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1989 J. Phys. A: Math. Gen. 22 1829

(http://iopscience.iop.org/0305-4470/22/11/023)

J. Phys. A: Math. Gen. **22** (1989) 1829–1858. Printed in the UK

Conformal invariance and the operator content of the XXZ model with arbitrary spin

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Received 24 October 1988

Abstract. This paper is concerned with the critical properties of the anisotropic Heisenberg chain, or XXZ model, with arbitrary integer or half-integer spin. The eigenspectra of these Hamiltonians, with periodic boundaries, are calculated for finite chains by solving numerically their associated Bethe ansatz equations. The resulting spectra are found to be in accord with the predictions of conformal invariance and the operator content is identified, for lattices with an even and odd number of sites. The results for spin 1 and spin $\frac{3}{2}$ indicate that the conformal anomaly c for these models, in the gapless regime, has the value $c = 3S/(1+S)$, independent of the anisotropy, and the exponents vary continuously with the anisotropy as in the eight-vertex model. The operator content of these models indicate that the underlying field theory governing these critical spin-S models are described by composite fields formed by the product of Gaussian and $Z(N)$ fields, with $N = 2S$. Finally some of the irrelevant operators which produce the leading finite-size corrections of the eigenenergies are identified.

1. Introduction

The critical fluctuations of statistical mechanical systems are believed to be described by massless field theories. If, in addition to scale invariance, the statistical systems have short-range interactions and translational and rotational symmetry then the underlying field theory is believed to be conformally invariant (Polyakov 1970). In two dimensions (or $(1+1)$-dimensional spacetime) the conformal invariance powerfully constrains the possible universality classes of critical behaviour (Belavin *et al* 1984a, b, Friedan *et al* 1984). A complete classification of these universality classes is therefore closely related to the classification of all unitary conformally invariant $(1+1)$-dimensional field theories. These classes are labelled by a single dimensionless number c, the central charge or the conformal anomaly of the associated Virasoro algebra, the irreducible representations of which determine the operator algebra describing the critical behaviour. If c is less than unity then unitarity quantises c to the values (Friedan *et al* 1984)

$$c = 1 - [6/m(m+1)] \qquad m = 3, 4, 5, \ldots . \tag{1.1}$$

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0305-4470/89/111829+30\$02.50

The first members of this minimal series correspond to the critical Ising model ($m=3$), tricritical Ising model ($m=4$), critical three-state Potts model ($m=5$), etc. In these series the operator algebra is finite and the scaling dimensions $(\Delta_{p,q}, \bar{\Delta}_{p,q})$ (related to the critical exponents) of the primary operators are given by the Kac formula

$$\Delta_{p,q}=\frac{[p(m+1)-qm]^2-1}{4m(m+1)} \qquad 1\leqslant p\leqslant m+1,\ 1\leqslant q\leqslant m. \tag{1.2}$$

In the limit $m\to\infty$, where $c=1$, the algebra is no longer finite and these conformal theories describe statistical models with continuously varying critical exponents like the Ashkin-Teller, eight-vertex and XXZ models. When $c\geqslant 1$ unitarity does not constrain the values of c. However when the primary fields obey a larger algebra than the Virasoro algebra it is possible to find a relationship between the central charge c and the possible scaling dimensions $\Delta_{p,q}$. These are the cases of models exhibiting supersymmetry (Friedan *et al* 1985, Bershadsky *et al* 1984), where

$$c=\tfrac{3}{2}\{1-[8/m(m+2)]\} \qquad m=3,4,\ldots \tag{1.3}$$

and exhibiting Z(N)-Zamolodchikov-Fateev parafermionic algebra (Zamolodchikov and Fateev 1985), where

$$c=2(N-1)/(N+2) \qquad N=2,3,4,\ldots \tag{1.4}$$

and Kac-Moody algebra (Knizhnik and Zamolodchikov 1984) where c depends of the charge k of the associated semisimple group G. In the case where G is the group SU(2) we have

$$c=3k/(1+k). \tag{1.5}$$

More recently it was shown (Kastor *et al* 1988, Bagger *et al* 1988, Ravanini 1988), using a Feigin-Fuchs construction (Feigin and Fuchs 1982, Dotsenko and Fateev 1984), that a more general set of unitary field theories can be derived from those described by SU(2) Kac-Moody algebra with charge k. The conformal anomaly is given by

$$c=\frac{3k}{k+2}\left(1-\frac{2(k+2)}{m(m+k)}\right) \qquad m=3,4,\ldots;\ k=1,2,\ldots \tag{1.6}$$

while the possible scaling dimensions $(\Delta,\bar{\Delta})$ of the primary operators are given by

$$\Delta_{p,q}=\frac{[p(m+k)-qm]^2-k^2}{4km(m+k)} \qquad 1\leqslant p\leqslant m-1,\ 1\leqslant q\leqslant m+k-1. \tag{1.7}$$

For $k=1$ and $k=2$ we recover the minimal and supersymmetric series respectively, while for $k>2$ we have more general series culminating, as $m\to\infty$, in the conformal anomaly of SU(2) Kac-Moody algebra with topological charge k. As we mentioned earlier, the minimal series ($k=1$ in (1.6)) culminates in a $c=1$ theory describing models with continuously varying exponents. It is important to know if the same also occurs for the general series (1.6). If so then there must exist critical statistical models with continuously varying exponents governed by an operator conformal algebra, with central charge given by (1.5).

In this paper we will study a special set of one-dimensional quantum antiferromagnetic Hamiltonians describing the dynamics of particles with arbitrary spin ($S=1, \frac{3}{2}, 2,\ldots$). These Hamiltonians are generalisations of the spin-$\frac{1}{2}$ antisotropic Heisenberg chain, or XXZ model, for arbitrary spins and are the natural candidates to exhibit continuously varying critical exponents. In the same way as the spin-$\frac{1}{2}$ XXZ

Hamiltonian (Yang and Yang 1966a, b), these models are exactly integrable (Sogo *et al* 1983, Sogo 1984, Babujian and Tsvelick 1986, Kirillov and Reshetikhin 1987a, b) in the thermodynamic limit through the Bethe ansatz. We will calculate, in the gapless regime of these models, the conformal anomaly of the underlying conformal algebra as well their operator content. These calculations will be done by exploiting a set of important relations (see Cardy 1987a for a review) between the eigenspectrum of the finite lattice system at the critical point, and the conformal anomaly and scaling dimensions of operators describing the critical behaviour. If we write the transfer matrix as $T=\exp(-aH)$, where a is the lattice spacing, then, in a strip of width L with periodic boundary conditions, the ground-state energy, $E_0(L)$, of the Hamiltonian H behaves, for large L, as (Blöte *et al* 1986, Affleck 1986a)

$$\frac{E_0(L)}{L}=e_\infty-\frac{\pi c\zeta}{6L^2}+\mathrm{o}(L^{-2}). \tag{1.8}$$

Here c is the central charge of the conformal class governing the critical behaviour, e_∞ is the ground-state energy per particle in the bulk limit ($L\to\infty$) and ζ is a model-dependent constant that must be determined, usually numerically, to ensure that the resulting equations of motion are conformally invariant (von Gehlen *et al* 1986). The structure of the higher-energy states are also determined by the primary operators of the theory (Cardy 1986a). For each primary operator O_α with dimension X_α and spin S_α, these exists a tower of states in the spectrum of H with energies $E^\alpha_{M,M'}(L)$ and momenta $P_{M,M'}(L)$ given by

$$E^\alpha_{M,M'}=E_0(L)+2\pi\zeta(X_\alpha+M+M')L^{-1}+\mathrm{o}(L^{-1}) \qquad M, M'=0,1,2,\ldots \tag{1.9a}$$

and

$$P_{M,M'}=(2\pi/L)(S_\alpha+M-M') \qquad M, M'=0,1,2,\ldots. \tag{1.9b}$$

Usually the eigenspectrum of finite-size spin Hamiltonians are calculated numerically using the Lanczos method or variants (Roomany *et al* 1980, Hamer and Barber 1981). For the statistical models we will consider in this paper, these methods permit us to consider only lattice sizes up to $L\sim 10$–13, depending on the value of S. However the existence of a Bethe ansatz for these models permit us to calculate the eigenenergies for much larger lattices ($L\sim 50$–100) by solving numerically the associated Bethe ansatz equations; we thereby obtain, by using (1.8) and (1.9), very accurate estimates of the conformal anomaly and scaling dimensions†.

This paper is organised as follows. In § 2 we present the models as well their associated Bethe ansatz equations (BAE). We also rederive these equations using the string hypothesis and show that they do not provide correct estimates of the finite-size effects. In § 3 we analyse the picture of zeros of the BAE by solving them numerically. The conformal anomaly for the spin-1 and spin-$\frac{3}{2}$ models are calculated numerically in § 4, while the operator content for even and odd lattice sizes are obtained in § 5. In § 6 we discuss the corrections of the eigenenergies due to the finite-size effects. Finally our conclusion is presented in § 7 and the analytical calculation of the finite-size corrections of the energies, using the string hypothesis, is derived in an appendix.

† A brief summary of some of our results has appeared in Alcaraz and Martins (1988c).

2. The spin-S XXZ quantum Hamiltonian

The spin $S=\frac{1}{2}$ isotropic Heisenberg model was the first model solved, in the thermodynamic limit, by using the Bethe ansatz (Bethe 1931). Since then much effort has been expended in order to obtain generalisations of this model which preserve exact integrability through the Bethe ansatz (see, e.g., Lieb and Wu 1972, Thacker 1981, Baxter 1982, Gaudin 1983 and Tsvelick and Weigmann 1983). The first generalisation is the spin-$\frac{1}{2}$ XXZ model (Yang and Yang 1966a, b) obtained by the introduction of a plane anisotropy. This model is described by the Hamiltonian

$$H_{XXZ}^{(1/2)}(\gamma) = -\frac{1}{2}\sum_{i=1}^{L}(\sigma_i^x\sigma_{i+1}^x+\sigma_i^y\sigma_{i+1}^y-\cos\gamma\sigma_i^z\sigma_{i+1}^z) \tag{2.1}$$

where σ_i^x, σ_i^y and σ_i^z are Pauli matrices defined at the lattice sites and γ is the anisotropic constant. A generalisation of the isotropic Heisenberg to arbitrary spin S (integer or half-integer), preserving integrability and the SU(2) symmetry, was obtained by Takhtajan (1982) and Babujian (1982, 1983). The anisotropic generalisation of these models, for the spin-1 case, the spin-1 XXZ model, was introduced by Zamolodchikov and Fateev (1980)

$$H_{XXZ}^{(1)}(\gamma)=\frac{1}{4}\sum_{i=1}^{L}\{\sigma_i-(\sigma_i)^2-2(\cos\gamma-1)(\sigma_i^{\perp}\sigma_i^z+\sigma_i^z\sigma_i^{\perp})$$
$$-2\sin^2\gamma(\sigma_i^z-(\sigma_i^z)^2+2(S_i^z)^2-2)\} \tag{2.2a}$$

where

$$\sigma_i=\boldsymbol{S}_i\cdot\boldsymbol{S}_{i+1}=\sigma_i^{\perp}+\sigma_i^z \qquad \sigma_i^z=S_i^zS_{i+1}^z. \tag{2.2b}$$

Here S^x, S^y and S^z are the (3×3) matrices of spin 1. The generalisation for arbitrary spin S, the spin-S XXZ quantum Hamiltonian (Sogo *et al* 1983, Sogo 1984, Babujian and Tsvelick 1986, Kirillov and Reshetikhim 1987a, b), is a complicated polynomial of spin-S matrices having an anisotropic parameter γ. These Hamiltonians are related to two-dimensional vertex models ($(2S+1)$-colour-vertex models), in which a particular link can assume $2S+1$ colours, and are extensions of the well studied six-vertex model (see, e.g., Baxter 1982). From their exact solution (Sogo 1984) the general spin-S Hamiltonian is gapless (critical) in the particular regime where $0\leqslant\theta=2S\gamma\leqslant\pi$. Therefore, due to the local character of the interactions and the fact that these Hamiltonians are related to translationally and rotationally invariant two-dimensional critical systems, we suppose (Cardy 1987a) that they are described, in its gapless regime, by conformally invariant field theories. In the isotropic limit, $\gamma=0$, these spin models reduce to the Takhtajan–Babujian models (Takhtajan 1982, Babujian 1982).

2.1. The Bethe ansatz equations

The general spin-S Hamiltonian, with periodic boundary conditions imposed, commutes with the total spin operator $\hat{S}^z=\Sigma_i S_i^z$. Consequently, for even (odd) values of the lattice size L, the associated Hilbert space can be separated into $2LS+1$ ($2LS$) disjoint sectors labelled by the eigenvalues of S, namely $n=0, \pm1, \pm2, \ldots, \pm LS$ ($n=\pm\frac{1}{2}, \pm\frac{3}{2}, \ldots, \pm LS$). Due to the spin-reversal symmetry the sectors with $n=k$ and $n=-k$ are degenerate and we can restrict, in the following, to the sectors $n\geqslant0$. In the Bethe ansatz formulation for these spin-S XXZ models with periodic boundaries

(Sogo *et al* 1983, Sogo 1984) the eigenenergies, for a given sector n, are given in terms of the $(SL-n)$ complex roots $(\lambda_1, \lambda_2, \ldots, \lambda_{SL-n})$ of the non-linear set of Bethe ansatz equations (BAE)

$$\frac{\sinh \gamma(\lambda_j - \mathrm{i}S)}{\sinh \gamma(\lambda_j + \mathrm{i}S)} = \prod_{k=1 \neq j}^{SL-n} \frac{\sinh \gamma(\lambda_j - \lambda_k - \mathrm{i})}{\sinh \gamma(\lambda_j - \lambda_k + \mathrm{i})} \qquad j = 1, \ldots, SL-n. \tag{2.3}$$

The energy and momentum of the eigenstates are given in terms of the roots of the BAE by

$$E = \frac{\sin^2(2S\gamma)}{2S} \sum_{j=1}^{SL-n} \frac{1}{\cos 2S\gamma - \cosh 2\lambda_j} \tag{2.4a}$$

and

$$P = \sum_{j=1}^{SL-n} 2 \tan^{-1}(\coth(S\gamma) \tan \lambda_j) \qquad (\mathrm{mod}\ 2\pi) \tag{2.4b}$$

respectively. The exact solution, in the limit $L \to \infty$, for the ground-state energy per particle e_∞ (Sogo 1984) is given by the expression

$$e_\infty(\gamma_1 S) = -\frac{\sin(2S\gamma)}{2S} \int_{-\infty}^{+\infty} \frac{\sinh[(\pi - 2S\gamma)x] \sinh(2S\gamma x)}{\sinh(\pi x) \sinh(2\gamma x)} \mathrm{d}x. \tag{2.5}$$

In table 1 we list e_∞ for some values of γ and S.

2.2. *The string hypothesis and the large-L limit*

All the analytic results, in the $L \to \infty$ limit, for the spin models we are considering, are obtained under the assumption that the string hypothesis, which asserts that as $L \to \infty$ the roots λ_j of (2.3) cluster in complex r-strings. Each r-string $\{\lambda_{j,k}^r\}$ is composed by r complex roots with the same real part λ_j^r (the string's centre) and equally spaced imaginary parts:

$$\lambda_{j,k}^r = \lambda_j^r + \tfrac{1}{2}(r + 1 - 2k) \qquad k = 1, 2, \ldots, r. \tag{2.6}$$

Within this assumption we can parametrise an arbitrary configuration of roots by giving the numbers ν_r of strings of size r, with the restriction $\Sigma_r r\nu_r = SL - n$. In terms of the strings configuration $\{\nu_r\}$ the BAE (2.3) reduces to the system of real equations for the string's centres $\lambda_j^r; j = 1, 2, \ldots, \nu_r$ (Sogo 1984):

$$L\psi_{r,2S}(\lambda_j^r) = 2\pi Q_j^r + \sum_{s=1}^{\infty} \sum_{k=1}^{\nu_s} \Xi_{r,s}(\lambda_j^r - \lambda_k^s) \tag{2.7a}$$

Table 1. Ground-state energy per site $e_\infty(S)$ (2.5), of the spin $S = 1$ and $S = \frac{3}{2}$ models for several values of γ.

γ	$e_\infty(1)$	$e_\infty(\frac{3}{2})$
$\pi/6$	−0.75	−0.619 3035
$\pi/4\sqrt{2}$	−0.722 0079	−0.563 3719
$\pi/5.5$	−0.707 7075	−0.535 5164
$\pi/3\sqrt{2}$	−0.544 8573	−0.256 0750
$\pi/4$	−0.5	−0.192 8775

where

$$\psi_{n,2S}(x) = \sum_{l=1}^{\min(r,2S)} \theta_{r+2S+1-2l}(x) \tag{2.7b}$$

$$\Xi_{r,s}(x) = \begin{cases} \theta_{|s-r|}(x) + 2\theta_{|s-r|+2}(x) + \ldots + 2\theta_{|s+r|-2}(x) + \theta_{|s+r|}(x) & r \neq s \\ 2\theta_2(x) + 2\theta_4(x) + \ldots + 2\theta_{2s-2}(x) + 2\theta_{2s}(x) & r = s \end{cases} \tag{2.7c}$$

and

$$\theta_r(x) = 2\tan^{-1}[\coth(\gamma r/2)\tan x]. \tag{2.7d}$$

The eigenenergies for a given distribution of $\{\nu_r\}$ strings are given, from (2.4) and (2.6), by

$$E = -\frac{1}{2}\sum_{k=1}^{\infty}\sum_{j=1}^{\nu_k} \psi'_{r,2S}(\lambda_j^k) \tag{2.8}$$

where the prime indicates the derivative. For L even, according to Sogo (1984), the ground state, which occurs in the $n=0$ sector, corresponds to a sea of $2S$-strings ($\nu_{2S} = L/2$, $\nu_r = 0$ for $r \neq 2S$), while the lowest state in the sector $n = 1$ corresponds to $\nu_{2S} = (L/2) - 1$, $\nu_{2S-1} = 1$, and so on. The numbers Q_j^r occurring in (2.7) are integers or half-integers, depending on the particular distribution $\{\nu_r\}$ of strings. For example, for the lowest energy in the sector n ($n \geqslant 0$), characterised by the distribution of strings, $\nu_{2S} = (L/2) - 1 - [n/2S]$, $\nu_{2S-\{n/2S\}} = 1$ ($[r/2S]$ and $\{r/2S\}$ are the integer part and the remaining fractional part of the ratio $r/2S$), these numbers are

$$Q_j^{2S} = -\tfrac{1}{2}(\nu_{2S-1}) + I - 1 \qquad I = 1, 2, \ldots, \nu_{2S} \tag{2.9a}$$

$$Q_j^{2S-\{n/2S\}} = 0. \tag{2.9b}$$

We should stress at this point that the string assumption (2.6) is expected to be valid only in the $L \to \infty$ limit; consequently the finite-size corrections of the eigenenergies, calculated using this assumption, will give us incorrect results. Although incorrect, these results will give us an idea of the true finite-size corrections of the eigenspectrum. The large-L corrections for real BAE like (2.7), obtained under the string assumption, can be calculated analytically by using a method pioneered by de Vega and Woynarovich (1985) and Hamer (1986) and refined by Woynarovich and Eckle (1987a, b). In the appendix we present the main steps in the calculation of the finite-size corrections of (2.7) and (2.8) for the lowest energies $E_n^{\mathrm{st}}(\gamma)$ of the sector $n = 0, 1, 2, \ldots$. From (A25), the ground-state energy $E_0^{\mathrm{st}}(\gamma)$, for the L-sites chain with periodic boundaries behaves, as $L \to \infty$, like

$$\frac{E_0^{\mathrm{st}}(\gamma)}{L} = e_\infty(\gamma) - \frac{\pi^2 \sin(2S\gamma)}{4S\gamma L^2}\left(-\tfrac{1}{6} + \mathcal{O}(L^{-1}) + \mathcal{O}(L^{-2/S}) + \mathcal{O}(L^{-4\gamma/(\pi-2S\gamma)})\right) \tag{2.10}$$

while, from (A26), the mass gap amplitude which corresponds to the lowest energy $E_n^{\mathrm{st}}(\gamma)$, of sector n, behaves as $L \to \infty$ like

$$\frac{E_n^{\mathrm{st}}}{L} - \frac{E_0^{\mathrm{st}}}{L} = \frac{\pi^2 \sin(2S\gamma)}{2S\gamma L^2}\left(x_P n^2 + \mathcal{O}(L^{-1}) + \mathcal{O}(L^{-2}) + \mathcal{O}(L^{-4\gamma/(\pi-2S\gamma)}) + \mathcal{O}(L^{-2/S})\right)$$

$$x_P = (\pi - 2S\gamma)/4\pi S. \tag{2.11}$$

It is interesting to analyse (2.10) and (2.11) in the limit where $\gamma \to 0$ (isotropic model). In this limit an infinite number of corrections sum to a logarithmic correction.

These corrections, for the ground-state energy $E_0^{\rm st}(0)$ and the lowest eigenenergy $E_n^{\rm st}(0)$, of sector n, are given by Alcaraz and Martins (1988b)

$$\frac{E_0^{\rm st}(0)}{L}=e_\infty(0)-\frac{\pi^2}{12L^2}+\mathcal{O}\left(\frac{1}{L^2(\ln L)^3}\right)+\mathcal{O}\left(\frac{\ln(\ln L)}{L^2(\ln L)^4}\right) \qquad (2.12)$$

and

$$\frac{E_n^{\rm st}(0)}{L}-\frac{E_0^{\rm st}(0)}{L}=\frac{\pi^2n^2}{4SL^2}+\mathcal{O}\left(\frac{1}{L^2\ln L}\right)+\mathcal{O}\left(\frac{\ln(\ln L)}{L^2(\ln L)^2}\right) \qquad (2.13)$$

respectively. The coefficients appearing in the L-power factors are functions of the spin S and γ, and can be calculated exactly. However, as we will see in §§ 4-7, our numerical studies reveal that although some of the L-power dependence of the finite-size eigenenergies for the true energies given by (2.3) and (2.4) are correctly estimated by (2.10)-(2.13), the corresponding amplitudes are not.

3. Numerical solutions of the Bethe ansatz equations

Some numerical work on the solution of the Bethe ansatz equations (BAE), for finite L, have been reported in the literature. Most of this work concentrates on the spin-$\frac{1}{2}$ XXZ Hamiltonian (2.1). The lowest eigenenergies (Des Cloiseaux and Pearson 1962, Avdeev and Dörfel 1985) and correlation functions (Grieger 1984, Borysowicz *et al* 1985) were calculated at the isotropic point ($\gamma=0$). The ground state and first excited state for $0\leqslant\gamma\leqslant\pi$ were calculated by Woynarovich and Eckle (1987a, b), while a general numerical analysis of the whole eigenspectrum of the $S=\frac{1}{2}$ XXZ model was carried out by Alcaraz *et al* (1987, 1988a). It is important to remark here that for most of the eigenstates of the spin $S=\frac{1}{2}$ model the BAE are real while for general S they are complex, becoming real only in the $L\to\infty$ limit, in the cases where the string assumption (2.6) is valid (see (2.7)). The little numerical work reported for the general spin-S model has concentrated on the isotropic point (Avdeev and Dörfel 1987, Alcaraz and Martins 1988a, b).

In this section we will report our numerical analysis of the BAE for the spin $S=1$ and $S=\frac{3}{2}$ XXZ Hamiltonians in the region where $0\leqslant\gamma\leqslant\pi/2S$. We solved the system of BAE (2.3) or (2.7) by using a Newton-type method for systems of size $L=3,4,\ldots,40$. These lattice sizes are large enough for the purpose of the present paper, although without much computational effort we can extend the lattice chains up to $L\sim100$. Instead of solving directly the complex BAE (2.3) we initially solve its real counterpart (2.7) and use this solution as the initial guess in solving (2.3). In table 2 we show, as an example, the roots $\{\lambda_j=\lambda_j^{\rm R}+{\rm i}\lambda_j^{\rm I}\}$ corresponding to the ground state for the $L=12$

Table 2. Complex roots $\lambda_j=\lambda_j^{\rm R}+{\rm i}\lambda_j^{\rm I}(j=1\text{-}3)$ of the system (2.3) corresponding to the ground state of the spin $S=1$, with $\gamma=\pi/10$ in a chain of $L=12$ sites. The other roots not shown in the table are obtained from these by the combinations $\pm\lambda_j^{\rm R}\pm{\rm i}\lambda_j^{\rm I}$. The roots $\pm\lambda_j^{2S}$ are the corresponding ones obtained by solving (2.7).

j	$\lambda_j^{\rm R}$	$\lambda_j^{\rm I}$	λ_j^{2S}
1	0.699 0380	0.543 2110	0.669 9014
2	0.283 9373	0.533 2110	0.284 0535
3	0.085 0243	0.516 1657	0.084 3019

sites spin-1 model at $\gamma = \pi/10$. We also show, in this table, the corresponding position $\{\lambda_j^{2S}\}$ of the $2S$-strings obtained by solving (2.7). Let us consider initially the cases where the lattice size is an even number.

3.1. *Lowest energy of sector n*

The ground state has zero momentum and belongs to the sector $n = 0$. Its corresponding distribution of roots, independently of γ, cluster in a sea of L string-like complexes of size $2S$ (see 2.6) where the imaginary parts are approximately equally spaced. The states with lowest energy in the other sectors also have zero momentum and their corresponding zeros cluster into $(L-[n/2S])$ string-like structures of size $2S$ and one string-like structure of size $\{n/2S\}$, where, as before, $[n/2S]$ and $\{n/2s\}$ are the integer part and the remaining fractional part of the ratio $(n/2S)$, respectively. In figures 1$(a$–$c)$ (spin 1), and figures 2$(a$–$c)$ (spin $\frac{3}{2}$) we draw in a schematic form, for an $L = 8$ chain and $\gamma = \pi/5$, the distribution of zeros for the lowest states in sectors $n = 0$, 1 and 2.

3.2. *Excited states with zero momentum*

For a given sector n several excitations occur, having a symmetric (with respect to the imaginary axis) distribution of zeros and consequently zero momentum. In figures 3$(a$–$g)$ we show a schematic sketch of the distribution of zeros for some of the most

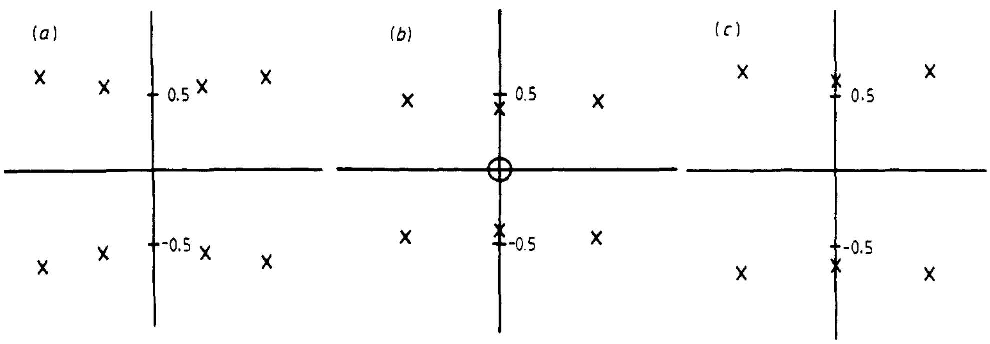

Figure 1. Typical distribution of zeros of the Bethe ansatz equations for the lowest-energy state in the sector n of the spin-1 model with $\gamma = \pi/5$ in a chain of width $L = 8$; the values of n are (a) $n = 0$ (ground state), (b) $n = 1$ and (c) $n = 2$.

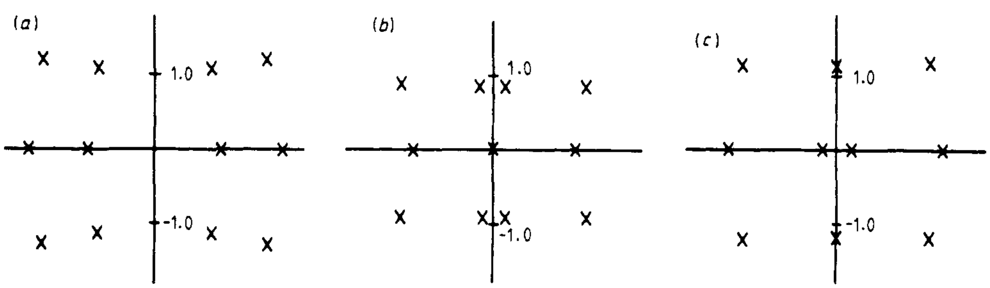

Figure 2. Typical distribution of zeros of the Bethe ansatz equations for the lowest-energy state in the sector n of the spin-$\frac{3}{2}$ model with $\gamma = \pi/5$ in a chain of width $L = 8$; the values of n are (a) $n = 0$ (ground state), (b) $n = 1$ and (c) $n = 2$.

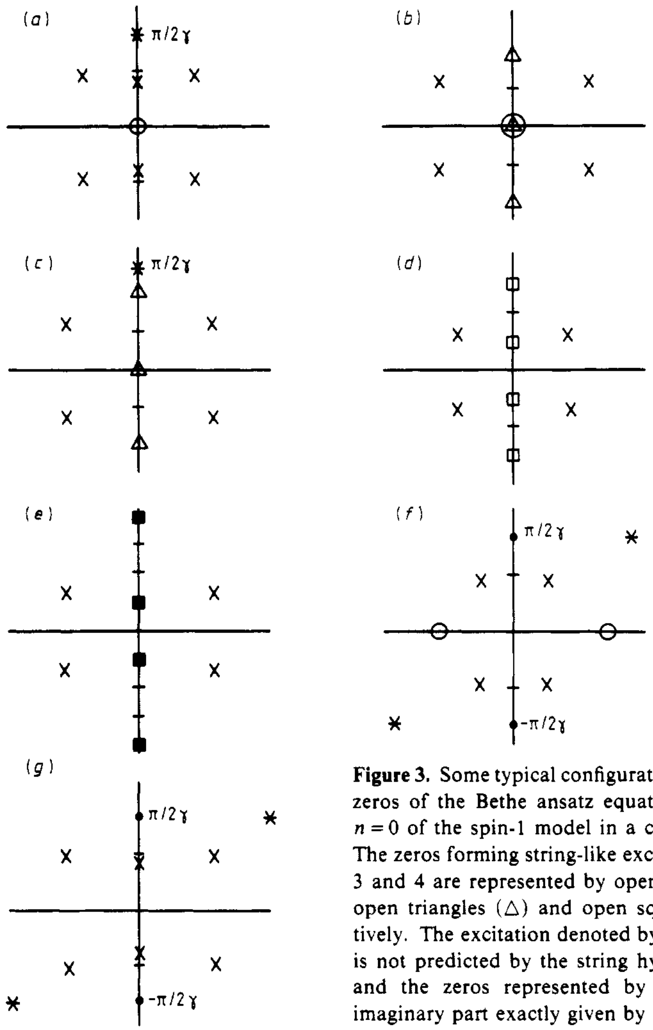

Figure 3. Some typical configurations of the complex zeros of the Bethe ansatz equations for the sector $n=0$ of the spin-1 model in a chain of $L=8$ sites. The zeros forming string-like excitations of size 1, 2, 3 and 4 are represented by open (○), crosses (×), open triangles (△) and open squares (□), respectively. The excitation denoted by full squares in (e) is not predicted by the string hypothesis (see text) and the zeros represented by asterisks have an imaginary part exactly given by $\pm\pi/2\gamma$.

significant excitations in the ground-state sector $n=0$, for the spin-1 system with $L=8$ sites. These are excitations in a sea of two-string particles (represented by crosses). The configuration in figure 3(a) is obtained by fixing two zeros, one at the origin (open circle) and other at $\lambda = \mathrm{i}\pi/2\gamma$ (asterisks), for all L, and solving for the remaining two-strings. In figures 3(b) and 3(c) the three strings (open triangles) are given exactly by (2.6), even for finite lattices. The squares in figure (3d) represent four string-like excitations. The excitations where the imaginary part is exactly $\pm\pi/2\gamma$, which are represented by asterisks in figure 3, are not predicted in the string assumption (2.6); however they can be included by considering a more general string hypothesis (Babujian and Tsvelick 1986, Kirillov and Reshetikhin 1987a, b). The excitation represented by full squares in figure 3(e) corresponds in the infinite-size limit to the zeros located at $(-2\mathrm{i}, -\mathrm{i}/2, \mathrm{i}/2, 2\mathrm{i})$, which is not predicted by either of these string assumptions (Alcaraz and Martins 1989). In figures 4(a–f) we also show the picture of zeros corresponding to the zero-momentum states in the $n=0$ sector of the spin-$\frac{3}{2}$ system with $L=8$. As before, several string-like and other excitations appear in a background of three string-like particles (crosses). From figures 3 and 4 and from the results of $S=\frac{1}{2}$

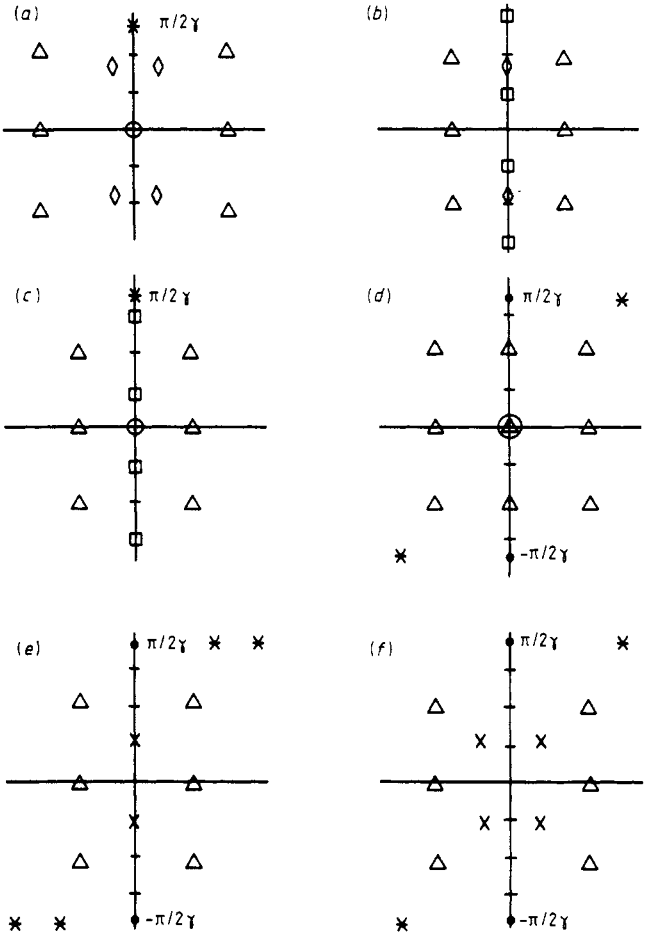

Figure 4. Some typical configurations of the complex zeros of the Bethe ansatz equations for the sector $n=0$ of the spin-$\frac{3}{2}$ model in a chain of $L=8$ sites. The zeros forming string-like excitations of size 1, 2, 3 and 4 are represented by open circles (○), crosses (×), open triangles (△) and open squares (□), respectively. The excitations denoted by open diamonds (◇) in (*a*) and (*b*) are not predicted by the string hypothesis (see text) and the zeros represented by asterisks (*) have the imaginary part $\pm\pi/2\gamma$.

(Alcaraz *et al* 1987, 1988a) and $S=2$ (Alcaraz and Martins 1988b) we verify that for arbitrary S, zeros will appear with their imaginary part exactly located, even for finite lattices, at $\lambda^{\pm}=\pm\pi/2\gamma$ or forming exact strings of size $(2S+1)$, given by (2.6). Similarly, as in the spin-1 case, configurations not predicted by the string hypothesis occur for higher spins (Alcaraz and Martins 1989). The distribution of zeros corresponding to the zero-momentum eigenenergies in the sectors where $n\neq 0$, are similar to those shown in figures 3 and 4, except that the number of $2S$-string-like structures in the background will depend on the particular value of n.

3.3. Excited states with non-zero momentum

The states with momentum $P=(2\pi k/L)$ $(k=1,2,\ldots,L-1)$ are characterised by a non-symmetric distribution of zeros. In figure 5 we show some of these distributions

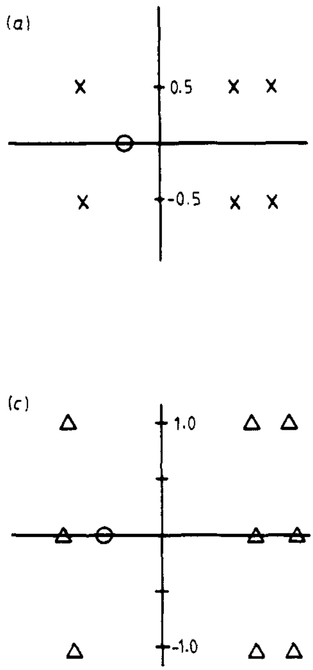

Figure 5. Schematic distribution of zeros corresponding to states with non-zero momentum P in a $L=8$ chain. (a) Spin 1, sector $n=1$, $P=2\pi/L$, (b) spin 1, sector $n=2$, $P=2\pi/L$ and (c) spin $\frac{3}{2}$, sector $n=2$, $P=2\pi/L$.

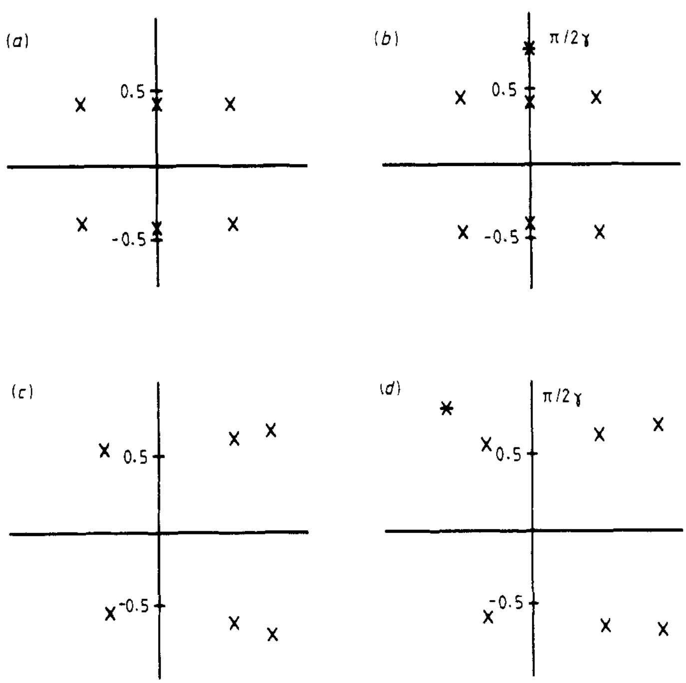

Figure 6. Some typical configurations of the complex zeros of the Bethe ansatz equations which occur in the sector n of the spin-1 Hamiltonian with $L=7$ sites. The states are: (a) ground state (sector $n=0$); (b) lowest-energy state in the sector $n=0$; (c) excited state in the sector $n=1$; (d) excited state in the sector $n=0$.

of zeros, together with the corresponding momenta, for the $L=8$ spin-1 and spin-$\frac{3}{2}$ systems.

Before closing this section let us mention the main features that occur in the distributions of zeros when the chain size L is an odd number. The results for spin-$\frac{1}{2}$ (Alcaraz *et al* 1988a) and our results for $S=1$ and $S=\frac{3}{2}$ indicate that the ground states occur in the sectors $n=\pm S$ and are consequently, at least, doubly degenerate. In figures 6(a) and 6(b) we show the pattern of zeros for the lowest-energy state of sectors $n=1$ (ground state) and $n=0$. In figures (6c) and (6d) we exhibit the structure of zeros for an excited state with non-zero momentum in the sectors $n=1$ and $n=0$, respectively.

4. Conformal anomaly

The finite-size effects of a two-dimensional statistical model in a strip of size L are equivalent to the finite-temperature effects of a one-dimensional quantum Hamiltonian, with temperature T ($L=\beta=1/T$). From this fact and the relation (1.8) (Blöte *et al* 1986, Affleck 1986a), the conformal anomaly c, or central charge of the associated Virasoro algebra may be estimated from the low-temperature behaviour of the specific heat of the associated infinite quantum Hamiltonian. From the specific heat calculations (Babujian 1982, 1983 and Takhtajan 1982), Affleck (1986a, b) calculated the conformal anomaly $c=3S/(1+S)$ for the spin-S XXZ Hamiltonian at the isotropic point $\gamma=0$. This central charge (see (1.5)), together with approximate mappings, leads to the conjecture (Affleck and Haldane 1987) that the criticality of these isotropic models is governed by Wess-Zumino-Witten-Novikov field-theoretic models with symmetry group SU(2) and topological charge $k=2S$. This conjecture was recently verified numerically by Alcaraz and Martins (1988a, b).

The low-temperature specific heat for the spin-S XXZ model was also calculated, in the bulk limit, for certain values of the anisotropy γ (Babujian and Tsvelick 1986; Kirillov and Reshetihkim 1987a, b). These calculations are based on the string hypothesis, and for $P=\pi/\gamma$ integer (Babujian and Tsvelick 1986) they produce a specific heat which gives us $c=3S/(1+S)$, as in the isotropic model. However for $P=\pi/\gamma$ irrational (not integer) (Kirillov and Reshetikhim 1987b) these results do not apply (Johannesson 1988). Consequently the finite-size calculations presented in this paper, which do not assume any string hypothesis, will be important in elucidating this point.

Our numerical results, for finite L, show that the state with lowest energy in the sector n, irrespective of the values of γ, is composed by the same sort of excitations (see § 3). The conformal anomaly c may be calculated from the finite-size corrections of the ground state of the finite lattice, $E_0(L)$, as in (1.8). The constant ζ, appearing in (1.8) and (1.9), can be calculated by comparing different energy levels associated with the same operator (same conformal tower). All the numerical analysis of the finite-size corrections for the eigenspectrum indicates that

$$\zeta=\frac{\pi\sin(2S\gamma S)}{4\gamma S}\qquad 0\leq\gamma\leq\pi/2S \tag{4.1}$$

which coincides with the velocity of sound originally calculated by Sogo (1984). From (1.8) and (4.1) we can therefore estimate the conformal anomaly from the large-L limit

Table 3. Finite-size estimators $c(L, \gamma)$ (4.2) for the conformal anomaly of the spin $S=1$ chain, for increasing L and several values of γ. In the last two lines we present the extrapolated and conjectured ($c=\frac{3}{2}$) results.

L	$\gamma=\pi/6$	$\gamma=\pi/5.5$	$\gamma=\pi/5$	$\gamma=\pi/4\sqrt{2}$	$\gamma=\pi/3\sqrt{2}$	$\gamma=\pi/3$
8	1.556 670	1.554 628	1.551 836	1.555 339	1.545 776	1.532 078
16	1.518 574	1.517 165	1.515 435	1.517 641	1.512 370	1.508 159
24	1.510 206	1.509 094	1.507 816	1.509 463	1.505 805	1.503 682
32	1.506 826	1.505 896	1.504 876	1.506 200	1.503 400	1.502 095
40	1.505 057	1.504 252	1.503 401	1.504 513	1.502 247	1.501 354
Extrapolated	1.500 00 (5)	1.500 00 (2)	1.500 00 (2)	1.500 00 (3)	1.500 00 (2)	1.500 00 (1)
Exact	1.5	1.5	1.5	1.5	1.5	1.5

Table 4. Conformal anomaly estimators $c(L, \gamma)$ (4.2), for several values of the spin $S=\frac{3}{2}$ chain. The extrapolated results together with the conjectured result ($c=1.8$) is presented in the last two lines.

L	$\gamma=\pi/6$	$\gamma=\pi/5.5$	$\gamma=\pi/5$	$\gamma=\pi/4\sqrt{2}$	$\gamma=\pi/4$	$\gamma=\pi/3\sqrt{2}$
8	1.874 366	1.868 455	1.861 212	1.870 463	1.844 910	1.849 180
16	1.822 895	1.819 802	1.816 722	1.820 793	1.812 113	1.813 130
24	1.811 823	1.809 746	1.807 913	1.810 388	1.805 703	1.806 147
32	1.807 472	1.805 924	1.804 667	1.806 390	1.803 357	1.803 604
40	1.805 262	1.804 035	1.803 103	1.804 397	1.802 231	1.802 387
Extrapolated	1.800 00 (4)	1.800 00 (4)	1.800 00 (2)	1.800 00 (4)	1.800 00 (2)	1.800 00 (1)
Exact	1.8	1.8	1.8	1.8	1.8	1.8

of the sequence

$$c(L, \gamma)=\frac{24\gamma LS}{\pi^2 \sin(2\gamma S)}(e_\infty L-E_0(L)). \tag{4.2}$$

Our numerical results for the spin-1 and spin-$\frac{3}{2}$ models reveal that for all values of γ ($0\leq\gamma\leq\pi/2S$), the above sequences give a conformal anomaly $c=3S/(1+S)$, like the isotropic model. In table 3 (spin-1) and table 4 (spin-$\frac{3}{2}$) we show the sequences (4.2) for $L=8$–40 and some values of γ. All the extrapolations presented in this paper were obtained by using the Van den Broeck and Schwartz (1979) approximants. The fact that the $S=\frac{1}{2}$ model (2.1) exhibits a critical line ($0\leq\gamma\leq\pi/2S$) of continuously varying exponents with a fixed conformal anomaly $c=1$, induces us to expect for all spin S the existence of critical exponents varying continuously with the values of γ. In this case the motion along the fixed line, for these general-spin models, should be governed by a marginal operator, with scaling dimensions $(\Delta, \bar{\Delta})=(1, 1)$.

5. The operator content of the periodic spin-S XXZ chain

We investigate in this section the operator content of the spin-S XXZ model, when the lattice size L is an even or odd number. In both cases the scaling dimensions of the operator describing the critical behaviour of the infinite system will be calculated using the relations (1.9), which relate these quantities to the mass gap amplitudes of the finite chain with periodic boundary conditions.

Using (1.9), the scaling dimension associated with the rth excited eigenstate $E_n^r(\gamma, L)$ of sector n will be given by the large-L limit of either of the sequences

$$\Lambda_L^r(\gamma, n) = \frac{L}{2\pi\zeta}(E_n^r(\gamma, L) - E_0(\gamma, L)) \tag{5.1}$$

or

$$\Omega_L^r(\gamma, n) = [(E_n^r(\gamma, L) - Le_\infty)6L + \pi c\zeta]/12\pi\zeta \tag{5.2}$$

where, as before, ζ is given by (4.1), $E_0(\gamma, L)$ is the ground state of the L-site chain, c is the conformal anomaly already calculated in § 4 and e_∞ is given by (2.5). The sequences (5.1) or (5.2) will be more convenient for the cases where L is an even or odd number, respectively. We will now consider separately the spin-1 and spin-$\frac{3}{2}$ models.

5.1. Spin-1 model

5.1. Even L. Let us consider initially the case where L is even. In this case the minimum-energy state, for whatever sector n, is a zero-momentum state and the ground state belongs to the sector $n = 0$. Our numerical results indicate that, associated with these states, there exists an operator $O_{n,0}$ with dimension $X_{n,0}(\gamma)$ given by

$$X_{n,0}(\gamma) = n^2 X_P + k/8 \qquad n = \pm 1, \pm 2, \ldots \tag{5.3a}$$

where

$$X_P = (\pi - 2\gamma)/4\pi \qquad k = (m+n) \bmod 2. \tag{5.3b}$$

In table 5 we show, for two values of γ, the sequences (5.1) corresponding to $X_{n,0}$ for L up to 40. We also present in these tables the extrapolated and conjectured results. Although we can extend our numerical calculations, without much computational effort, to lattices up to $L \sim 100$, this is not necessary because the convergence rate of the sequences (5.1), except around $\gamma = 0$ (see § 7), permit us to obtain convincing results by considering lattice sizes up to $L \sim 40$. The dimensions (5.3) depend continuously on γ, like the spin-$\frac{1}{2}$ model, and the operators $O_{1,0}$ and $O_{2,0}$ are generalisations of the polarisation and energy operators of the eight-vertex model (Baxter 1982), respectively. The constant $k/8$ appearing in (5.3), which has the value 1 for n odd (0

Table 5. Scaling dimension estimators $\Lambda_L^0(\gamma, n)$ (5.1) associated with the lowest-energy state of the sectors $n = 1$, 2 and 3 of the spin $S = 1$ chain for $\gamma = \pi/5.5$ and $\gamma = \pi/3$. The conjectured results are given by $X_{1,0}$, $X_{2,0}$ and $X_{3,0}$ in (5.3).

	$\Lambda_L^0(\gamma, 1)$		$\Lambda_L^0(\gamma, 2)$		$\Lambda_L^0(\gamma, 3)$	
L	$\gamma = \pi/5.5$	$\gamma = \pi/3$	$\gamma = \pi/5.5$	$\gamma = \pi/3$	$\gamma = \pi/5.5$	$\gamma = \pi/3$
8	0.293 770	0.216 797	0.604 082	0.337 335	1.431 334	0.897 076
16	0.288 377	0.211 744	0.622 176	0.334 283	1.516 489	0.891 919
24	0.286 854	0.210 429	0.627 626	0.333 745	1.537 152	0.887 609
32	0.286 136	0.209 838	0.630 176	0.333 560	1.545 324	0.884 968
40	0.285 717	0.209 505	0.631 627	0.333 767	1.549 395	0.883 225
Extrapolated	0.284 08 (9)	0.208 33 (4)	0.636 3 (4)	0.333 33 (3)	1.556 (7)	0.874 99 (8)
Exact	0.284 091	0.208 333	0.636 363	0.333 . . .	1.556 82	0.875

for n even) is related to the fact that, for such states, the configuration of zeros for the BAE have (do not have) a single one-particle excitation in addition to the sea of two-string excitations.

Let us now calculate the scaling dimensions associated with excited states in a given sector n. Let us, for the moment, restrict ourselves to the mass gap amplitudes associated with eigenstates with zero momentum. The distribution of zeros for the BAE for these states are symmetric with respect to the imaginary axis, and in figures 3(a–g) we can see some typical examples of them. Our numerical studies indicate that, for a given sector n, there exist two series of dimensions $X_{n,m}$ and $Y_{n,m}$ associated with the zero-momenta states where

$$X_{n,m}(\gamma) = n^2 X_P + (m^2/16X_P) + \tfrac{1}{2}|n \times m| + \tfrac{1}{8}k \tag{5.4a}$$

and

$$Y_{n,m}(\gamma) = X_{n,m}(\gamma) + 1 \qquad (n+m) = 0 \bmod 2 \tag{5.4b}$$

with $n,m = 0, \pm 1, \pm 2, \ldots$ and $k = (n+m) \bmod 2$. We see clearly that, apart from some additional constants, the above dimensions have the same structure as the dimensions appearing in the Gaussian model (Kadanoff and Brown 1979). In table 6 we show, for two values of γ, the corresponding finite-size sequences (5.1) for some scaling dimensions. It is interesting, at this point, to give an idea of the particular distribution of zeros of the BAE producing (5.4). The dimensions $X_{n,-1}$ are obtained from the configuration of zeros where one of the zeros, forming the minimum-energy state of sector n, jumps to the imaginary axis at $\lambda = \mathrm{i}\pi/2\gamma$ (excitation of type A), as in figure 3(a) for the sector $n = 0$. On the other hand, the dimensions $X_{n,+1}$ are produced by the configuration where three zeros jump to the imaginary axis forming an exact three-string excitation, as in figure 3(b) for the sector $n = 0$. The dimensions $X_{n,-2}$ are formed when four zeros, forming the state with lowest energy in the sector n, cluster in one three-string excitation and one excitation of the type A, described above, while $X_{n,2}$ are produced when the four zeros prefer to form a string of size four (see figures 3(c) and 3(d)). The other family of dimensions $Y_{n,m}$, which obeys the selection rule

Table 6. Finite-size sequences (5.1) associated with the scaling dimensions $X_{n,m}$ and $Y_{n,m}$ for the spin $S = 1$ model with an even number of sites for $\gamma = \pi/6$ and $\gamma = \pi/3\sqrt{2}$. The conjectured results are given by (5.4).

γ	L	$X_{0,-1}$	$X_{0,1}$	$X_{1,1}$	$X_{2,1}$	$Y_{2,0}$	$Y_{1,1}$
$\pi/6$	8	0.426 975	0.664 442	0.815 966	1.691 706	1.452 700	1.577 605
$\pi/6$	16	0.442 636	0.603 717	0.887 411	1.876 763	1.575 718	1.760 964
$\pi/6$	24	0.450 957	0.580 027	0.917 468	1.942 698	1.611 650	1.827 359
$\pi/6$	32	0.456 323	0.566 946	0.934 843	1.977 775	1.627 939	1.862 686
$\pi/6$	40	0.460 167	0.558 465	0.946 485	2.000 164	1.637 041	1.885 134
$\pi/6$	Extrapolated	0.500 (1)	0.500 (8)	1.040 (9)	2.16 (7)	1.666 (6)	2.04 (1)
$\pi/6$	Exact	0.5	0.5	1.041 666	2.166...	1.666...	2.041 666
$\pi/3\sqrt{2}$	8	0.547 607	0.698 164	0.928 352	1.759 540	1.385 526	1.677 497
$\pi/3\sqrt{2}$	16	0.570 430	0.651 720	1.012 558	1.957 544	1.480 061	1.893 878
$\pi/3\sqrt{2}$	24	0.578 752	0.635 043	1.042 452	2.019 710	1.503 739	1.966 977
$\pi/3\sqrt{2}$	32	0.583 073	0.626 436	1.045 760	2.048 909	1.513 286	2.002 778
$\pi/3\sqrt{2}$	40	0.585 735	0.621 160	1.066 744	2.065 621	1.518 125	2.023 837
$\pi/3\sqrt{2}$	Extrapolated	0.597 9 (5)	0.597 9 (4)	1.105 0 (4)	2.126 (5)	1.528 (2)	2.105 (1)
$\pi/3\sqrt{2}$	Exact	0.597 952	0.597 952	1.105 100	2.126 547	1.528 955	2.105 100

$(n+m)=0 \bmod 2$, is formed from the configuration which produces $X_{n,m}$, by the two zeros of the 2-string sea by two real excitations or two type-A excitations as in figure 3(*g*).

It is important to observe that (5.4*a*) exhibits the dimension $Y_{0,0}$, which is fixed to the unity, independent of the anisotropy γ (see table 7). Moreover, since the dimensions (5.4) are continuous functions of γ, we should find, from standard renormalisation group arguments, a dimension $X_{\text{mar}}=2$, for all γ, corresponding to the marginal operator O_{mar} governing the motion along the fixed critical line (Kadanoff and Brown 1979, Cardy 1987b). In fact, the configuration of zeros in which we have two one-particle excitations with imaginary part $\pm\pi/2\gamma$, like that of figure 3(*f*), produce the dimension $x=2$, for all γ. In table 7 we show, for some values of γ, the sequences (5.1) which correspond to this marginal operator, as well to $Y_{0,0}$.

Table 7. Finite-size sequences (5.1) associated with the scaling dimensions $Y_{0,0}$ and X_{mar} for $\gamma=\pi/6$, $\pi/5$ and $\pi/3\sqrt{2}$. The conjectured results are $Y_{0,0}=1$ and $X_{\text{mar}}=2$ for all values of γ.

	$Y_{0,0}$			X_{mar}		
L	$\gamma=\pi/6$	$\gamma=\pi/5$	$\gamma=\pi/3\sqrt{2}$	$\gamma=\pi/6$	$\gamma=\pi/5$	$\gamma=\pi/3\sqrt{2}$
8	0.851 557	0.890 211	0.925 984	1.613 828	1.662 672	1.728 701
16	0.920 530	0.952 621	0.974 573	1.801 863	1.852 085	1.902 064
24	0.945 918	0.972 031	0.986 972	1.867 114	1.912 079	1.948 881
32	0.959 052	0.980 920	0.991 981	1.900 062	1.939 859	1.968 238
40	0.967 068	0.985 860	0.994 520	1.919 923	1.955 389	1.978 169
Extrapolated	0.999 9 (8)	0.999 9 (8)	0.999 9 (8)	1.999 9 (4)	1.999 (8)	1.999 (8)
Exact	1	1	1	2	2	2

The fact that the conformal anomaly has the value $c=\frac{3}{2}=1+\frac{1}{2}$ and the existence of the marginal operator, peculiar to $c=1$ theories, induces us to interpret the present model in terms of composite operators

$$\psi^{n,m}_{\Delta_\text{I},\bar{\Delta}_\text{I}}=\sigma_{\Delta_\text{I},\bar{\Delta}_\text{I}}\phi^{n,m}_{\Delta^+,\Delta^-} \tag{5.5a}$$

formed by the product of an Ising-type ($c=\frac{1}{2}$) operator $\sigma_{\Delta_\text{I},\bar{\Delta}_\text{I}}$ with dimensions $(\Delta_\text{I},\bar{\Delta}_\text{I})$ and a Gaussian-type ($c=1$) operator (U(1) symmetric), $\phi^{n,m}_{\Delta^+,\Delta^-}$ with dimensions (Δ^+,Δ^-), which describes an excitation with spin wavenumber n and a vorticity m, where

$$\Delta_\text{I},\bar{\Delta}_\text{I}=0,\tfrac{1}{2},\tfrac{1}{16} \tag{5.5b}$$

$$\Delta^{\pm}=\tfrac{1}{2}[n\sqrt{X_P}\pm(m/4\sqrt{X_P})]^2. \tag{5.5c}$$

Consequently the scaling dimension and spin of the composite operator (5.4*a*) are given by

$$d^{n,m}_{\Delta_\text{I},\bar{\Delta}_\text{I}}=\Delta_\text{I}+\bar{\Delta}_\text{I}+n^2X_P+(m^2/16X_P) \tag{5.5d}$$

and

$$S^{n,m}_{\Delta_\text{I},\bar{\Delta}_\text{I}}=\Delta_\text{I}-\bar{\Delta}_\text{I}+\tfrac{1}{2}|n\times m| \tag{5.5e}$$

respectively. In fact we can interpret, in a closed form, all the dimensions (5.4), related to zero-momenta states, as arising from the conformal towers of the primary operators $\psi^{n,m}_{\Delta_\text{I},\bar{\Delta}_\text{I}}$. For example, we show in table 8 the position (M and M' of (1.9)) in the

Table 8. The location (M and M' in (1.9)) of the dimensions $X_{n,m}$ and $Y_{n,m}$ given by (5.4), in the conformal towers of the primary operators $\psi^{n,m}_{\Delta_I,\bar{\Delta}_I}$ with spin $S^{n,m}_{\Delta_I,\bar{\Delta}_I}$.

	n	m	Δ_I	$\bar{\Delta}_I$	$\lvert n\times m\rvert/2$	M	M'	$S^{n,m}_{\Delta_I,\bar{\Delta}_I}$
$X_{0,0}$	0	0	0	0	0	0	0	0
$Y_{0,0}$	0	0	$\frac{1}{2}$	$\frac{1}{2}$	0	0	0	0
$X_{0,1}$	0	1	$\frac{1}{16}$	$\frac{1}{16}$	0	0	0	0
$X_{1,1}$	1	1	0	$\frac{1}{2}$	$\frac{1}{2}$	0	0	0
$Y_{1,1}$	1	1	$\frac{1}{2}$	0	$\frac{1}{2}$	0	1	1
$X_{2,1}$	2	1	$\frac{1}{16}$	$\frac{1}{16}$	1	0	1	1
$X_{2,2}$	2	2	0	0	2	0	2	2
$Y_{2,0}$	2	0	$\frac{1}{2}$	$\frac{1}{2}$	0	0	0	0

conformal tower of the primary operator $\psi^{n,m}_{\Delta_I,\bar{\Delta}_I}$, for some of the dimensions (5.4). More generally from (5.4) and table 8 we clearly see that the Ising and Gaussian fields couple in a peculiar way depending on the parity of n and m: $\psi^{n,m}_{0,0}$ and $\psi^{n,m}_{1/2,1/2}$, for n, $m=2\mathbb{Z}$ (even); $\psi^{n,m}_{0,1/2}$ and $\psi^{n,m}_{1/2,0}$ for n, $m=2\mathbb{Z}+1$ (odd) and $\psi^{n,m}_{1/16,1/16}$, for $n-m=2\mathbb{Z}+1$ (odd). These results also predict that the lowest level ($M=M'=0$) in the conformal tower of primary operators with non-zero spin should correspond to an eigenstate with momentum different from zero. In fact we verified these predictions numerically. For example, the eigenenergy, in the sector $n=1$, corresponding to the configuration of the type shown in figure 5(a), (momentum $P=2\pi/L$) produces the dimension of the spin-1 primary field $\psi^{1,1}_{1/2,0}$. As another typical example we mention the particular state, with momentum $P=2\pi/L$ in the sector $r=2$ (figure 5(b)), which produces the dimension of the spin-1 operator $\psi^{2,1}_{1/16,1/16}$. In table 9 we show our numerical estimates for the amplitudes derived from these two non-zero momentum states.

It is interesting to observe that the dimension $X_{\mathrm{mar}}=2$, corresponding to the marginal operator, is not given directly by (5.5). We can try to interpret this dimension as representing the $M=M'=1$ (the corresponding level will have zero momentum, as it should) daughter of the identity operator $\psi^{0,0}_{0,0}$ or the first level ($M=M'=0$) of a spinless primary marginal operator of the Virasoro algebra. In this latter case, in order to include this primary field in (5.5), the dimensions Δ^+ and Δ^- of the Gaussian field $\phi^{n,m}_{\Delta^+,\Delta^-}$ should be interpreted as the irreducible representations of an algebra larger

Table 9. Scaling dimensions estimators (5.1) corresponding to the dimensions $d^{2,1}_{1/16,1/16}$ and $d^{1,1}_{1/2,0}$ for $\gamma=\pi/6$ and $\gamma=\pi/5$. These dimensions are related to states with momentum $P=2\pi/L$ and their conjectures values are given by (5.5d) (see text).

	$d^{2,1}_{1/16,1/16}$		$d^{1,1}_{1/2,0}$	
L	$\gamma=\pi/6$	$\gamma=\pi/5$	$\gamma=\pi/6$	$\gamma=\pi/5$
8	1.083 739	1.070 432	0.999 616	1.013 155
16	1.137 619	1.119 800	1.037 710	1.056 296
24	1.150 266	1.130 371	1.042 759	1.063 193
32	1.155 510	1.134 465	1.043 858	1.065 275
40	1.158 299	1.136 527	1.044 068	1.066 103
Extrapolated	1.166 6 (5)	1.141 (6)	1.041 (6)	1.066 (7)
Exact	1.166 . . .	1.141 666	1.041 666	1.066 . . .

than the Virasoro algebra. From the fact that when $\gamma=0$ the conjectured underlying algebra is an SU(2) Kac–Moody algebra (Affleck 1986a, b, Affleck and Haldane 1987) we expect that, as in the spin-$\frac{1}{2}$ model (Alcaraz *et al* 1988a, b) the Gaussian field dimensions Δ^+ and Δ^- are the irreducible representations of the U(1) Kac–Moody algebra. As discussed by Cardy (1987b), a marginal primary operator in a non-decomposable $c>1$ theory can only occur through a very unusual combination of the coefficients in the operator product expansion of the associated operator algebra. This is not the case for the present model since, from (5.5), we can decompose its $c>1$ conformal algebra into a product of a $c=1$ (which has the marginal operator) and a $c=\frac{1}{2}$ algebra.

All these results indicate that the operator content for the spin-1 model, with periodic boundaries, is given by

$$\mathscr{E}^{e}_{s=1}(\gamma)=\Bigg([(0,0)_V+(\tfrac{1}{2},\tfrac{1}{2})_V]\otimes\sum_{\substack{n=2\mathbb{Z}\\ m=2\mathbb{Z}}}+[(0,\tfrac{1}{2})_V+(\tfrac{1}{2},0)_V]\otimes\sum_{\substack{n=2\mathbb{Z}+1\\ m=2\mathbb{Z}+1}}$$
$$+(\tfrac{1}{16},\tfrac{1}{16})_V\otimes\sum_{\substack{n=2\mathbb{Z}\\ m=2\mathbb{Z}+1}}+(\tfrac{1}{16},\tfrac{1}{16})_V\otimes\sum_{\substack{n=2\mathbb{Z}+1\\ m=2\mathbb{Z}}}\Bigg)(\Delta^+,\Delta^-)_{KM} \tag{5.6}$$

where $(\Delta_I,\bar{\Delta}_I)_V$ and $(\Delta^+,\Delta^-)_{KM}$ are the irreducible representations of the $c=\frac{1}{2}$ (Ising) Virasoro algebra and the U(1) Kac–Moody algebra (Gaussian), respectively.

It is important to mention here that (5.6) are precisely the dimensions occurring in the generalised Coulomb gas picture, recently proposed for this model by Di Francesco *et al* (1988).

The Ising dimensions occurring in (5.6) can be identified (Cardy 1986b), with the operator content $z_2(r,s)$ of the sector $s=0$ or 1 (even or odd parity) of the Ising model with toroidal boundary condition $r=0$ or 1 (periodic or antiperiodic) and (5.6) can be written in the more simplified form

$$\mathscr{E}^{e}_{s=1}(\gamma)=\sum_{r=0}^{1}\sum_{s=0}^{1}z_2(r,s)\otimes\sum_{\substack{n=2\mathbb{Z}+r\\ m=2\mathbb{Z}+s}}(\Delta^+,\Delta^-)_{KM} \tag{5.7}$$

5.1.2. Odd L. In this subsubsection we will calculate, from the mass gap amplitudes, the operator content of the spin-1 XXZ model, when the number of sites is an odd number. Due to the antiferromagnetic character of the spin chains we are studying, the ground state, when the lattice size is odd, is frustrated. This implies that in the infinite-size limit the ground state of these odd lattices tends toward an excited state with a topological excitation induced by this frustration. In this sense this effect is similar to that produced by the introduction of other toroidal boundary conditions, which are not periodic, in the even-L chain.

In the same way, as occurred when L is even, the dimensions obtained by extrapolating (5.2) can be explained as being derived from the conformal towers of the composite operator $\psi^{n,m}_{\Delta_I,\bar{\Delta}_I}$ introduced in (5.5). As we discussed at the end of § 3, the ground state, in this case, is a zero-momentum eigenstate of the sector $n=1$ (see figure 6(a)). Its associated dimension, obtained from (5.2), is given by $d^{1,0}_{1/16,1/16}$ in (5.5d). The lowest energy in the sector $n=0$ (see figure 6(b)), which also has zero momentum, produces the dimension $d^{0,1}_{1/16,1/16}$. The non-zero-momentum states of sector $n=1$ and $n=0$, shown in figures 6(c) and 6(d), give us the dimensions $d^{1,1}_{0,0}$ and $d^{0,0}_{1/2,0}$, respectively. In table 10 we show the sequences (5.2) corresponding to the above sequences.

Table 10. Scaling dimensions estimators (5.2) for the spin $S=1$ model with $\gamma=\pi/6$ and $\gamma=\pi/5$, in a lattice with an odd number of sites, we list sequences corresponding to $d^{1,0}_{1/16,1/16}$, $d^{0,1}_{1/16,1/16}$, $d^{1,1}_{0,1}$ and $d^{0,0}_{1/2,0}$ (see text).

	$d^{1,0}_{1/16,1/16}$		$d^{0,1}_{1/16,1/16}$		$d^{1,1}_{0,0}$		$d^{0,0}_{1/2,0}$	
L	$\gamma=\pi/6$	$\gamma=\pi/5$	$\gamma=\pi/6$	$\gamma=\pi/5$	$\gamma=\pi/6$	$\gamma=\pi/5$	$\gamma=\pi/6$	$\gamma=\pi/5$
7	0.274 186	0.261 698	0.385 096	0.428 289	0.549 052	0.565 966	0.511 146	0.506 089
15	0.283 218	0.268 830	0.421 333	0.471 938	0.547 987	0.568 587	0.507 253	0.503 801
23	0.286 117	0.271 035	0.436 461	0.489 223	0.546 277	0.568 179	0.505 037	0.502 441
31	0.287 539	0.272 094	0.445 418	0.498 803	0.545 247	0.567 833	0.503 828	0.501 738
35	0.288 009	0.272 440	0.448 654	0.502 195	0.544 882	0.567 702	0.503 413	0.501 506
Extrapolated	0.291 66 (6)	0.274 9 (9)	0.500 (3)	0.541 6 (2)	0.541 (5)	0.566 (5)	0.499 9 (4)	0.499 9 (4)
Exact	0.291 66...	0.275	0.5	0.541 666	0.541 66...	0.566...	0.5	0.5

Collecting all the amplitudes we have derived, our numerical analysis indicates the following operator content for the spin-1 model, for the infinite-L (odd) chain:

$$\mathscr{E}^{\mathrm{o}}_{s=1}(\gamma)=\Bigg([(0,\tfrac{1}{2})_{\mathrm{V}}+(\tfrac{1}{2},0)_{\mathrm{V}}]\otimes\sum_{\substack{n=2\mathbb{Z}\\ m=2\mathbb{Z}}}+[(0,0)_{\mathrm{V}}+(\tfrac{1}{2},\tfrac{1}{2})_{\mathrm{V}}]\otimes\sum_{\substack{n=2\mathbb{Z}+1\\ m=2\mathbb{Z}+1}}$$

$$+(\tfrac{1}{16},\tfrac{1}{16})_{\mathrm{V}}\otimes\sum_{\substack{n=2\mathbb{Z}\\ m=2\mathbb{Z}+1}}+(\tfrac{1}{16},\tfrac{1}{16})_{\mathrm{V}}\otimes\sum_{\substack{n=2\mathbb{Z}+1\\ m=2\mathbb{Z}}}\Bigg)(\Delta^+,\Delta^-)_{\mathrm{KM}} \tag{5.8}$$

where the notation is the same as in (5.6). The result (5.8) contradicts the conjectured results (Di Francesco *et al* 1988) obtained for these odd L lattices, from a combination of partition functions of generalised Coulomb gases.

It is interesting to observe that if we add (5.6) to (5.8) and divide by two, we can express the Ising part of the resulting operator content in terms of a larger algebra formed by the combination of two Virasoro ($c=\frac{1}{2}$) conformal towers:

$$\mathscr{E}_{s=1}(\gamma)=\frac{1}{2}\Bigg((0\oplus\tfrac{1}{2},0\oplus\tfrac{1}{2})\otimes\sum_{n-m=2\mathbb{Z}}+(\tfrac{1}{16}\oplus\tfrac{1}{16},\tfrac{1}{16}\oplus\tfrac{1}{16})\otimes\sum_{n-m=2\mathbb{Z}+1}\Bigg)(\Delta^+,\Delta^-)_{\mathrm{KM}}. \tag{5.9}$$

5.2. Spin $\frac{3}{2}$

5.2.1. Even L. Let us restrict our attention initially to the case of even lattice sizes. From the lowest state in the sector n (zero momentum, see figures 2(a)-(c)) the extrapolated values of the sequences (5.1) give the dimensions

$$X_{n,0}=n^2X_P+t_n \tag{5.10a}$$

where

$$X_P=(\pi-3\gamma)/6\pi \tag{5.10b}$$

and $t_n=0$ or $\frac{2}{15}$ depending on whether n is a multiple of $3(n=3\mathbb{Z})$ or not ($n=3\mathbb{Z}+1$ or $n=3\mathbb{Z}+2$), respectively. As in the spin-1 model, these dimensions depend continuously on γ. In table 11 we show some of our numerical estimates for the above dimensions. The above constants t_n are some of the dimensions appearing in the Kac table (1.2) of the $c=\frac{4}{5}$ Virasoro algebra, which corresponds to the three-state Potts

Table 11. Scaling dimensions estimators $\Omega_L^0(\gamma, n)$ (equation (5.1)) associated with the lowest-energy state of the sectors $n = 1$, 2 and 3 of the spin $S = \frac{3}{2}$ chain for $\gamma = \pi/3\sqrt{2}$ and $\gamma = \pi/3$. The conjectured results are given by $X_{1,0}$, $X_{2,0}$ and $X_{3,0}$ in (5.10).

	$\Omega_L^0(\gamma, 1)$		$\Omega_L^0(\gamma, 2)$		$\Omega_L^0(\gamma, 3)$	
L	$\gamma = \pi/3\sqrt{2}$	$\gamma = \pi/6$	$\gamma = \pi/3\sqrt{2}$	$\gamma = \pi/6$	$\gamma = \pi/3\sqrt{2}$	$\gamma = \pi/6$
8	0.196 617	0.236 134	0.339 730	0.474 425	0.441 280	0.709 246
16	0.189 050	0.226 211	0.333 608	0.472 258	0.439 591	0.733 202
24	0.186 825	0.223 184	0.331 931	0.471 192	0.439 384	0.740 277
32	0.185 743	0.221 690	0.331 139	0.470 505	0.439 335	0.743 442
40	0.185 096	0.220 790	0.330 672	0.470 019	0.439 321	0.745 177
Extrapolated	0.182 1 (3)	0.216 66 (5)	0.328 5 (8)	0.466 6 (7)	0.439 33 (8)	0.749 9 (5)
Exact	0.182 149	0.216 6...	0.328 595	0.466...	0.439 340	0.75

model. Our results for spin 1 and the fact that the conformal anomaly of this model $c = \frac{9}{5} = 1 + \frac{4}{5}$ induce us to interpret this spin-$\frac{3}{2}$ model in terms of the composite operator

$$\psi^{n,m}_{\Delta_3, \bar{\Delta}_3} = \sigma_{\Delta_3, \bar{\Delta}_3} \phi^{n,m}_{\Delta^+, \Delta^-} \tag{5.11a}$$

formed by the product of the Z(3)-type operator $\sigma_{\Delta_3, \bar{\Delta}_3}$ ($c = \frac{4}{5}$) with dimensions $(\Delta_3, \bar{\Delta}_3)$ and the Gaussian-type ($c = 1$) operator, $\phi^{n,m}_{\Delta^+, \Delta^-}$ with dimensions

$$\Delta^{\pm} = \tfrac{1}{2}[n\sqrt{X_P} \pm (m/6\sqrt{X_P})]^2. \tag{5.11b}$$

From (1.2) the possible scaling dimensions of the primary Z(3) fields are

$$\Delta_3, \bar{\Delta}_3 = 0, \tfrac{1}{40}, \tfrac{1}{15}, \tfrac{1}{8}, \tfrac{2}{5}, \tfrac{2}{3}, \tfrac{21}{40}, \tfrac{7}{5}, \tfrac{13}{8}, 3 \tag{5.11c}$$

the total dimension and spin of the operator $\psi^{n,m}_{\Delta_3, \bar{\Delta}_3}$ will be given by

$$d^{n,m}_{\Delta_3, \bar{\Delta}_3} = \Delta_3 + \bar{\Delta}_3 + n^2 X_P + (m^2/36 X_P) \tag{5.11d}$$

and

$$S^{n,m}_{\Delta_3, \bar{\Delta}_3} = \Delta_3 - \bar{\Delta}_3 + \tfrac{1}{3}|nm|. \tag{5.11e}$$

Consequently the dimensions (5.9) can be identified as being associated with the spinless operator $\psi^{n,0}_{0,0}$ or $\psi^{n,0}_{1/15,1/15}$ depending on whether n is a multiple of 3 or not, respectively.

From the excited states with zero momentum in a given sector n, we obtained several families of dimensions. For example, the states with the distributions of zeros with correspond to figures 4(a)-(f) give us the dimensions $d^{0,-1}_{1/15,1/15}$, $d^{0,1}_{1/15,1/15}$, $d^{0,2}_{1/15,1/15}$, $d^{0,0}_{2/5,2/5}$, $d^{0,0}_{7/5,7/5}$ and $X_{\text{mar}} = 2$, respectively. In tables 12 and 13 we show some of the sequences (5.1) obtained from the zero-momentum states.

We calculate all the amplitudes numerically and our experience of the spin-1 model indicates the following operator content for the spin-$\frac{3}{2}$ model, with periodic boundary conditions:

$$\mathscr{E}^{e}_{s=3/2}(\gamma) = \sum_{r=0}^{2} \sum_{s=0}^{2} z_3(r, s) \otimes \sum_{n=3\mathbf{Z}+r} \sum_{m=3\mathbf{Z}+s} (\Delta^+, \Delta^-)_{\text{KM}} \tag{5.12a}$$

Table 12. Scaling dimensions estimators (5.1) associated with zero-momentum states of the spin $S=\frac{3}{2}$ model with $\gamma=\pi/6$. The associated dimensions $d^{n',m'}_{\Delta_3,\bar{\Delta}_3}$ are conjectured by (5.11d). The last column corresponds to the daughter $M=0$, $M'=1$ (see equation (1.9)) of the primary operator with spin 1 and dimensions $d^{1,1}_{0,2/3}$.

L	$d^{0,-1}_{1/15,1/15}$	$d^{0,1}_{1/15,1/15}$	$d^{2,0}_{2/3,2/3}$	$d^{1,1}_{1/15,2/5}$	$d^{3,0}_{2/5,2/5}$	$d^{1,1}_{0,2/3}+1$
8	0.432 962	0.612 011	1.470 906	1.045 961	1.421 125	1.629 843
16	0.441 860	0.548 797	1.591 220	0.998 577	1.509 423	1.829 941
24	0.446 560	0.526 212	1.624 541	0.973 072	1.531 421	1.901 644
32	0.449 455	0.514 312	1.638 920	0.952 199	1.540 146	1.938 870
40	0.451 451	0.506 849	1.646 611	0.947 531	1.544 455	1.961 916
Extrapolated	0.466 (8)	0.466 (7)	1.666 (4)	0.883 (7)	1.55 (2)	2.084 (1)
Exact	0.466 . . .	0.466 . . .	1.666 . . .	0.833 3 . . .	1.55	2.083 3 . . .

where

$$z_3(0,0)=(0,0)_V+(\tfrac{2}{5},\tfrac{2}{5})_V+(\tfrac{2}{5},\tfrac{7}{5})_V+(\tfrac{7}{5},\tfrac{2}{5})_V+(\tfrac{7}{5},\tfrac{7}{5})_Y+(3,0)_V+(0,3)_V+(3,3)_V \quad (5.12b)$$

$$z_3(1,1)=z_3(2,2)=(\tfrac{1}{15},\tfrac{2}{5})_V+(\tfrac{1}{15},\tfrac{7}{15})_V+(\tfrac{2}{3},0)_V+(\tfrac{2}{3},3)_V \quad (5.12c)$$

$$z_3(1,2)=z_3(2,1)=(\tfrac{2}{5},\tfrac{1}{15})_V+(\tfrac{7}{5},\tfrac{1}{15})_V+(0,\tfrac{2}{3})_V+(3,\tfrac{2}{3})_V \quad (5.12d)$$

$$z_3(1,0)=z_3(0,1)=z_3(0,2)=z_3(2,0)=(\tfrac{1}{15},\tfrac{1}{15})_V+(\tfrac{2}{3},\tfrac{2}{3})_V. \quad (5.12e)$$

The dimensions $(\Delta_3,\bar{\Delta}_3)_V$ and $(\Delta^+,\Delta^-)_{KM}$ are the irreducible representations of the $c=\frac{4}{5}$ (three-state Potts model) Virasoro algebra and the U(1) Kac–Moody algebra (Gaussian), respectively.

As in the $S=1$ model, the above dimensions for even lattices (5.12), are precisely the dimensions appearing in the partition function of the gneralised Coulomb gas recently introduced by Di Francesco *et al* (1988). It is important to observe that only a subset of all the possible dimensions (5.11c) occurs in (5.12b)–(5.12e). In fact, in a manner, analogous to the $S=1$ model, the dimensions $z_3(r,s)$ are exactly the operator content of the sector of charge s (0, 1 or 3) of the three-state Potts quantum Hamiltonian with toroidal boundary condition $S_{L+1}=S_1\exp[\mathrm{i}(2\pi/3)r]$ $(r=0,1,2)$, where S_i are Z(3) operators (see, e.g., von Gehlen and Rittenberg 1986).

Table 13. Finite-size sequences corresponding to the scaling dimensions $d^{0,0}_{2/5,2/5}$ and X_{mar} (equation (5.11)) for the spin $S=\frac{3}{2}$ chain with $\gamma=\pi/6$ and $\gamma=\pi/5$. The conjectured results are $d^{0,0}_{2/5,2/5}=\frac{4}{5}$ and $X_{\mathrm{mar}}=2$ for all values of γ.

	$d^{0,0}_{2/5,2/5}$		X_{mar}	
L	$\gamma=\pi/6$	$\gamma=\pi/5$	$\gamma=\pi/6$	$\gamma=\pi/5$
8	0.767 180	0.803 640	1.668 626	1.757 219
16	0.793 840	0.813 440	1.885 240	1.916 682
24	0.800 091	0.812 790	1.914 165	1.957 605
32	0.802 244	0.811 422	1.941 377	1.974 075
40	0.803 107	0.810 198	1.956 563	1.982 381
Extrapolated	0.80 (2)	0.80 (1)	1.999 (2)	1.999 9 (3)
Exact	0.8	0.8	2	2

5.2.2. Odd L. We now close this section by discussing the operator content obtained in the case where the lattice size L is an odd number. As in the $S=1$ model, due to the antiferromegnetic character of the interactions, the ground state is frustrated. The ground state is a non-zero-momentum state in the sector $n=\frac{3}{2}$. Using the sequence (5.2) we verify that its associated dimension is $d^{3/2,1/2}_{1/15,1/15}$. On the other hand the lower state, in the sector $n=\frac{1}{2}$, is associated to the dimension $d^{1/2,1/2}_{1/15,2/5}$.

The BAE for these odd-L lattices are very difficult to solve numerically and we calculated only a few mass gap amplitudes. The amplitudes we derived together with the results (5.9) for the spin-1 (L odd) and (5.12) for the spin-$\frac{3}{2}$ (L even) indicate the following operator content for the spin-$\frac{3}{2}$ model, for the infinite-L (odd) chain

$$\mathscr{E}^{\mathrm{o}}_{s=3/2}(\gamma)=\sum_{r=0}^{2}\sum_{s=0}^{2} z_3(r,s)\otimes\sum_{n=3Z+r+3/2}\;\sum_{m=3Z+s+3/2}(\Delta^+,\Delta^-)_{\mathrm{KM}} \tag{5.13}$$

where the notation is the same as in (5.12).

6. Corrections to finite-size scaling

In this section we will discuss briefly some of the dominant corrections appearing in (1.8) and (1.9) due to the finite size of the system. In fact these relations are valid only in the $L\to\infty$ limit. For finite L the eigenenergy $E_\alpha(L)$ corresponding to the operator O_α, with dimension X_α, has the correction $R_\alpha(L)$, i.e.

$$\frac{E_\alpha(L)}{L}=Le_\infty+\frac{2\pi\zeta}{L}\left(X_\alpha-\frac{c}{12}+R_\alpha(L)\right). \tag{6.1}$$

These corrections arise (Cardy 1986a) since the physical finite-lattice Hamiltonian deviates from the conformally invariant Hamiltonian, H^*, of the continuum theory, by terms involving irrelevant operators, i.e.

$$H=H^*+\sum_\beta a_\beta O_\beta \tag{6.2}$$

where O_β are irrelevant operators with scaling dimensions $X_\beta>2$ and a_β are the coupling constants, unknown in principle.

Applying standard perturbation theory (Cardy 1986a, von Gehlen *et al* 1986, Reinicke 1987, Alcaraz *et al* 1988a), up to second order, the correction term $R_\alpha(L)$ in (6.1) can be expressed in terms of the coefficients $C_{\alpha,\beta,\delta}$ of the operator product expansion (Kadanoff 1979, Kadanoff and Brown 1979):

$$R_\alpha(L)=2\pi\sum_\beta a_\beta C_{\alpha,\alpha,\beta}\left(\frac{2\pi}{L}\right)^{x_\beta-2}+4\pi^2\sum_{\beta,\beta',\alpha'}{}^{\prime}\frac{a_\beta a_{\beta'}C_{\alpha',\alpha,\beta}(2\pi/L)^{x_\beta+x_{\beta'}-4}}{x_\alpha-x_{\alpha'}}+\ldots \tag{6.3}$$

where the term, $\alpha'=\alpha$ is excluded from the second sum. Consequently we can understand, from the finite-size eigenenergies, which of the irrelevant operators govern the corrections due to the finite size.

The irrelevant operators, in the identity block, will always be present (Cardy 1986a, Reinicke 1987) in (6.2). The most dominant of these operators has dimension $X_I=4$ leading to a term $\mathcal{O}(L^{-2})$ in $R_\alpha(L)$. The other irrelevant operators entering (6.3) depend on the particular Hamiltonian under consideration and on the particular symmetries and selection rules which determine the coefficients $C_{\alpha,\beta,\gamma}$ in (6.3). The key question is now to identify from our finite-size results the dominant irrelevant operators entering (6.2).

Let us discuss initially the above corrections for the eigenenergies derived under the string assumption (see § 2.1 and the appendix). From (2.10) the first two terms for the corrections $R_\alpha(L)$ ($X_0 = 0$ in (6.1)), corresponding to the ground state E_0^{st}, are of $\sigma(L^{-2})$, $\sigma(L^{-2/s})$ and $\sigma(L^{-4\gamma/(\pi-2s\gamma)})$. As we already discussed, we do not expect that the amplitudes corresponding to these powers are the same as the true energies obtained without any string assumption. Moreover due to the fact that the string assumption only perceives the Gaussian part (gives $c = 1$, for all S, for example), it may be that certain powers of L are not correctly estimated by this assumption. For example, our numerical analysis of the correct energies reveals that the term $o(L^{-4/3})$, for all γ, predicted for the ground state of the spin-$\frac{3}{2}$ model, is not present. On the other hand, other terms not predicted by (2.10) and (2.11) are present in the finite-size corrections of the true energies.

The dominant finite-size corrections of the true energies (2.4) may be estimated in several ways. Assuming in (6.1)

$$R_\alpha(L) \sim B_\alpha L^{-w_\alpha} \tag{6.4}$$

We can calculate the power w_α from the large-L behaviour of the sequence

$$W_\alpha(L) = \left[\ln\left(\frac{R_\alpha(L)}{R_\alpha(L+1)}\right)\right]\left[\left(\frac{L+1}{L}\right)\right]^{-1}. \tag{6.5}$$

In figures 7(a) and 7(b) we show, for several values of γ, the extrapolated values w_0 and w_1 for the ground state and lowest energy state for the sector $n = 1$ of the spin-1 model. These numerical results indicate that, for the ground state,

$$W_0 = \begin{cases} 4\gamma/(\pi - 2\gamma) & \text{if } \gamma < \pi/4 \\ 2 & \text{if } \gamma > \pi/4 \end{cases} \tag{6.6a}$$

while for the lowest state in the sector $n = 1$

$$W_1 = \begin{cases} 4\gamma/(\pi - 2\gamma) & \text{if } \gamma < \pi/6 \\ 1 & \text{if } \gamma > \pi/6 \end{cases}. \tag{6.6b}$$

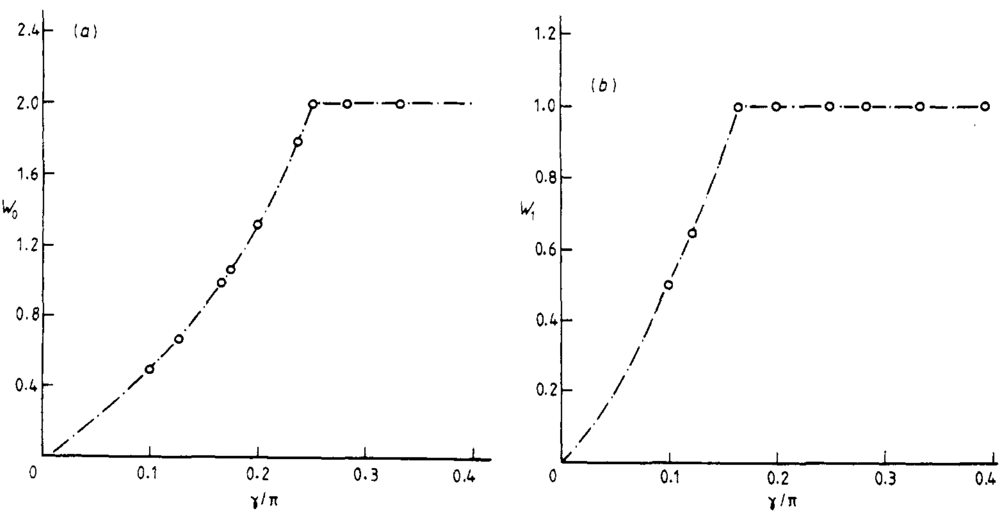

Figure 7. Plot of the extrapolated values (circles) of the estimators (a) W_0 and (b) W_1 defined in (6.5).

Moreover, the numerical results indicate that at $\gamma=\pi/4$ ($\gamma=\pi/6$) R_0 (R_1) exhibits a behaviour which depends logarithmically on the lattice size, as also occurs in the spin-$\frac{1}{2}$ model (Alcaraz *et al* 1988a).

The results (6.6*a*) and (6.6*b*) and the corresponding results for the spin-$\frac{3}{2}$ model together with (2.10) and (2.11) clearly induce us to conjecture that the correction term $o(L^{-4\gamma/(\pi-2S\gamma)})$, is always present in (6.1) and (6.3). As in the spin-$\frac{1}{2}$ model we can understand this term, using (6.3), as arising from the second-order correction of the irrelevant operator with dimension

$$X_r=\frac{\pi}{S(\pi-2S\gamma)}+\frac{2S-1}{S}. \tag{6.7}$$

As in the spin-$\frac{1}{2}$ model (Alcaraz *et al* 1988a), the results (6.6*a*) and (6.6*b*) indicate that the first-order correction term produced from (6.7) vanishes. The dimension (6.7) corresponds to the primary operator $\psi^{0,2}_{1/2,1/2}$ in (5.5) for the spin-1 model and to the operator $\psi^{0,2}_{2/3,2/3}$ in (5.11) for the spin-$\frac{3}{2}$ model. It is important to observe that $x_r\to 2$ as $\gamma\to 0$. This fact implies that higher-order perturbation terms in (6.3), arising from this term, become important as γ decreases. Strictly at $\gamma=0$, an infinite number of terms become equally important in (6.5), and the original corrections renormalise, giving rise to logarithmic corrections (Cardy 1986c). These logarithmic corrections, occurring at $\gamma=0$, were studied previously in Alcaraz and Martins (1988a, b).

The correction term $o(L^{-1})$ appearing in (6.6*b*) is also predicted by (2.11) and may arise from the first-order correction term of an irrelevant operator, with dimension $X_r=3$. Such operators occur from the combination of the marginal Gaussian operator, with dimension $(\Delta,\bar{\Delta})=(1,1)$, and the Ising operator with dimension $(\Delta_I,\bar{\Delta}_I)=(\frac{1}{2},\frac{1}{2})$.

In the same way as in the spin-$\frac{1}{2}$ model, our results indicate different corrections for the excited states. For example the corrections, arising from (6.7), occur at first order for the level corresponding to the operators $\psi^{0,\pm 1}_{0,0}$ of the spin-1 model.

An analysis more complete than that presented here, of the finite-size corrections for these spin models is an interesting point for future work. It is interesting to know which particular combinations of Gaussian and $Z(2S)$-parafermionic operators are present in (6.2).

7. Comments and conclusion

The central objective of the work described in this paper has been to study the critical properties of the spin-S XXZ model. We now close this paper with some comments and generalisations.

The results shown in tables 3 and 4 for the conformal anomaly and in tables 5-11 for the scaling dimensions clearly indicate that the relations (1.8) and (1.9), derived under the assumption of conformal invariance of the critical model, are consistent for all values of γ, even for irrational values of $P=\pi/\gamma$. The value of the conformal anomaly being constant $c=3S/(1+S)$, for all γ, and the scaling dimensions depending continuously on γ.

The results of §§ 4-6, for the spin-1 and spin-$\frac{3}{2}$ models, induce us to generalise these results for higher spins. The conformal anomaly

$$c=3S/(1+S)=1+2(2S-1)/(2S+2) \tag{7.1}$$

can be decomposed into the sum of the conformal anomaly of a $c=1$ (Gaussian) and a Z(2S) Fateev-Zamolodchikov algebra (see (1.4)). From (7.1) we expect, in the same way as in the spin-1 and spin-$\frac{3}{2}$ models, that the general spin-S model is described in terms of the composite operator

$$\psi^{n,m}_{\Delta_{2s},\bar{\Delta}_{2s}} = \sigma_{\Delta_{2s},\bar{\Delta}_{2s}}\phi^{n,m}_{\Delta^+,\Delta^-} \qquad (7.2)$$

formed by the product of the Z(2S)-type operator $\sigma_{\Delta_{2s},\bar{\Delta}_{2s}}$, with dimensions $(\Delta_{2s}, \bar{\Delta}_{2s})$ $(c=(2S-1)/(S+1))$, and the Gaussian operator $(c=1)$ describing an excitation of spin wavenumber n and vorticity m, whose dimensions are given by

$$\Delta^{\pm} = \frac{1}{2}\left(n\sqrt{X_P} \pm \frac{m}{4S\sqrt{X_P}}\right)^2 \qquad X_P = \frac{\pi - 2S\gamma}{4\pi S}. \qquad (7.3)$$

The operator content, for even lattices, for the spin-1 model given by (5.6) and (5.7) and for the spin-$\frac{3}{2}$ model given by (5.12) lead to the conjecture that, for general S, the operator content is given by

$$\mathscr{E}^{e}_{\mathscr{S}}(\gamma) = \sum_{r=0}^{2S-1}\sum_{s=0}^{2S-1} z_{2S}(r,s) \otimes \sum_{\substack{n=(2S)\mathbf{Z}+r \\ m=(2S)\mathbf{Z}+s}} (\Delta^+, \Delta^-)_{\mathrm{KM}} \qquad (7.4)$$

where $(\Delta^+, \Delta^-)_{\mathrm{KM}}$ (see 7.3) are the highest weights of the U(1) Kac-Moody algebra and $z_{2S}(r, s)$ refers to the operator content of the quantum Z(2S) Fateev-Zamolodchikov Hamiltonian (Alcaraz and Lima Santos 1986). These Z(2S)-symmetric Hamiltonians are divided into sectors of Z(2S) charges $s = 0, 1, \ldots, 2S-1$ and there were $r = 0, 1, \ldots, 2S-1$ types of toroidal boundary conditions. The operator content $z_{2S}(r, s)$ refers to the sector s of the Hamiltonian with boundary condition r.

In the case where the lattice size is an odd number, our results (5.8) for spin 1 and (5.13), for spin-$\frac{3}{2}$, imply the conjecture for general spin S

$$\mathscr{E}^{o}_{\mathscr{S}}(\gamma) = \sum_{r=0}^{2S-1}\sum_{s=0}^{2S-1} z_{2s}(r,s) \otimes \sum_{\substack{n=(2S)\mathbf{Z}+r+S \\ m=(2S)\mathbf{Z}+s+S}} (\Delta^+, \Delta^-)_{\mathrm{KM}}. \qquad (7.5)$$

We studied analytically (§ 2 and the appendix) and numerically (§ 6) the correction due to finite-size effects of the eigenenergies (see (1.8) and (1.9)). From these results we conjecture that, for general spin S, one of the most important operators governing these corrections is the spinless operator (7.2) with $n=0$, $m=2$, $\Delta_{2S} = \bar{\Delta}_{2S} = (2S-1)/2S$ and dimension

$$d^{0,2}_{\Delta_{2S},\Delta_{2S}} = \frac{\pi}{S(\pi - 2S\gamma)} + \frac{2S-1}{S}. \qquad (7.6)$$

As $\gamma \to 0$ the dimension $d^{0,2}_{\Delta_{2S},\bar{\Delta}_{2S}} \to 2$ and this operator produces several large finite-size corrections. Strictly at $\gamma = 0$, this operator becomes marginal and logarithmic corrections occur as in (2.12) and (2.13).

It is known (Alcaraz *et al* 1987, 1988a, b) that the operator content of the whole minimal series (1.1) can be obtained from the $(c=1)$ spin-$\frac{1}{2}$ XXZ model with twisted boundary conditions, specified by the angle ϕ

$$(S^X_{L+1} \pm \mathrm{i}S^Y_{L+1}) = \exp(\pm\mathrm{i}\phi)(S^X_1 \pm \mathrm{i}S^Y_1) \qquad S^Z_{L+1} = S^Z_1. \qquad (7.7)$$

In a forthcoming publication the conformal anomaly and dimensions predicted by the general series ((1.6) and (1.7) with $K=2S$), will be obtained from the general spin-S XXZ model with the above boundaries imposed.

Acknowledgments

It is a pleasure to acknowledge profitable conversations with R Köberle and V Rittenberg. This research was supported in part by Conselho Nacional de Desenvolvimento Científico e Technológico—CNPq and Fundação de Amparo à Pesquisa do Estado de São Paulo—FAPESP—Brasil.

Appendix. The leading finite-size corrections

In this appendix we will derive, based on the string hypothesis (2.6), the leading finite-size corrections for the eigenenergies of the spin-S XXZ model. Our calculations will be based on the anlytical method pioneered by de Vega and Woynarovich (1985) and Hamer (1986) and refined by Woynarovich and Eckle (1987a, b) (see also Hamer *et al* 1987).

We will calculate the finite-size corrections of the lowest energies $E_n(L)$ of the sector $n=0,1,2,\ldots$ of these spin models in a chain of L sites. These eigenenergies are given by (2.7) and (2.8) with Q_j^n given by (2.9). For a given distribution of strings $\{\nu_k\}$ it is convenient to define the density of roots $\sigma_L^n(\lambda)$ for the $2S$-strings (λ_j^{2S}, $j=1,2,\ldots,\nu_k$) in the sector n of the finite system by

$$\sigma_L^n(\lambda)=\frac{\mathrm{d}Z_L^n}{\mathrm{d}\lambda} \qquad \text{(A1}a\text{)}$$

where

$$Z_L^n(\lambda_j^{2S})=\frac{Q_j^n}{2\pi}=\frac{1}{2\pi}\left(\psi_{2S,2S}(\lambda_j)-\frac{1}{L}\sum_{k=1}^{\infty}\sum_{i=1}^{\nu_k}\Xi_{2,K}(\lambda_j^{2S}-\lambda_i^k)\right) \qquad \text{(A1}b\text{)}$$

with the functions ψ and Ξ as defined in (2.7). When $L\to\infty$ the roots tend toward a continuous distribution with density given by

$$\sigma_\infty(\lambda)=\frac{1}{2\pi}\left(\psi'_{2S,2S}(\lambda)-\int_{-\infty}^{+\infty}\sigma_\infty(u)\Xi'_{2S,2S}(\lambda-u)\,\mathrm{d}u\right) \qquad \text{(A2)}$$

where, as usual, the prime indicates the derivative. This integral equation has the solution (Sogo 1984)

$$\sigma_\infty(\lambda)=\frac{1}{2\gamma\cosh(\pi\lambda/\gamma)} \qquad \text{(A3)}$$

and from (2.8) the energy per site is given by

$$e_\infty=-\frac{\sin\theta}{2S}\int_{-\infty}^{+\infty}\sigma_\infty(\lambda)\psi'_{2S,2S}(\lambda)\,\mathrm{d}\lambda \qquad \text{(A4)}$$

where $\theta=2S\gamma$. Using equations (2.7), (2.8) and (A1)-(A4) and performing some lengthy algebraic manipulations, we can express the difference of the energy and density of roots from their bulk-limit ($L\to\infty$) values by

$$\frac{E_n}{L}-e_\infty=-\frac{\sin\theta}{2S}\int_{-\infty}^{+\infty}\sigma_\infty(u)S(u)\,\mathrm{d}u \tag{A5}$$

and

$$\sigma_L^n-\sigma_\infty=-\frac{1}{L}\Xi'_{2S,2S-n}-\frac{1}{2\pi}\int_{-\infty}^{+\infty}P(\lambda-u)S(u)\,\mathrm{d}u \tag{A6}$$

respectively, where

$$S(u)=\frac{1}{L}\sum_j\delta(\lambda_j-u)-\sigma_L^n(u) \tag{A7}$$

$$P(\lambda)=\int_{-\infty}^{+\infty}\exp(\mathrm{i}\lambda\omega)K(\omega)\,\mathrm{d}\omega \tag{A8}$$

$$[1-K(\omega)]^{-1}=G_+(\omega)G_-(\omega) \tag{A9}$$

and

$$G_+(\omega)=G_-(-\omega)=\frac{\sqrt{4S(\pi-\theta)}\exp(\phi(\omega))\Gamma(1-\frac{1}{2}\mathrm{i}\omega)\Gamma(1-\mathrm{i}\gamma\omega/2\pi)}{\Gamma(1-\mathrm{i}(\pi-\theta)\omega/2\pi)\Gamma(\frac{1}{2}-\mathrm{i}\gamma\omega/2\pi)\Gamma(1-\mathrm{i}\theta\omega/2\pi)} \tag{A10}$$

with

$$\phi(\omega)=\tfrac{1}{2}\mathrm{i}\omega(\ln[\pi/(\pi-\theta)]+(\theta/\pi)\ln[(\pi-\theta)/\theta]). \tag{A11}$$

The leading finite-size corrections (Woyanarovich and Eckle 1987a, b Hamer *et al* 1987), for large L, are given by

$$\frac{E_n}{L}-e_\infty=\frac{2\pi}{S}\sin(2S\gamma)\int_\Lambda^\infty\sigma_\infty(\lambda)\sigma_L^n(\lambda)\,\mathrm{d}\lambda-\frac{1}{2L}\sigma_\infty(\lambda)-\frac{\sigma_\infty(\Lambda)}{12L^2\sigma_L^n(\Lambda)} \tag{A12}$$

$$\begin{aligned}\sigma_L^n(\lambda)-\sigma_\infty(\lambda)&\\ &=\frac{1}{2\pi}\int_\Lambda^\infty\sigma_L^n(u)P(\lambda-u)\,\mathrm{d}u-\frac{P(\lambda-\Lambda)}{4\pi L}+\frac{P'(\lambda-\Lambda)}{12L^2\sigma_L^n(\Lambda)}\\ &\quad+\left(\int_{-\infty}^{-\Lambda}\sigma_L^n(u)\frac{P(\lambda-u)}{\pi}\,\mathrm{d}u-\frac{P(\lambda+\Lambda)}{2\pi L}-\frac{P'(\lambda+\Lambda)}{24L^2\sigma_L^n(\Lambda)}-\frac{1}{L}\Xi'_{2S,2S-n}\right)\end{aligned} \tag{A13}$$

where Λ is the largest-magnitude root determined by the boundary condition

$$\int_\Lambda^\infty\sigma_L^n(\lambda)\,\mathrm{d}\lambda=\frac{1}{2L}+\left(1-\frac{2S\gamma}{\pi}\right)\frac{n}{L}. \tag{A14}$$

The first-order corrections $\mathcal{O}(1/L^2)$ are calculated by neglecting the terms in the large bracket in (A13), which are responsible for higher-order corrections.

Defining

$$R(\lambda)=P(\lambda)/2\pi \qquad f(\lambda)=\sigma_\infty(\lambda+\Lambda) \tag{A15}$$

$$X^n(\lambda)=\sigma_L^n(\lambda+\Lambda) \qquad t=\lambda+\Lambda \tag{A16}$$

we can write (A13) as

$$X^n(t)=f(t)+\int_0^\infty X^n(u)R(t-u)\,\mathrm{d}u-\frac{R(t)}{L}+\frac{R'(t)}{12L^2\sigma_L^n(\Lambda)} \tag{A17}$$

which is precisely the standard form of the Wiener-Hopf equation (see, for example, Morse and Feshbach 1953). This equation is solved by introducing the Fourier transforms

$$\tilde{X}_\pm^n=\int_{-\infty}^{+\infty}\exp(\mathrm{i}\omega t)X_\pm^n(t)\,\mathrm{d}t \qquad X_\pm^n(t)=\begin{cases}x^n(t) & t\gtrless 0\\ 0 & t\gtrless 0\end{cases} \tag{A18}$$

and the corresponding Fourier pairs $f(t)\leftrightarrow\tilde{f}(t)$, $R(t)\leftrightarrow\tilde{R}(t)$. After some algebraic manipulation $\tilde{X}_\pm^n(\omega)$ can be expressed by

$$\tilde{X}_+^n(\omega)=C^n(\omega)+G_+(\omega)[Q_+(\omega)+P(\omega)] \tag{A19}$$

where

$$C^n(\omega)=\frac{1}{2L}-\frac{\mathrm{i}\omega}{12L^2\sigma_L^n(\Lambda)} \qquad Q_+(\omega)=\frac{G_-(\mathrm{i}\pi/\gamma)\exp(-\pi\Lambda/\gamma)}{\pi-\mathrm{i}\gamma\omega} \tag{A20}$$

$$P(\omega)=-\frac{1}{2L}+\mathrm{i}\frac{g}{12L^2\sigma_L^n(\Lambda)}-\mathrm{i}\frac{\omega}{12L^2\sigma_L^n(\Lambda)}$$

$$g=\frac{\mathrm{i}}{12}\left[2-\frac{2\pi}{\pi-2S\gamma}+\frac{\pi}{\gamma}\left(3-\frac{1}{S}\right)\right]. \tag{A21}$$

From (A17) and the definitions (A15) and (A16) we obtain

$$G_+(\mathrm{i}\pi/\gamma)\exp(-\pi\Lambda/\gamma)=\frac{1}{2L}+\frac{(\pi-2S\gamma)n}{L\pi G_+(0)}-\mathrm{i}\frac{g}{12L^2\sigma_L^n(\Lambda)} \tag{A22}$$

and

$$\sigma_L^n(\Lambda)=\frac{g^2}{24L^2\sigma_L^n(\Lambda)}+\mathrm{i}\frac{g}{2L}+\frac{G_-(-\mathrm{i}\pi/\gamma)}{\gamma}\exp(-\pi\Lambda/\gamma). \tag{A23}$$

Finally, using (A19), (A22) and (A23) in (A12) and approximating (A3), $\sigma_\infty(\lambda)\approx\exp(-\pi\Lambda/\gamma)/\gamma$ we obtain the first-order correction for the lowest eigenenergy of sector n $(0,1,2,\ldots)$

$$\frac{E_n}{L}=e_\infty+\frac{\pi^2\sin(2S\gamma)}{4S\gamma L^2}\left(-\tfrac{1}{6}+2X_P n^2\right) \qquad X_P=\frac{\pi-2S\gamma}{4S\pi}. \tag{A24}$$

The next corrections of (A24) are obtained by using (A22) and (A23) and include the large brackets of equation (A13). These terms introduce corrections of $o(P(2\Lambda)/L)$ in $\sigma_L^n(\Lambda)$ and $\exp(-\pi\Lambda/\gamma)$. For spins $S\geqslant 1$ we obtain for the ground state $(n=0)$, the corrections

$$\frac{E_0}{L}=e_\infty+\frac{\pi^2\sin(2S\gamma)}{4S\gamma L^2}\left[-\tfrac{1}{6}+\mathcal{O}(L^{-2})+\mathcal{O}(L^{-4\gamma/(\pi-2S\gamma)})+\mathcal{O}(L^{-2/S})\right] \tag{A25}$$

while the corresponding corrections for the mass gap amplitude of sector $n \neq 0$ are given by

$$\frac{E_n}{L}-\frac{E_0}{L}=\frac{\pi^2 \sin(2S\gamma)}{2S\gamma L^2}[X_P n^2+\mathcal{O}(L^{-1})+\mathcal{O}(L^{-2})+\mathcal{O}(L^{-2/S})+\mathcal{O}(L^{-4\gamma/(\pi-2S\gamma)})] \qquad \text{(A26)}$$

where X_P is defined in (A24).

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