - \frac{\pi}{6N}\sum_j v_j \tag{3.9}$$

where v_j are the Fermi velocities (2.20) of the n_j-strings and

$$\varepsilon(M_j/N, D_j/N) = \sum_j \int_j \mathrm{d}\lambda\ \varepsilon^{(0)}_j(\lambda)\rho_j(\lambda|\Lambda^{\pm}). \tag{3.10}$$

In (3.9) we made use of the fact, that $\rho_j(\lambda|\Lambda^{\pm})$ differs from $\rho_{j,N}(\lambda)$ by terms of order $1/N^2$ only, and that

$$\pm\frac{\partial}{\partial\Lambda^{\pm}_j}\varepsilon^{(0)}_j(\Lambda^{\pm}_j) + \sum_k \int_k \varepsilon^{(0)}_k(\lambda) f^{\pm}_{jk}(\lambda) = \pm\frac{\partial}{\partial\Lambda^{\pm}_j}\varepsilon_j(\Lambda^{\pm}_j) \tag{3.11}$$

which can be seen by comparing the formal solutions of (3.8*b*) for $f^{\pm}_{jk}$ and of (2.16) for the dressed energies ε_j in terms of Neumann's series.

In the thermodynamic limit $N\to\infty$ with $\mu_j \equiv M_j/N$, $\delta_j \equiv d_j/N$ kept finite $\varepsilon(\mu, \delta)$ is the energy density of the infinite system. In this limit the ground state is obtained by minimising $\varepsilon(\mu, \delta)$ with respect to μ and δ or, equivalently, to $\Lambda^{\pm}$. This condition gives the following conditions:

$$\begin{aligned} 0 \overset{!}{=} \partial\varepsilon/\partial\Lambda^{\pm}_j &= \pm\varepsilon^{(0)}_j(\Lambda^{\pm}_j)\rho_j(\Lambda^{\pm}_j|\Lambda^{\pm}) + \sum_n \int_n \varepsilon^{(0)}_j(\lambda)\frac{\partial\rho_j(\lambda|\Lambda^{\pm})}{\partial\Lambda^{\pm}_j} \\ &= \pm\varepsilon_j(\Lambda^{\pm}_j)\rho_j(\Lambda^{\pm}_j|\Lambda^{\pm}) \end{aligned} \tag{3.12}$$

where $\varepsilon_j(\lambda)$ are the dressed energies (2.16) of the n_j-strings. Hence, $\Lambda^{\pm}_0$ for the ground state are defined by the condition that the dressed energies vanish at the Fermi points. From symmetry one has $\Lambda^{\pm}_0 = \pm\Lambda_0$. Our results for the infinite chain in section 2 show that we have here $\Lambda_{j,0} = \infty$ for all j. With (3.12) we can expand ε to second order in $\Lambda^{\pm} \mp \Lambda_0$. Denoting the minimal value of ε as ε_∞, we find

$$\varepsilon(\Lambda^{\pm}) = \varepsilon_\infty + \pi\sum_j v_j\{[\rho_j(\Lambda_{j,0}|\pm\Lambda_0)(\Lambda^{+}_j - \Lambda_{j,0})]^2 + [\rho_j(-\Lambda_{j,0}|\pm\Lambda_0)(\Lambda^{-}_j + \Lambda_{j,0})]^2\} \tag{3.13}$$

where v_j are again the Fermi velocities (2.20) of the n_j-strings.

Finally we have to express the result (3.13) for the energy in terms of the deviation of the numbers M_j and D_j from their ground state values. This amounts to calculation of the Jacobian of the transformation between the $\Lambda^{\pm}_j$ and the μ_j, δ_j. From (3.6) we find (again we can replace $\rho_{j,N}(\lambda)$ by $\rho_j(\lambda|\Lambda^{\pm})$ within our accuracy since the $\Lambda^{\pm}$ have to be calculated to order $1/N$ only)

$$\rho_j(\pm\Lambda_{j,0}|\Lambda^{\pm})\left(\frac{\partial\Lambda_j^{\pm}}{\partial\mu_k}\right)\bigg|_{\Lambda_j=\pm\Lambda_{j,0}} = \pm\tfrac{1}{2}(Z^{-1})_{jk} \tag{3.14a}$$

$$\rho_j(\pm\Lambda_{j,0}|\Lambda^{\pm})\left(\frac{\partial\Lambda_j^{\pm}}{\partial\delta_k}\right)\bigg|_{\Lambda_j=\pm\Lambda_{j,0}} = Z_{kj}. \tag{3.14b}$$

The matrix Z is defined as $Z_{ik}=\xi_{ik}(\Lambda_{k,0})$ where $\xi(\lambda)$ is the dressed charge matrix [6, 8, 20, 23, 24] which is the solution of the following set of integral equations:

$$\xi_{ik}(\lambda)+\sum_j\int_j \mathrm{d}\mu\,\xi_{ij}(\mu)T_{jk}(\lambda-\mu)=\delta_{ik}. \tag{3.15}$$

Although it is not possible to solve these equations in general, it is shown in the appendix that the matrix Z appearing in (3.14) satisfies the following relation for large values of the $\Lambda_0^{\mp}$

$$\lim_{\Lambda\to\infty}[ZZ^{\mathrm{T}}]=\left(1+\int_{-\infty}^{\infty}\mathrm{d}\mu\,T(\mu)\right)^{-1}. \tag{3.16}$$

With (3.14) we can rewrite the expansion (3.13) of $\varepsilon(\mu,\delta)$ as

$$\varepsilon(\mu,\delta)\simeq\varepsilon_\infty+2\pi(\tfrac{1}{4}\boldsymbol{m}^{\mathrm{T}}(Z^{-1})^{\mathrm{T}}V(Z^{-1})\boldsymbol{m}+\boldsymbol{d}^{\mathrm{T}}ZVZ^{\mathrm{T}}\boldsymbol{d}) \tag{3.17}$$

where $m_j=\mu_j-\mu_{j,0}$, $d_j=\delta_j$ and $V=\mathrm{diag}(v_1,v_2,\ldots,v_n)$.

Taking (3.9) and (3.17), we obtain for the ground state energy of the finite chain (to order $1/N$)

$$E_0(N)-N\varepsilon_\infty=-\frac{\pi}{6N}\sum_j v_j. \tag{3.18}$$

This can be interpreted as the generalisation of the relation (1.1) for the scaling of the ground state energy to critical theories with different Fermi velocities and $c_j\equiv1$ for all j.

For excited states of the type considered here the energy gaps scale as

$$E_N(M_j,D_j)-E_0(N)=\frac{2\pi}{N}(\tfrac{1}{4}(\boldsymbol{M}-\boldsymbol{M}_0)^{\mathrm{T}}(Z^{-1})^{\mathrm{T}}V(Z^{-1})(\boldsymbol{M}-\boldsymbol{M}_0)+\boldsymbol{D}^{\mathrm{T}}ZVZ^{\mathrm{T}}\boldsymbol{D}). \tag{3.19}$$

The inclusion of particle-hole-like excitations as well as of strings with length other than those present in the ground state configuration (2.18) modifies the densities (3.7) by terms of order $1/N$. Consideration of particle-hole pairs near the Fermi points of the Dirac sea modifies (3.19) to [8, 14]

$$\begin{aligned}E_N(M_j,D_j,I_j^{\pm})-E_0(N)\\ =\frac{2\pi}{N}\bigg[&\tfrac{1}{4}(\boldsymbol{M}-\boldsymbol{M}_0)^{\mathrm{T}}(Z^{-1})^{\mathrm{T}}V(Z^{-1})(\boldsymbol{M}-\boldsymbol{M}_0)\\ &+\boldsymbol{D}^{\mathrm{T}}ZVZ^{\mathrm{T}}\boldsymbol{D}+\sum_j v_j(I_j^{+}+I_j^{-})\bigg]\end{aligned} \tag{3.20}$$

where I_j^+ (I_j^-) are non-negative integers describing excitations in the vicinity of the right (left) Fermi point of the j-strings, respectively. The momentum of this state is found to be

$$P=\frac{2\pi}{N}\left(\boldsymbol{M}\cdot\boldsymbol{D}+\sum_j (I_j^+-I_j^-)\right). \tag{3.21}$$

Excitation of an n_α-string with $\alpha \notin \{j_0\}$ can be included in the above analysis by replacing $a_{j,2S}$ by $a_{j,2S}-T_{j\alpha}/N$ in (3.5). As an example, we add an n_α-string $\alpha \notin \{j_1\}$ (i.e. a string with vanishing dressed energy) at $\lambda=0$ to the state with $D_j \equiv 0$. In the system considered here, namely one with $\Lambda_0^\mp=\pm\infty$, the leading finite-size correction to the energy is again given by (3.19) but with $\boldsymbol{M}_0$ shifted

$$M_{j,0}^{(\alpha)}=M_{j,0}+\sum_k\left(1+\int_{-\infty}^{\infty}\mathrm{d}\mu\ T(\mu)\right)_{jk}^{-1}\int_{-\infty}^{\infty}\mathrm{d}\mu\ T_{k\alpha}(\mu). \tag{3.22}$$

(The inverse has to be taken in the space with $j,k\in\{j_0\}$).

Just as with the N-dependence of the ground state energy (3.18), the finite-size corrections (3.20) to the energies of excited states can be interpreted as being generated by suitable generalisations of the primary operators in a conformal Gaussian model [12] with coupling constant $\propto X$. These have scaling dimensions

$$X_{(m,n)}=\frac{1}{4X}m^2+Xn^2. \tag{3.23}$$

Results similar to (3.20) have be obtained earlier for different systems by Izergin *et al* [20] and by Woynarovich [8]. It generalises the findings of de Vega [18] for q-state vertex models and Suzuki [19] for nested Bethe ansatz models with only one Fermi velocity $v_j\equiv v$, as can be seen by using the relation (3.16) for the matrix Z.

This derivation of the finite-size corrections to the spectrum relies on the accuracy of the string hypothesis (2.4). It is well known, however, that the positions of the single roots $\lambda_j^{(n)}$ can differ from the ones predicted by (2.4) by terms of $1/N$ rather that $\exp(-\delta N)$ [16, 17]. Nevertheless, it has been found in previous work on the higher-spin XXZ chains with a single Fermi velocity [3] that the dependence of the scaling dimensions on the anisotropy is predicted correctly by this approach, the true values differing from (3.20) by constant terms only. Furthermore, these constant terms could be attributed to operators of a $Z(k)$ parafermionic theory, and hence could take certain discrete values only. We show below that a similar behaviour is true in the multicomponent case considered here and use (3.20) as a starting point to obtain the corrections to the operator dimensions arising from the $1/N$ deviations from the string assumption.

4. Numerical results for the $S=\frac{7}{2}$ chain with two Dirac seas

The simplest of the spin chain models considered here which has more than one Fermi velocity is found to be the chain with $S=\frac{7}{2}$ in the allowed interval

$$\tfrac{5}{2}<\pi/\gamma<3. \tag{4.1}$$

From (2.18) we find that the ground state of the infinite chain is a sea of 2- and 5-strings with positive and negative parity, respectively, in the entire interval. The integral equations (2.13) for the ground-state densities are solved by Fourier transformation. This leads to a linear system of equations for the transforms of the densities:

$$(\delta_{jk}+T_{jk}(\omega))\rho_k(\omega)=a_{j,2S}(\omega) \tag{4.2}$$

with (remember that $p_0=\pi/\gamma$)

$$1+T_{22}(\omega)=4\frac{\sinh(p_0-2)\omega\cosh^2\omega}{\sinh(p_0\omega)} \tag{4.3a}$$

$$T_{25}(\omega)=T_{52}(\omega)=4\frac{\sinh(2p_0-5)\omega\cosh^2\omega}{\sinh(p_0\omega)} \tag{4.3b}$$

$$1+T_{55}(\omega)=2\frac{\sinh(2p_0-5)\omega}{\sinh(p_0\omega)}[\cosh(p_0-5)\omega+4\cosh(p_0-2)\omega\cosh\omega]. \tag{4.3c}$$

The resulting Fourier transforms of the densities are

$$\rho_2(\omega)=\frac{\cosh(8-3p_0)\omega}{2\cosh\omega\cosh(3-p_0)\omega} \tag{4.4a}$$

$$\rho_5(\omega)=\frac{1}{2\cosh(3-p_0)\omega}. \tag{4.4b}$$

(For sake a clarity we use the string lengths n_j instead of the Takahashi indices j to label the components of T, ρ etc in this section.) $\rho_n(\omega=0)=\frac{1}{2}$, hence the ground state of the finite-N spin chain is a configuration of $N/2$ 2-strings and $N/2$ 5-strings if N is even. (For odd N the ground state configuration is different, this is an example of the non-analytic N dependence of finite-size properties [14].) The energy density of the ground state is

$$\varepsilon_\infty=-\frac{2}{\gamma}\int_{-\infty}^{+\infty}d\omega\frac{1}{\cosh(p_0-3)\omega\sinh(p_0\omega)}\{\cosh(8-3p_0)\omega\sinh(3p_0-7)\omega$$
$$+\tfrac{1}{2}\sinh(2p_0-5)\omega[1+2\cosh2\omega+4\cosh(2p_0-5)\omega\cosh\omega]\}. \tag{4.5}$$

The other string lengths that are allowed from (2.7) in the entire interval (4.1) are 1^+, 1^- and 3^+ (superscripts indicate the corresponding parity). Strings of length $n\geqslant 8$ exist, too, but their existence is restricted to subsets of the interval (4.1). The ground state densities of these strings vanish; their hole densities are found to be

$$\rho_{1,+}^{\mathrm{h}}(\omega)\equiv0 \tag{4.6a}$$

$$\rho_{1,-}^{\mathrm{h}}(\omega)=\frac{\cosh(8-3p_0)\omega}{\cosh\omega} \tag{4.6b}$$

$$\rho_3^{\mathrm{h}}(\omega)=\begin{cases}\dfrac{\cosh(8-3p_0)\omega}{\cosh(3-p_0)\omega} & \text{for } p_0<\frac{8}{3}\\ 1/(2\cosh(\omega/3)) & \text{for } p_0=\frac{8}{3}\\ 0 & \text{for } p_0>\frac{8}{3}.\end{cases} \tag{4.6c}$$

The Fermi velocities of the two Dirac seas are found from the asymptotics of $\rho_{2,5}(\lambda)$ as $\lambda\to\pm\infty$:

$$v_2=p_0=\frac{\pi}{\gamma}\qquad v_5=\frac{p_0}{(3-p_0)}=\frac{\pi}{3\gamma-\pi}. \tag{4.7}$$

The leading term in the low-temperature expansion of the free energy of the $S=\frac{7}{2}$ XXZ chain with anisotropies in the interval (4.1) can be found from the results of Kirillov and Reshetikhin [11] (note that their ground state configuration is not correct if $\sigma=m_r$ in (2.17), (2.18) [4]. This difference, however, can be included in their final result for the free energy in a straightforward way):

$$F(T)=F_0-\frac{\pi T^2}{6}\left(\frac{3}{2}\frac{1}{v_2}+\frac{1}{v_5}\right)+o(T^2). \tag{4.8}$$

Using a Newton-type method, we have solved the Bethe ansatz equations (2.1) for small systems numerically. The results allow us to compare the predictions (3.18) and (3.20) from the string hypothesis for the scaling behaviour with the exact numerical values. The results for the ground state energy of finite lattices indicate the following for the scaling of E_0 with N (see table 1):

$$E_0(N)-N\varepsilon_\infty=-\frac{\pi}{6N}\left(\tfrac{3}{2}v_2+v_5\right)+o\left(\frac{1}{N}\right). \tag{4.9}$$

Both (4.8) and (4.9) indicate that the critical field theory corresponding to this spin chain in the continuum limit is a not Lorentz invariant model with sectors labelled by $c_2=\frac{3}{2}$ and $c_5=1$. This result does not agree with the analytical prediction (3.18) of $c_2=c_5=1$. However, as mentioned above, this is a consequence of the usage of the string hypothesis (2.4) for the derivation of (3.18). Analysing our numerical data, we find indeed that the individual roots in 5-strings approach the values (2.4) exponentially fast with N, while the ones in 2-strings are described by (2.4) to order $1/N$ only (see table 2).

Table 1. Finite-size scaling data $-(6N/\pi)(E_0(N)-N\varepsilon_\infty)$ for the ground state energy of the $S=\frac{7}{2}$ chain with different values of the anisotropy in the interval $\frac{5}{2}<(\pi/\gamma)<3$. Also shown are the VBS extrapolations (see [25]) and the conjecture (4.9).

N	$\frac{\pi}{\gamma}=\frac{51}{20}$	$\frac{\pi}{\gamma}=\frac{13}{5}$	$\frac{\pi}{\gamma}=\frac{8}{3}$	$\frac{\pi}{\gamma}=\frac{11}{4}$	$\frac{\pi}{\gamma}=\frac{14}{5}$
4	8.751 56	10.706 83	12.605 73	15.808 87	18.800 35
8	9.259 48	10.485 06	12.154 82	15.328 21	18.416 25
12	9.401 43	10.438 70	12.069 30	15.220 43	18.318 43
16	9.444 92	10.422 03	12.039 18	15.180 26	18.275 06
20	9.462 87	10.414 22	12.025 18	15.161 09	18.252 55
24	9.472 06	10.409 94	12.017 54	15.150 45	18.239 31
Extrapolated	9.474	10.400	12.000	15.125	18.203
Conjectured	9.491 67	10.4	12	15.125	18.2

To compare numerical finite-size data for excited states with the analytical prediction (3.20) we have to calculate the matrix Z first. Although the 2×2 matrix Z is not uniquely determined by (3.16), this relation is sufficient to obtain Z from our numerical data. From (4.3) we find

$$\left(1+\int_{-\infty}^{\infty}\mathrm{d}\mu\; T(\mu)\right)=(1+T(\omega=0))=\frac{2}{\pi}\begin{pmatrix}2(\pi-2\gamma) & 2(2\pi-5\gamma)\\ 2(2\pi-5\gamma) & 5(2\pi-5\gamma)\end{pmatrix}. \tag{4.10a}$$

Table 2. Deviations of the positions of individual roots from the string hypothesis (2.4) for the ground state with $\gamma = 3\pi/8$ as a function of N. δy_2 is the difference of the imaginary part of the roots of the 2-string closest to the real axis and the string-hypothesis value (namely 1). δy_5 is the equivalent quantity for the root of the 5-string closest to the real axis with imaginary part $\frac{14}{3}$ from (2.4).

N	$N\delta y_2$	δy_5
4	0.356 030 05	0.003 942 50
8	0.305 019 61	0.000 211 84
12	0.268 032 90	0.000 018 88
16	0.258 729 30	0.000 001 96
20	0.254 554 50	0.000 000 22
24	0.252 198 43	0.000 000 03

We also need the inverse of this matrix

$$(1+T(\omega=0))^{-1} = \frac{1}{2}\begin{pmatrix} \frac{5}{2} & -1 \\ -1 & (\pi-2\gamma)/(2\pi-5\gamma) \end{pmatrix}. \tag{4.10b}$$

Using (3.16), (3.19) and from our numerical results for the finite-size scaling of the states with $(\Delta M_2, \Delta M_5)$ chosen as $(-1, 0)$ and $(0, -1)$ we can calculate the matrix elements of Z^{-1}. For example, a numerical value for $(Z^{-1})_{22}$ is given by

$$((Z^{-1})_{22})^2 = \frac{4\gamma}{\pi}\left(\frac{\pi-3\gamma}{\pi-2\gamma}\frac{N\delta E}{2\pi}+1\right) \tag{4.11}$$

where δE is $(E_{(-1,0)}(N) - E_0(N))$. Our numerical results (see table 3) indicate that Z^{-1}, and hence Z, both have the following structure:

$$Z = \begin{pmatrix} a & b \\ 0 & d \end{pmatrix}. \tag{4.12}$$

With this additional information, the non-zero elements of Z can be calculated from (3.16) with (4.10) to be

$$a = \frac{1}{2}\left(\frac{\pi}{\pi-2\gamma}\right)^{1/2} \qquad b = -\left(\frac{2\pi-5\gamma}{2\pi-4\gamma}\right)^{1/2} \qquad d = \frac{1}{2}\left(\frac{2\pi-4\gamma}{2\pi-5\gamma}\right)^{1/2}. \tag{4.13}$$

Z^{-1} is of the same form with a, b, d replaced by $\bar{a}$, $\bar{b}$, $\bar{d}$

$$\bar{a} = 2\left(\frac{\pi-2\gamma}{\pi}\right)^{1/2} \qquad \bar{b} = \frac{2(2\pi-5\gamma)}{\sqrt{\pi(\pi-2\gamma)}} \qquad \bar{d} = 2\left(\frac{2\pi-5\gamma}{2\pi-4\gamma}\right)^{1/2}. \tag{4.14}$$

(These values have been used as the conjecture with which we compare our numerical results in table 3.)

This expression for the dressed charge matrix allows us to identify the finite-size corrections in other excited states. A consistency check is obtained by analysing the state with $(\Delta M_2, \Delta M_5) = (-1, -1)$. Equation (3.19) predicts

$$\frac{N}{2\pi}(E_{(-1,-1)}(N) - E_0(N)) = \frac{18\pi^2 - 104\pi\gamma + 147\gamma^2}{2\gamma(\pi-3\gamma)}. \tag{4.15}$$

In table 4 this prediction is compared with our numerical data for different values of the anisotropy γ and N up to 20.

Table 3. Elements of $\hat{Z}^{-1}$ from finite-lattice calculations for different values of the anisotropy γ. (*a*) $((\hat{Z}^{-1})_{22})^2$, (*b*) $((\hat{Z}^{-1})_{52})^2$, (*c*) $((\hat{Z}^{-1})_{55})^2$, (*d*) $((\hat{Z}^{-1})_{25})^2$. The conjectures are given by (4.14). (Entries marked ## could not be calculated due to numerical instabilities.)

(*a*) N	$\frac{\pi}{\gamma}=\frac{13}{5}$	$\frac{\pi}{\gamma}=\frac{8}{3}$	$\frac{\pi}{\gamma}=\frac{11}{4}$	$\frac{\pi}{\gamma}=\frac{14}{5}$
4	0.914 520	1.011 885	1.131 513	1.202 532
8	0.920 700	1.001 608	1.098 047	1.154 975
12	0.921 992	1.000 628	1.093 828	1.157 695
16	0.922 459	1.000 337	1.092 511	1.145 489
20	##	1.000 211	1.091 924	1.144 519
Extrapolated	0.923	1.000	1.091	1.143
Conjectured	0.923 077	1.0	1.090 909	1.142 857

(*b*) N	$\frac{\pi}{\gamma}=\frac{13}{5}$	$\frac{\pi}{\gamma}=\frac{8}{3}$	$\frac{\pi}{\gamma}=\frac{11}{4}$	$\frac{\pi}{\gamma}=\frac{14}{5}$
4	0.008 557	−0.011 885	−0.040 604	−0.059 675
8	0.002 306	−0.001 608	−0.007 137	−0.012 118
12	0.001 768	−0.000 628	−0.002 919	−0.014 110
16	0.000 617	−0.000 337	−0.001 602	−0.002 632
20	##	−0.000 211	−0.001 015	−0.001 932
Extrapolated	0.006	−0.000 07	−0.000 3	−0.000 04
Conjectured	0	0	0	0

(*c*) N	$\frac{\pi}{\gamma}=\frac{13}{5}$	$\frac{\pi}{\gamma}=\frac{8}{3}$	$\frac{\pi}{\gamma}=\frac{11}{4}$	$\frac{\pi}{\gamma}=\frac{14}{5}$
4	0.765 93	1.059 8	1.295 9	1.380 12
8	0.690 50	1.015 3	1.321 7	##
12	0.677 20	1.006 8	1.327 4	1.473 1
16	0.672 58	1.003 8	1.329 7	1.481 8
Extrapolated	0.670	1.002	1.330	
Conjectured	0.666 667	1.0	1.333 333	1.5

(*d*) N	$\frac{\pi}{\gamma}=\frac{13}{5}$	$\frac{\pi}{\gamma}=\frac{8}{3}$	$\frac{\pi}{\gamma}=\frac{11}{4}$	$\frac{\pi}{\gamma}=\frac{14}{5}$
4	0.003 30	0.190 2	0.522 28	0.762 74
8	0.078 73	0.234 7	0.496 37	##
12	0.088 73	0.243 2	0.490 78	0.669 86
16	0.093 35	0.246 2	0.488 48	0.661 06
Extrapolated	0.097	0.248	0.488	
Conjectured	0.102 564	0.25	0.484 848	0.642 857

Table 4. Finite-size scaling of the gap between the ground state and the excited state with $\Delta M_2 = \Delta M_5 = -1$ for different values of the anisotropy. The numerical results are compared to the prediction (4.15).

N	$\frac{\pi}{\gamma}=\frac{13}{5}$	$\frac{\pi}{\gamma}=\frac{8}{3}$	$\frac{\pi}{\gamma}=\frac{11}{4}$	$\frac{\pi}{\gamma}=\frac{14}{5}$
4	2.272 103	3.649 760	5.986 202	8.027 459
8	2.177 193	3.533 909	5.806 842	7.766 289
12	2.161 722	3.514 459	5.773 071	7.714 418
16	2.156 488	3.507 914	5.761 917	7.699 535
20		3.504 960	5.757 060	7.694 477
Extrapolated	2.157	3.501	5.752	7.691
Conjectured	2.15	3.5	5.75	7.7

The finite-size scaling properties in all of the excited states considered above as compared to the finite-N ground state are described correctly by the prediction (3.20) based on the string hypothesis, despite the different value of c_2. This fact has been observed earlier in the investigation of higher-spin XXZ chains with a single Fermi velocity [3, 4]: the operators identified from the scaling behaviour of states consisting of sea strings only were found to be composite operators formed by the product of a Gaussian-type operator and the identity operator in the parafermionic sector of this model, the latter having zero dimension. To find a non-zero contribution from the parafermionic sector, one has to consider states with strings other than the sea strings present. In the following we shall investigate the scaling of energies of states with a single 1^+-string added at $\lambda = 0$. As mentioned in section 3, this amounts to a shift (3.22) of $\boldsymbol{M}_0$ in (3.20). The shift is given by

$$\delta \boldsymbol{M}_0 = (1 + T(\omega = 0))^{-1}\begin{pmatrix} T_{21}(\omega=0) \\ T_{51}(\omega=0)\end{pmatrix}. \tag{4.16}$$

In the interval (4.1) we have

$$T_{21}(\omega = 0) = 2(\pi - 2\gamma)/\pi \qquad T_{51}(\omega=0) = 2(2\pi - 5\gamma)/\pi \tag{4.17}$$

and hence $\delta\boldsymbol{M}_0 = (\frac{1}{2}, 0)$. From (3.20) we obtain the following predictions for the finite-size corrections to the energies of states with $N/2 - 1$ 2-strings and $N/2$ 5-strings:

$$\frac{N}{2\pi}(E^{(1)}_{(-1,0)}(N) - E_0(N)) = \frac{\pi - 2\gamma}{4\gamma} + v_2 X_2 \tag{4.18}$$

and with $M_2 = N/2$, $M_5 = N/2 - 1$:

$$\frac{N}{2\pi}(E^{(1)}_{(0,-1)}(N) - E_0(N)) = \frac{9\pi^2 - 61\pi\gamma + 96\gamma^2}{4\gamma(\pi - 3\gamma)} + v_2 X_2. \tag{4.19}$$

Here X_2 is the contribution of the continuum field theory that gives rise to the change of c_2 from the Gaussian value 1 to the one found in (4.8) and (4.9), namely $\frac{3}{2}$. From the known conformal properties for the higher-spin XXZ chains with a single Fermi velocity, we conjecture that this is again the Z(2) or Ising model. Hence, we expect to find $X_2 = \Delta_2 + \bar{\Delta}_2$ where Δ_2, $\bar{\Delta}_2$ are the operator dimensions of the Ising model.

$$\Delta_2, \bar{\Delta}_2 = 0, \tfrac{1}{16}, 1. \tag{4.20}$$

Table 5. Finite-size scaling of the gap between the ground state and the excited states with an additional 1-string at $\lambda = 0$ and $(\Delta M_2, \Delta M_5)$ chosen as (*a*) $(-1, 0)$ and (*b*) $(0, -1)$ for different values of the anisotropy. The numerical results are compared with the predictions (*a*) (4.18) and (*b*) (4.19) with $X_2 = \frac{1}{8}$.

(*a*) N	$\frac{\pi}{\gamma} = \frac{13}{5}$	$\frac{\pi}{\gamma} = \frac{8}{3}$	$\frac{\pi}{\gamma} = \frac{11}{4}$	$\frac{\pi}{\gamma} = \frac{14}{5}$
4	0.497 404	0.513 422	0.509 362	0.479 579
8	0.484 820	0.509 077	0.536 034	0.546 058
12	0.481 177	0.506 143	0.536 398	0.552 689
16	0.479 468	0.504 610	0.535 696	0.553 572
20	0.478 516	0.503 683	0.535 062	0.553 531
Extrapolated	0.476	0.502	0.536	0.554
Conjectured	0.475	0.5	0.531 25	0.55

(*b*) N	$\frac{\pi}{\gamma} = \frac{11}{4}$	$\frac{\pi}{\gamma} = \frac{14}{5}$
4	4.027 632	5.429 828
8	4.025 642	5.550 635
12	4.027 458	5.989 890
16	4.028 619	5.608 099
20	4.029 340	5.618 445
Extrapolated	4.031	5.642
Conjectured	4.031 25	5.65

Comparison of our numerical results shows that the scaling of the energy gaps for these states is indeed described accurately by the predictions (4.18), (4.19) with $X_2 = \frac{1}{8}$ (see table 5).

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Note added in proof. Since the submission of our original manuscript we managed to find the Wiener–Hopf factorisation (A6) of the kernel $1 + T(\omega)$ of the internal equations in section 4 (e.g. (4.2)). It is of the form

$$G^{-}(\omega) = \begin{pmatrix} a(-\omega) & b(-\omega) \\ 0 & d(-\omega) \end{pmatrix}$$

($G^{+}(\omega)$ is given by (A7)) with $a(-\omega)$, $b(-\omega)$, $d(-\omega)$ analytic functions for $\mathrm{Im}(\omega) < 0$ given by

$$a(\omega)a(-\omega) = \sinh(p_0\omega)/(4\sinh(p_0 - 2)\omega\cosh^2\omega)$$

$$d(\omega)d(-\omega) = \sinh(p_0 - 2)\omega/(2\sinh(2p_0 - 5)\omega\cosh(p_0 - 3)\omega)$$

$$b(\omega)b(-\omega) = \sinh(2p_0 - 5)\omega/(2\sinh(p_0 - 2)\omega\cosh(p_0 - 3)\omega)$$

(the factorisation of these equations in terms of gamma functions is straightforward). The analytical prediction (A9) for the elements of the dressed charge matrix agrees with our numerical results (equations (4.12), (4.13) and 4.14)).

Appendix. The dressed charge matrix

For zero magnetic field, the Λ_j either vanish or are infinite. In this case (3.15) can be solved by Fourier transformation, giving (in the subspace of Takahashi indices $j \in \{j_0\}$)

$$\xi(\lambda) \equiv \xi(0) = \left(1 + \int_{-\infty}^{\infty} \mathrm{d}\mu\, T(\mu)\right)^{-1}. \tag{A1}$$

However, for large but finite Λ_j this holds for $|\lambda| \ll \Lambda_j$ only. $\xi_{ik}(\Lambda_k)$ can be obtained by application of the Wiener–Hopf (WH) method. For large Λ_k the functions

$$\bar{\xi}_{ik}(x) = \xi_{ik}(\Lambda_k - x) \tag{A2}$$

are solutions of a multicomponent WH-type integral equation

$$\bar{\xi}_{ik}(x) + \sum_j \int_0^{\infty} \mathrm{d}y\, \bar{\xi}_{ij}(y)\, T_{jk}(\Lambda_j - \Lambda_k + x - y) = \delta_{ik}. \tag{A3}$$

Fourier transformation yields

$$\xi^{+}(\omega)\, U(\omega)(1 + T(\omega))\, U(\omega)^{-1} + \xi^{-}(\omega) = \frac{\mathrm{i}}{\omega + \mathrm{i}0} \tag{A4}$$

where $\xi^{\pm}(\omega) = \int \mathrm{d}x\, \Theta(\pm x)\bar{\xi}(x)\, \mathrm{e}^{\mathrm{i}\omega x}$ are analytic functions for $\mathrm{Im}(\omega) \overset{>}{(<)} 0$ ($\Theta(x)$ is the step function), and

$$U(\omega) = \mathrm{diag}\{\exp(\mathrm{i}\omega\Lambda_1), \ldots, \exp(\mathrm{i}\omega\Lambda_n)\}. \tag{A5}$$

To solve these equations one has to find a factorisation of the kernel of the above equations

$$1 + T(\omega) = G^{+}(\omega)[G^{-}(\omega)]^{-1} \qquad \lim_{\omega\to\infty} G^{+}(\omega) = \lim_{\omega\to\infty} G^{-}(\omega) = 1 \tag{A6}$$

where $G^{+}(\omega)$ ($G^{-}(\omega)$) are analytic matrix functions in the open upper (lower) half of the complex plane and are continuous on the real axis.

Although there is no constructive method for obtaining such a factorisation for general multicomponent WH equations, for a self-adjoint matrix function which is continuous and has non-zero determinant on the extended real line (such as $(1 + T)$) this factorisation is known to exist [26] and because of the symmetries of $T(\omega)$, namely $T(\omega) = T(-\omega)$ and $T = T^{\mathrm{T}}$ it follows

$$[G^{+}(-\omega)^{\mathrm{T}}] = [G^{-}(\omega)]^{-1}. \tag{A7}$$

In terms of these matrices the solution of (A4) is

$$\xi^{+}(\omega) = \frac{\mathrm{i}}{\omega + \mathrm{i}0} G^{-}(0)[U(\omega)G^{+}(\omega)U(\omega)^{-1}]^{-1}. \tag{A8}$$

Contour integration gives

$$\lim_{\Lambda\to\infty} \xi_{ik}(\Lambda_k) = \frac{1}{\pi}\int_{-\infty}^{\infty} \mathrm{d}\omega\, \xi^{+}_{ik}(\omega) = -\mathrm{i} \lim_{\omega\to\infty} [\omega \xi^{+}_{ik}(\omega)] = G^{-}_{ik}(0). \tag{A9}$$

Together with (A6) and (A7), this yields the following relation:

$$\lim_{\Lambda\to\infty} \xi(0) = \lim_{\Lambda\to\infty} [ZZ^{\mathrm{T}}]. \tag{A10}$$

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