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LETTER TO THE EDITOR

Conformal anomaly and critical exponents of the spin-1 Takhtajan–Babujian model

Francisco C Alcaraz and Márcio J Martins

Departamento de Física, Universidade Federal de São Carlos, CP-676, 13560 São Carlos, SP, Brazil

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Abstract. We consider the critical behaviour of the spin-1 Hamiltonian of the Takhtajan-Babujian model. The Bethe ansatz equations for this antiferromagnet in a finite chain are investigated analytically and numerically. The conformal anomaly and critical exponents are obtained by exploiting their relations with the eigenspectrum of the finite system. Our results strongly support the conjecture that the Wess-Zumino-Witten non-linear σ model with topological charge $k=2$ is the underlying field theory for this statistical mechanics model.

Since the exact solution of the spin $S=\frac{1}{2}$ Heisenberg model by using the Bethe ansatz (Bethe 1931) many efforts have been made in order to obtain other models also soluble by this ansatz (see, e.g., Lieb and Wu 1972, Thacker 1981, Baxter 1982, Gaudin 1983, Tsvelick and Weigmann 1983). Looking for a generalisation of the Heisenberg model to higher spin S Takhtajan (1982) and Babujian (1982, 1983) were able to find a set of critical (gapless) quantum-spin antiferromagnetic models in which the Bethe ansatz may be formulated. These models for an L-site chain are defined by the Hamiltonian

$$H=\sum_{n=1}^{L} Q_{2S}(\boldsymbol{S}_n\cdot\boldsymbol{S}_{n+1}) \tag{1a}$$

where $\boldsymbol{S}_n$ (S_n^x, S_n^y, S_n^z) are SU(2) operators of arbitrary integer or half-integer spin S attached at the site n. The polynomial $Q_{2S}(x)$, of degree $2S$, is defined by

$$Q_{2S}(x)=-J\sum_{l=0}^{2S}\sum_{k=l+1}^{2S}\left(\frac{1}{k}\right)\prod_{j=0,j\neq l}^{2S}\left(\frac{x-x_j}{x_l-x_j}\right) \tag{1b}$$

where $x_l=\frac{1}{2}[l(l+1)-2S(S+1)]$ and $J(>0)$ is the coupling constant. Apart from a harmless constant the case $S=\frac{1}{2}$ reduces to the well known Heisenberg Hamiltonian

$$H=\frac{J}{4}\sum_{n=1}^{L}\boldsymbol{S}_n\cdot\boldsymbol{S}_{n+1} \tag{2}$$

while the case $S=1$ gives us

$$H=\frac{J}{4}\sum_{n=1}^{L}[\boldsymbol{S}_n\cdot\boldsymbol{S}_{n+1}-(\boldsymbol{S}_n\cdot\boldsymbol{S}_{n+1})^2] \tag{3}$$

which contains a quadratic term in the spin variables.

More recently Affleck (1986a, b) by relating the infinite system at finite temperature and the finite system at zero temperature calculated the conformal anomaly for these spin models from their low-temperature specific heat behaviour. Their conformal anomaly (or central charge of their conformal algebra) has the value

$$c = 3S/(1+S) \tag{4}$$

and coincides with the central charge of the two-dimensional Wess-Zumino-Witten model (WZW) with symmetry group G = SU(2) and topological charge $k = 2S$ (Khizhnik and Zamolodchikov 1984). This leads to the conjecture (Affleck 1986a, b, c) that the WZW is the underlying field theory which describes the critical behaviour of the spin models (1). This implies (Khizhnik and Zamolodchikov 1984, Affleck and Haldane 1987) that these spin models should have operators whose scaling dimensions X_j are

$$X_j = j(j+1)/(1+S) \qquad j = 0, \tfrac{1}{2}, 1, \ldots, S. \tag{5}$$

In the case of spin $\frac{1}{2}$ the dimension $X_{1/2} = \frac{1}{2}$ corresponds to the energy operator as well to the polarisation operator (Baxter 1982, Alcaraz *et al* 1987a, b). In the case of spin $S = 1$ we should have two relevant operators with dimensions $X_{1/2} = \frac{3}{8}$ and $X_1 = 1$, beyond the identity operator ($X_0 = 0$).

In this letter an independent test of predictions (4) and (5) will be made by calculating directly the conformal anomaly as well as the anomalous dimensions corresponding to several operators in the case of the spin $S = 1$ Hamiltonian (3). These calculations will be done by exploiting a set of remarkable relations (see Cardy (1987) for a recent review) between these quantities and the eigenspectrum of the statistical mechanics model.

The relevant relations, for our purposes, may be stated as follows. To each primary operator ϕ, with anomalous dimension X_ϕ and spin S_ϕ, in the operator algebra of the critical infinite chain there exists a set of states in the quantum Hamiltonian, in a periodic chain of L sites, whose energy and momentum are given by

$$E_{n,n'} = E_0^{(0)} + (2\pi/L)\zeta(X_\phi + n + n') + O(L^{-1}) \qquad n, n' = 0, 1, 2, \ldots \tag{6a}$$

$$P_{n,n'} = (2\pi/L)(S_\phi + n - n') \qquad n, n' = 0, 1, 2, \ldots \tag{6b}$$

respectively as $L \to \infty$. The ground-state energy of the finite chain is $E_0^{(0)}$ and ζ is introduced in order to ensure that the resulting equations of motion are conformally invariant (von Gehlen *et al* 1986). For the Hamiltonian (1), with arbitrary spin, the value $\zeta = \pi/2$ can be inferred from the known energy-momentum dispersion relations (Takhtajan 1982). In addition to the relations (6) the conformal invariance of the infinite system also predicts (Blöte *et al* 1986, Affleck 1986a) that the L-site ground-state energy $E_0^{(0)}$, at criticality, should behave as

$$E_0^{(0)}/L = e_\infty - \pi c\zeta/6L^2 + O(L^{-2}) \qquad L \to \infty. \tag{7}$$

Here c is the central charge of the conformal class governing the critical behaviour of the infinite system and e_∞ is the ground-state energy per site in the infinite lattice limit which for the Hamiltonian (3) has the exact value $e_\infty = -1$ (Takhtajan 1982, Babudjian 1982, 1983) where hereafter we will assume $J = 1$ in (1)-(3).

Previous finite-size studies of spin-1 systems (Blöte 1978, Botet and Jullien 1983, Botet *et al* 1983, Sólyom and Ziman 1984, Betsuyaku and Tokota 1986, Oitmaa *et al* 1986, Moreo 1987, Blöte and Capel 1986, Bonner *et al* 1987, Blöte and Bonner 1987) are basically restricted in finite-size scaling (Barber 1983) for lattice size up to $L=12$†. However the existence of a Bethe ansatz for the special family of models given in (1) will permit us to study these specific models for much bigger lattices. For the particular case of spin 1 we will consider lattice sizes up to $L=84$; although we can go even further ($L\sim 300$) these data will be sufficient for our numerical analysis.

The general spin-S Hamiltonian, with periodic boundary conditions imposed, commutes with the total spin operator $\hat{S}^z=\Sigma_n S_n^z$. Consequently the associated Hilbert space can be decomposed in $2L+1$ disjoint sectors labelled by the eigenvalues of $\hat{S}^z$; $r=0, \pm 1, \pm 2, \ldots$. Because of spin-reversal symmetry the sectors $r=+l$ and $r=-l$ are degenerate, and we can thus restrict ourselves only to sectors $r\geqslant 0$. From the Bethe ansatz (BA) formulation for these models (Takhtajan 1982, Babujian 1982) the eigenenergies, for the sector r, will be given in terms of the complex roots $(\lambda_1, \lambda_2, \ldots, \lambda_{L-r})$ of the $(L-r)$ coupled non-linear BA equations

$$\left(\frac{\lambda_j-\mathrm{i}S}{\lambda_j+\mathrm{i}S}\right)^L=\prod_{k=1\neq j}^{SL-r}\left(\frac{\lambda_j-\lambda_k-\mathrm{i}}{\lambda_j-\lambda_k+\mathrm{i}}\right) \qquad j=1,2,\ldots,SL-r. \tag{8}$$

The energy and momentum of the eigenstates are

$$E=-\sum_{j=1}^{SL-r}\frac{S}{\lambda_j^2+S^2} \tag{9a}$$

and

$$P=\sum_{j=1}^{SL-r}(2\tan^{-1}\lambda_j-\pi) \qquad \mod 2\pi \tag{9b}$$

respectively.

Recently several works have been reported (de Vega and Woynarovich 1985, Hamer 1985, 1986, Woynarovich and Eckle 1987a, b, de Vega and Karowski 1987, Woynarovich 1987, Hamer *et al* 1987) in which the finite-size corrections for the eigenenergies, in the large-L limit, can be computated analytically for systems with a Bethe ansatz formulation. However, these calculations were done based on methods where the assumption of real roots should hold, which is not the case in (8) for $S>\frac{1}{2}$. A standard way of transforming the system of complex roots to a system of real ones is the string hypothesis, which states that as $L\to\infty$ the numbers λ_j cluster in complexes of n-strings. Each n-string contains n complex roots of the form

$$\lambda_{j,k}^n=\lambda_j^n+\tfrac{1}{2}\mathrm{i}(n+1-2k) \qquad k=1,2,\ldots,n \tag{10}$$

where λ_j^n are real numbers corresponding to the centre of the n-string. With the assumption (10) we can parametrise an arbitrary configuration given the number of strings of size n such that $\Sigma_n n\nu_n=SL-r$. For a given configuration the system (8) reduces to the system of equations for λ_j^n, $j=1,2,\ldots,\nu_n$:

$$L\psi_{n,S}(\lambda_j^n)=2\pi Q_j^n+\sum_m\sum_{k=1}^{\nu_m}\phi_{n,m}(\lambda_j^n-\lambda_k^m) \tag{11}$$

where $\psi_{n,s}$ and $\phi_{n,m}$ are combinations of $\tan^{-1}$ functions and Q_j^n are integers or half-integer depending on the particular eigenenergy (see, for example, Babujian 1983).

† It is important to mention that the previous attempts to verify the conjectures (4) and (5) (Blöte and Capel 1986, Bonner *et al* 1987, Blöte and Bonner 1987, see also references therein) produced no convincing numerical agreement due to the small system sizes and the presence of logarithmic corrections.

The ground state, which occurs in the $r=0$ sector, corresponds to a sea of $2S$-strings ($\nu_{2S}=L/2S$), the lowest state in the $r=1$ sector to $\nu_{2S}=L/2S-1$, $\nu_{2S-1}=1$, and so on.

We should stress that the assumption (10) is valid only in the limit $L\to\infty$ whenever the state contains n-strings ($n>1$), consequently we do not expect, in general, that (11) will give us the correct finite-size corrections to the eigenspectrum in order to estimate the quantities in (6) and (7). These corrections, within the string hypothesis, can be calculated by the analytical method developed by Woynarovich and Eckle (1987a). The ground-state energy $E_0^{\rm st}$, with the string hypothesis, for the L-site chain behaves as

$$E_0^{\rm st}/L=e_\infty-\pi^2/12L^2+\mathrm{O}[1/L^2(\ln L)^3] \qquad L\to\infty \tag{12}$$

while the lowest energy in the r sector $E_r^{\rm st}$ behaves as

$$E_r^{\rm st}-E_0^{\rm st}=\pi^2r^2/4SL^2+\mathrm{O}(1/L^2\ln L) \qquad L\to\infty. \tag{13}$$

Equations (12) and (7), with $\zeta=\pi/2$, give us a value $c=1$ for all the spins in contradiction to the expected result (4). From (6a) the mass-gap amplitudes corresponding to the r sectors ($r\neq 0$) are related to the scaling dimensions X_r of operators occurring in the model. These dimensions govern the power-law decay of the several correlation functions of the critical model. From (13) and (6) we obtain $X_r=r^2/4S$ also in contradiction with the predicted result (5). In the case $S=\frac{1}{2}$ equations (12) and (13) give us the expected results $c=1$ and $X_{1/2}=\frac{1}{2}$ because, in this case, $E_r^{\rm st}$ consist of a sea of particles (1-string) and the string hypothesis is exact for finite L. Although the string assumption does not give in general the correct term of order $1/L^2$, equations (12) and (13) tell us that the eigenenergies will have also logarithmic behaviour beyond power corrections, like the $S=\frac{1}{2}$ Heisenberg model (Alcaraz *et al* 1987a, b, Woynarovich and Eckle 1987a). These corrections will slow down strongly the convergence rate of the finite-size estimators.

In order to obtain the correct energies we have to solve the original BA equations (8). For the spin-1 Hamiltonian (3) we solved these equations by using a Newton-type method. We first solve the more simple set of real equations (11) and use this solution together with (10) to produce the initial guess for the complex root system (8). In table 1 we show the ground-state energies E_0 for lattice size up to $L=84$. We also show the corresponding energies $E_0^{\rm st}$ obtained by solving (11). From (7), using $\zeta=\pi/2$ and $e_\infty=-1$ the conformal anomaly c can be obtained extrapolating the sequence

$$c_L\equiv-(E_0+L)12L/\pi^2. \tag{14}$$

Table 1. Finite-size sequence for the extrapolation of the conformal anomaly. E_0 and $E_0^{\rm st}$ are ground-state energy obtained using and not using the string hypothesis, respectively.

L	$-E_0/L$	$-E_0^{\rm st}/L$	$-(E_0-L)12L/\pi^2$	$-(E_0^{\rm st}-L)12L/\pi^2$
8	1.020 085 617	1.013 350 454	1.562 956	1.038 861
20	1.003 122 013	1.002 077 559	1.518 365	1.010 403
36	1.000 958 385	1.000 638 099	1.510 172	1.005 483
52	1.000 458 541	1.000 305 374	1.507 532	1.003 968
68	1.000 267 910	1.000 178 445	1.506 217	1.003 236
84	1.000 175 476	1.000 116 889	1.505 418	1.002 799

In table 1 we show this sequence for the true energies E_0 and for the energies E_0^{st} obtained by solving (11). Using VBS approximants (Hamer and Barber 1981) we obtain $c = 1.500\,(4) \pm 0.0004$ in excellent agreement with the prediction (4). Using the sequence (14) with E_0^{st} we obtain $c = 1.000\,(2) \pm 0.000\,(4)$ in perfect agreement with (12). From (6) the scaling dimensions X_r corresponding to the mass-gap amplitudes between the lowest energy E_r in the r sector and the ground state E_0 can be obtained in the limit $L \to \infty$ of the sequence

$$X_r(L) \equiv (E_r - E_0)L^2/\pi^2. \tag{15}$$

In table 2 we show these estimates, with the corresponding VBS extrapolations, for $r = 1$-5 and lattices up to $L = 84$. As we have already indicated, the expected logarithmic corrections make the series slowly convergent and give us poor estimates. In order to cancel at least part of the logarithmic corrections, i.e. those already present in the string hypothesis, we consider the sequence

$$D_r(L) \equiv [(E_r - E_0) - (E_r^{\mathrm{st}} - E_0^{\mathrm{st}})]L^2/\pi^2 \tag{16}$$

which will give us the correction we should add to the results (13) obtained using the string hypothesis. In table (3) we show these estimates for $r = 1$-5, together with their VBS extrapolations. We clearly see, in comparison with table 2, that the convergence rate increases and the extrapolations are much better, which indicate that the leading logarithmic correction that was present in the sequences of table 2 is no longer present. Using the extrapolated results of table 3 together with the exact expression (13) we

Table 2. Mass-gap amplitudes and extrapolations for sectors $r = 1$-5; see equation (15).

L	$X_1(1)$	$X_2(L)$	$X_3(L)$	$X_4(L)$	$X_5(L)$
8	0.336 784	0.740 494	1.672 538	2.407 210	3.644 041
20	0.337 846	0.803 857	1.886 674	2.960 138	4.662 006
36	0.339 962	0.829 474	1.958 973	3.155 378	5.002 364
52	0.341 389	0.841 900	1.991 375	3.239 970	5.144 823
68	0.342 426	0.849 709	2.011 296	3.289 661	5.227 074
84	0.343 229	0.855 258	2.025 270	3.323 434	5.282 452
Extrapolated	0.3 (5)	0.9 (4)	2.2 (5)	3.7 (7)	6.60 (6)

Table 3. Finite-size sequences of the quantities $D_r(L)$ for $r = 1$-5; see equation (16).

L	$D_1(L)$	$D_2(L)$	$D_3(L)$	$D_4(L)$	$D_5(L)$
8	0.118 550	0.014 8478	0.061 6628	0.036 8408	0.045 0017
20	0.121 419	0.005 3599	0.088 5157	0.018 4639	0.064 9935
36	0.122 445	0.003 0060	0.101 4681	0.009 9641	0.077 3298
52	0.122 889	0.002 0877	0.107 3706	0.006 6169	0.087 2656
68	0.123 146	0.001 8149	0.110 7617	0.004 9272	0.093 6852
84	0.123 317	0.001 5791	0.112 9719	0.003 9367	0.098 1576
Extrapolated	0.124 (6)	0.000 (3)	0.124 (4)	0.000 (7)	0.124 (5)

obtain the following estimates: $X_1=0.375\,(6)$, $X_2=1.000\,(3)$, $X_3=2.374\,(4)$, $X_4=4.000\,(7)$ and $X_5=6.374\,(5)$. We observe that X_1 and X_2 correspond to relevant operators and are in perfect agreement with the predictions (5).

From table 3 we see that while D_r converges to $\frac{1}{8}$ for the sectors with r odd, for r even there seems to be no indication of a correction ($D_r=0$) of order $1/L^2$. We believe the reason for such distinct behaviour is related to the fact that, while for r even the lowest state is a sea of 2-string-like particles, for odd values of r we also have single particles in addition to these particles. Our results suggest the following dimensions, for general r:

$$X_r=\begin{cases}\frac{1}{4}r^2 & r=2,4,6,\ldots\\ \frac{1}{4}r^2+\frac{1}{8} & r=1,3,5,\ldots.\end{cases} \tag{17}$$

We have also obtained some excited eigenenergies of states containing 3-string-like particles in the r sectors. Their corresponding dimensions, however, are the same as those occurring in the $r+1$ sector given in (17).

In summary, by solving the Bethe ansatz equations of the spin-1 model formulated by Babujian (1982) and Takhtajan (1982) we have calculated the conformal anomaly and scaling dimensions corresponding to several operators (17). Our results strongly support the conjecture that the WZW model, with $K=2$, is the underlying field theory describing the criticality of this spin model.

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