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LETTER TO THE EDITOR

Finite-size corrections for spin-S Heisenberg chains and conformal properties

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Abstract. We compare recent results on finite-size corrections for the isotropic (XXX) Heisenberg chain (and its integrable generalisations) with former numerical and analytic calculations. For the ground state and its lowest excitations, leading and non-leading terms are considered. Our analysis confirms the predictions of conformal invariance and sheds some new light on the fine structure of finite-size corrections.

The recent interest in finite-size corrections of exactly integrable models is mainly due to the fact that they are closely related to conformal invariance, which was discovered by Cardy (1984, 1986) and others (Blöte *et al* 1986, Affleck 1986). Strictly speaking, this is true for the corrections in the critical region only, where they are power-like for such quantities as energy, etc. In the non-critical region they show an exponential behaviour, in accordance with the fact that there is a finite mass gap in the excitation spectrum.

Using the concept of conformal invariance, some finite-size corrections can be proposed. On the other hand, independent analytic methods have been developed to calculate them for some models (Woynarovich and Eckle 1987, Hamer *et al* 1987).

Therefore it seems to be reasonable to re-examine some of the numerical and analytic results we obtained previously by solving the Bethe ansatz equations (BAE). Unfortunately, some of our results have not been noticed by other authors so far, though a comparison should be worthwhile. In this letter we deal with the Heisenberg antiferromagnetic spin chain

$$H = \frac{1}{4}\sum_{n=1}^{N} (\boldsymbol{G}_n \cdot \boldsymbol{G}_{n+1}) \tag{1}$$

or its integrable generalisation to spin S

$$H = \sum_{n=1}^{N} P(\boldsymbol{S}_n \cdot \boldsymbol{S}_{n+1}) \qquad \boldsymbol{S}_n^2 = S(S+1) \tag{2}$$

where P is a polynomial of degree $2S$ (see e.g. Babujian 1983), and we have set $J = 1$. The mass gap of these models is zero, so we are really in the critical region. From the general formula

$$\Delta E_0^{(N)} = E_0^{(N)} - E_\infty = -\pi c v / 6N \tag{3}$$

of Blöte *et al* (1986) and Affleck (1986), the latter obtained $c=3S/(S+1)$ for the central charge and $v=\pi/2$ for the 'effective' velocity (from low-energy dispersion relation), transforming (3) into

$$N\Delta E_0^{(N)}=-\frac{\pi^2 S}{4(S+1)}. \tag{4}$$

The same considerations used to obtain equation (3) lead to the specific heat capacity for low temperatures

$$\frac{C_N}{N}=\frac{2S}{S+1}T+\mathrm{O}(T^3). \tag{5}$$

This value was first calculated by solving the BAE by Babujian (1983). It is interesting to note that he was only able to give a rather complicated expression for C_N when $S\geqslant\frac{3}{2}$ and the calculation of the result relied completely on the basis of the string hypothesis (SH), which was later shown to be only 'partly' true (Avdeev and Dörfel 1985a). On one hand, one may argue that thermodynamics is correctly given by SH; on the other hand, the low-temperature limit favours the lower part of the spectrum where SH is definitely not valid. The picture becomes even more puzzling if one remembers the result of Alcaraz and Martins (1988), who showed that for $S=1$ the SH would imply the incorrect result

$$N\Delta E_0^{(N)}=-\pi^2/12. \tag{6}$$

For $S=\frac{1}{2}$, in the ground state the strings are real roots and (4) confirms the former results of Avdeev and Dörfel (1985b) and Hamer (1985).

For $S\geqslant 1$, the SH predicts for the ground state $N/2$ strings of length $2S$. Avdeev and Dörfel (1985c) have solved the BAE numerically and obtained deformed strings (of order $1/N$). In table 1 we present their extrapolated energy corrections obtained from calculations up to $SN\leqslant 128$ compared with $\Delta E_0^{(N)}$ from equation (4).

Table 1 clearly confirms equations (4) and (3) and the concept of conformal invariance. For higher S, the deviations are due to the fact that extrapolation requires higher N than we were able to use.

Furthermore, we have compared the ground-state energies of Alcaraz and Martins (1988) for $S=1$, published up to $N=84$, with those of Avdeev and Dörfel (1985c), which have been calculated up to $N=128$, and obtained complete agreement.

Table 1. The extrapolated finite-size corrections $\lim_{N\to\infty}(N\Delta E_0^{(N)})$ of the ground state compared with the theoretical prediction $(N\Delta E_0^{(N)})_{\text{theor}}=-\pi^2S/4(S+1)$ from $S=1$ to $S=\frac{9}{2}$.

S	$\lim_{N\to\infty}(-N\Delta E_0^{(N)})$	$(-N\Delta E_0^{(N)})_{\text{theor}}$
$\frac{1}{2}$	0.8230	0.8225
1	1.235	1.2337
$\frac{3}{2}$	1.484	1.4804
2	1.65	1.6449
$\frac{5}{2}$	1.77	1.7624
3	1.86	1.8506
$\frac{7}{2}$	1.93	1.9191
4	1.98	1.9740
$\frac{9}{2}$	2.03	2.0188

A new analytic method for calculating finite-size corrections for solutions of the BAE was introduced by Woynarovich and Eckle (1987) using Wiener–Hopf integration. This powerful method is independent of the predictions of conformal invariance and provides us with an algorithm for obtaining nearly all interesting corrections of the low-energy spectrum for $S=\frac{1}{2}$. The string deformation for $S \geq 1$ makes its generalisation a rather formidable task (for an attempt see Avdeev and Dörfel (1985b). It is therefore useful to observe how their results improve the coincidence with former numerical results.

Woynarovich and Eckle have calculated the first non-leading corrections to (4):

$$-N\Delta E_0^{(N)} = \frac{\pi^2}{12}\left(1+\frac{0.3433}{\ln^3 N}\right). \tag{7}$$

In table 2 we compare this analytic prediction with numerical results of Avdeev and Dörfel (1985b).

Table 2. The exact ground-state energy correction multiplied by $(-N)$ and the analytic prediction from equation (7).

N	$-N\Delta E_0^{(N)}$ (numerical)	$-N\Delta E_0^{(N)}$ (theory)
4	0.0096	0.9284
6	0.8634	0.8716
8	0.8473	0.8537
10	0.8397	0.8456
16	0.8311	0.8357
32	0.8262	0.8292
64	0.8244	0.8264
130	0.8237	0.8249
256	0.8233	0.8241

The deviations for large N fit with the next correction of order $O(1/\ln^4 N)$. It is surprising that (7) already works rather well for $N \leq 10$.

The extended version of Hamer *et al* (1987) gives the possibility of estimating the root of largest magnitude Λ and the density $\sigma_N(\Lambda)$.

Remember that for the density

$$\sigma_\infty(\lambda) = 1/2\cosh(\pi\lambda) \tag{8}$$

one has

$$\Lambda_0 = \frac{1}{\pi}\ln\frac{2N}{\pi} \tag{9}$$

and

$$\sigma_\infty(\Lambda_0) = \pi/2N \simeq \exp(-\pi\Lambda_0). \tag{10}$$

After a little algebra one finds

$$\sigma_N(\Lambda) = \frac{\pi}{48N}\left(11+\sqrt{\frac{409}{3}}\right)\left[1+O\left(\frac{1}{\ln^2 N}\right)\right] \tag{11}$$

and

$$\Lambda = \frac{1}{\pi} \ln\left(\frac{2N}{\sqrt{\pi l}} \frac{33+\sqrt{409\times 3}}{35+\sqrt{409\times 3}}\right)\left[1+\mathrm{O}\left(\frac{1}{\ln^3 N}\right)\right]$$
$$= \Lambda_0 + \Delta + \mathrm{O}\left(\frac{1}{\ln N}\right) \tag{12}$$

where $\Delta = 0.013\,8113$.

This fits very well with former numerical results which are presented in table 3.

The parameter Δ sets some kind of a new scale, which manifests itself in all higher corrections to $\sigma_N(\lambda)$ for $\lambda \geqslant \Lambda$. In this region a splitting

$$\sigma_N(\lambda) = \sigma_\infty(\lambda) + \Delta\sigma_N(\lambda) \tag{13}$$

makes no sense for perturbation theory, because the second part becomes much larger than the first part (the opposite of the situation for small $|\lambda| \ll \Lambda$). The complicated structure of Δ and its cumbersome calculation give us no hint of a physical interpretation of that scale, as we have for the energy correction in (3) in the form of the central charge.

Table 3. The largest root Λ (numerical result) compared with Λ_0 and $\Lambda_0 + \Delta$ for two different values of N.

	$N = 10$	$N = 256$
Λ_0	0.589 192	1.621 342
$\Lambda_0 + \Delta$	0.603 004	1.635 153
Λ	0.598 087	1.635 314

Concluding this part of our letter we compare $\sigma_N(\Lambda) = 0.005\,797\,47$ for $N = 256$ from (11) with its numerical value

$$\sigma_N(\Lambda) = 0.005\,789\,41.$$

The coincidence here is worse, but can still be explained by the corrections in (11) which come from the terms dropped in (18) in Woynarovich and Eckle (1987).

Now it is interesting to compare the results concerning the lowest excited states for $S = \frac{1}{2}$ and $S = 1$. Let us start with the standard XXX model. Though some results were already obtained by Alcaraz *et al* (1987), a general solution of the problem was presented by Woynarovich (1987). Solving the BAE, he was able to calculate in an analytic way the leading order of momenta and energies of all low-lying states and thus obtained the scaling dimensions of the relevant operators already predicted by conformal invariance. One may then ask how his results fit with the former analysis of Destri and Lowenstein (1982) and of Babelon *et al* (1983). A good comparison can be made with the case where no complex λ are present in the solutions of the BAE. In our normalisation the formulae of Woynarovich (which we were able to confirm) take the form

$$E_L^{(N)} - E_0^{(N)} = \frac{\pi^2}{N}\left[\frac{H^{+2} + H^{-2}}{4} + \left(\sum_n^{H^+} n_h^+ - \frac{H^+(H^+-1)}{2}\right)\right.$$
$$\left. + \left(\sum_{n'}^{H^-} n_{h'}^- - \frac{H^-(H^--1)}{2}\right)\right] \tag{14}$$

$$P_L^{(N)}-P_0^{(N)}=\frac{2\pi}{N}\left[\frac{H^{-2}-H^{+2}}{4}-\left(\sum_n^{H^+} n_h^+ - \frac{H^+(H^+-1)}{2}\right)\right.$$
$$\left.+\left(\sum_{n'}^{H^-} n_{h'}^- - \frac{H^-(H^--1)}{2}\right)\right]+\pi H^+ \tag{15}$$

with

$$H^+ + H^- = H = 2L. \tag{16}$$

Here L is the spin of the state and H^+ (H^-) is the number of holes near Λ ($-\Lambda$). The integers $n_h^\pm$ are defined by $n_h^\pm = J_{\max} \mp J_h$. Therefore the values in the round brackets in (14) and (15) are non-negative integers, measuring the distance of the holes from their maximum positions. Though it is clear that the analysis of Destri and Lowenstein (1982) cannot be applied, the deviations are not so strong. They consist mainly in the fact that additivity for the energies and momenta of holes is no longer valid, which consequently must violate the dispersion relation. The violating terms proportional to $(H^+)^2$ (instead of H^+) can be thought to contain an energy of 'interaction' for the holes missed in former analysis. The 'interaction' of holes on different ends is $o(1/N)$ and is therefore not present in (14). If H^+ and H^- are fixed, additivity is restored, at least as long as the holes do not move too far away from the ends.

On the basis of a generalisation of the methods of Destri and Lowenstein (1982), Avdeev and Dörfel (1985a, c) have estimated for general S the energy of the lowest triplet state (its momentum is π)

$$E_{\text{triplet}}^{(N)}-E_0^{(N)}=\frac{\pi^2}{4N}\left[\frac{1}{S}-\frac{1}{\ln N}+\frac{\ln(8S/\pi)}{\ln^2 N}+O\left(\frac{1}{\ln^3 N}\right)\right] \tag{17}$$

where they used $\sigma_\infty(\lambda)$ and the concept of a hole-induced density correction. Because $H^+ = H^- = 1$, it is not surprising that the leading term coincides with the correct answer in (14) (we have no 'interaction' of holes). But it is worthwhile noting that the first non-leading coefficient in this special case is correct, too. This can be seen from the results of Woynarovich and Eckle (1987), where they have obtained for the lowest states with $H^+ = H^- = L$

$$E_L^{(N)}-E_0^{(N)}=\frac{\pi^2 L^2}{2N}\left[1-\frac{1}{2\ln N}+O\left(\frac{\ln(\ln N)}{\ln^2 N}\right)\right]. \tag{18}$$

The question as to whether this is purely accidental or a result of some deeper symmetry requires further work.

In the case of complex λ, Woynarovich did not publish his findings for energy and momentum in detail, because he was mainly interested in reproducing the tower structure required by conformal invariance. Therefore we cannot follow the process by which wide pairs, strings and quartets violate additivity, as should be expected. For the lowest singlet (except the ground state) he has obtained the same energy as for the lowest triplet (to leading order), which was also predicted by Avdeev and Dörfel (1985c).

For $S=1$ a general analysis is still lacking due to the string deformations.

On the basis of conformal invariance and numerical results, Alcaraz and Martins (1988) suggested for the lowest excitations with spin L

$$E_L^{(N)}-E_0^{(N)}=\frac{\pi^2}{4N}\begin{Bmatrix} L^2 & L\text{ even} \\ L^2+\frac{1}{2} & L\text{ odd}\end{Bmatrix}+O\left(\frac{1}{N\ln N}\right). \tag{19}$$

For $L=1$ their numerical results up to $N=84$ coincide with those of Avdeev and Dörfel (1985c). We just may add to their values of X_1 (LHS of (19) multiplied by N/π^2) the result $X_1=0.344\,7143$ for $N=126$. Non-deformed strings would, instead of (19), imply

$$\tilde{E}_L^{(N)}-\tilde{E}_0^{(N)}=\frac{\pi^2L^2}{4N}+O\left(\frac{1}{N\ln N}\right) \tag{20}$$

(for $L=1$ see (17)) which yields

$$\tilde{E}_L^{(N)}-E_L^{(N)}=\frac{\pi^2}{N}\begin{cases}\frac{1}{24} & L\text{ even}\\ -\frac{1}{12} & L\text{ odd}\end{cases}+O\left(\frac{1}{N\ln N}\right). \tag{21}$$

This formula is also true for $L=0$. The change in sign is connected with the fact that for an even number of holes on one end (even L) the strings stretch, and for an odd number they shrink, which has been established numerically by Avdeev and Dörfel (1985c).

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