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LETTER TO THE EDITOR

An analytic treatment of finite-size corrections in the spin-1 antiferromagnetic XXZ chain

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Abstract. It is known that the standard method for calculating finite-size corrections in Bethe ansatz solvable systems is not applicable to the Takhtajan–Babujian model and its anisotropic XXZ generalisation. We develop a new analytic method explicitly avoiding root densities and associated problems. Nonlinear integral equations are derived whose solutions yield the correct central charges $c = 1$ and $c = \frac{3}{2}$ for the spin-$\frac{1}{2}$ and spin-1 XXZ chains, respectively. In the spin-1 case we obtain as a by-product the finite-size deviation of the Bethe ansatz roots from the 2-string formation.

There has been a recent growth of interest in calculating finite-size corrections in exactly solvable two-dimensional statistical mechanics models and their related quantum spin chains. One motivation is that at criticality such corrections are known to characterise an underlying conformal field theory (for a review, see e.g. [1]). In particular, for periodic boundary conditions, the leading finite-size correction to the ground state energy E_0 of the spin chain is related [2, 3] to the central charge c:

$$E_0 \sim Ne_0 - \pi\zeta c/6N \tag{1}$$

where N is the system size and ζ is a scale factor [4].

For models solvable via the Bethe ansatz, de Vega and Woynarovich have given a systematic procedure for calculating finite-size corrections [5]. This method, based on manipulations of root densities, has since been extended and applied to a number of models to derive c and various scaling dimensions (see e.g. [6, 7] and references therein).

On the other hand, for quantum spin chains c can also be obtained from the low-temperature heat capacity [3]. In this way, Affleck obtained the value

$$c = \frac{3s}{s+1} \tag{2}$$

for the integrable spin-s Takhtajan–Babujian (TB) model [8, 9]. However, the nature of the complex string solutions to the Bethe ansatz equations for E_0 has so far prevented

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a derivation of this result via (1). Nevertheless, the Bethe ansatz equations can still be solved numerically for relatively large N and small values of s [10–13]. In each case the estimates for c are in agreement with (2). More recently de Vega and Woynarovich have succeeded in deriving the finite-size behaviour of the roots [14].

In this letter we develop a different approach for calculating finite-size corrections, explicitly avoiding root densities. Our first goal has been to obtain the result (2) for the TB model. Here we present our results for the spin-1 case. In order to set the notation and for later comparison, we begin with a treatment of the spin-$\frac{1}{2}$ XXZ chain.

The Hamiltonian H of the more general spin-s XXZ chain (the TB model follows from H in the isotropic limit) and the momentum operator P can be expressed in terms of the transfer matrix $T(v)$ of the related $(2s+1)$-state vertex model (see e.g. [15–16]) as

$$H = \text{constant} \times (\ln T)'(v_0) \qquad P = \mathrm{i} \ln T(v_0) \tag{3}$$

where v_0 is a special value of the spectral variable v. The eigenspectrum of H can be obtained in terms of the eigenvalues $\Lambda(v)$ of $T(v)$

$$E = \text{constant} \times (\ln \Lambda)'(v_0) \qquad P = \mathrm{i} \ln \Lambda(v_0). \tag{4}$$

The spin-$\frac{1}{2}$ XXZ chain is related to the six-vertex model (see e.g. [17]). The eigenvalues $\Lambda(v)$ of the corresponding transfer matrix are determined from

$$\Lambda(v)q(v) = \Phi(v - \mathrm{i}\theta/2)q(v + \theta\mathrm{i}) + \Phi(v + \mathrm{i}\theta/2)q(v - \theta\mathrm{i}) \tag{5}$$

where

$$\Phi(v) = (\sinh v)^N \qquad q(v) = \prod_{j=1}^{N_-} \sinh(v - v_j). \tag{6}$$

Here N is the length of the chain and N_- is the number of down spins of the eigenstate. The unknown numbers v_j are determined by the Bethe ansatz equations $p(v_j) = -1$ where $p(v)$ is defined by

$$p(v) := \frac{\Phi(v - \mathrm{i}\theta/2)q(v + \theta\mathrm{i})}{\Phi(v + \mathrm{i}\theta/2)q(v - \theta\mathrm{i})}. \tag{7}$$

In the following we restrict ourselves to N even and also assume that $0 < \theta < \pi/2$ which covers a part of the planar XXZ chain in the neighbourhood of the (isotropic) antiferromagnetic Heisenberg model. The functions $q(v)$, $\Phi(v)$ and $\Lambda(v)$ are $\pi\mathrm{i}$ periodic:

$$q(v + \pi\mathrm{i}) = (-1)^{N/2} q(v) \qquad \Phi(v + \pi\mathrm{i}) = \Phi(v) \qquad \Lambda(v + \pi\mathrm{i}) = \Lambda(v). \tag{8}$$

The ground state is characterised by $N_- = N/2$ real numbers v_j distributed symmetrically about 0. We define functions $Q(v)$ and $P(v)$ as

$$\begin{aligned} Q(v) &:= (2\mathrm{i})^{-N/2} q(v) \left\{ \cosh\left[\frac{1}{2}\left(v - \frac{\pi}{2}\mathrm{i}\right)\right]\right\}^N \\ P(v) &:= \left\{ \coth\left[\frac{\pi}{2\theta}\left(v - \frac{\theta}{2}\mathrm{i}\right)\right]\right\}^N p(v) \end{aligned} \tag{9}$$

which are analytic, non-zero on the following strips and have zero logarithm in the far left/right limit (ANZZ)

$$\begin{aligned} 0 < \mathrm{Im}\,(v) < \pi \qquad & \text{for} \quad Q(v) \\ -\theta < \mathrm{Im}\,(v) < \theta \qquad & \text{for} \quad P(v). \end{aligned} \tag{10}$$

Due to the ANZZ property $\ln Q(v)$, $\ln P(v)$ can be Fourier transformed, e.g.

$$\ln Q(v) = \int_{-\infty}^{\infty} \hat{Q}(k) \mathrm{e}^{\mathrm{i}kv}\, \mathrm{d}k \tag{11}$$

with inverse transform

$$\hat{Q}(k) = \frac{1}{2\pi} \int_{-\infty+r\mathrm{i}}^{\infty+r\mathrm{i}} \ln Q(v) \mathrm{e}^{-\mathrm{i}kv}\, \mathrm{d}v \tag{12}$$

where r is somewhere between 0 and π.

From (7) and (8) we derive the first relation

$$\begin{aligned} &\hat{P}(k) + (\mathrm{e}^{-(\pi-\theta)k} - \mathrm{e}^{-\theta k})\hat{Q}(k) \\ &\quad = \frac{1}{2\pi} \int_{-\infty}^{\infty} \ln\left\{ \mathrm{i} \coth\left[\frac{\pi}{2\theta}\left(v - \frac{\theta}{2}\mathrm{i}\right)\right] \frac{\sinh(v - \mathrm{i}\theta/2)}{\sinh(v + \mathrm{i}\theta/2)} \right. \\ &\qquad \times \left. \frac{\cosh[(v + \mathrm{i}\theta - \mathrm{i}\pi/2)/2]}{\cosh[(v + \mathrm{i}\pi/2 - \mathrm{i}\theta)/2]} \right\}^N \mathrm{e}^{-\mathrm{i}kv}\, \mathrm{d}v. \end{aligned} \tag{13}$$

A second relation is derived from the fact that $h(v) := (1 + p(v))/2Q(v)$ is ANZZ in $-\theta < \mathrm{Im}(v) < \theta$. Cauchy's theorem then guarantees that

$$\int_{-\infty+a\mathrm{i}}^{\infty+a\mathrm{i}} \ln h(v) \mathrm{e}^{-\mathrm{i}kv}\, \mathrm{d}v = \int_{-\infty+b\mathrm{i}}^{\infty+b\mathrm{i}} \ln h(v) \mathrm{e}^{-\mathrm{i}kv}\, \mathrm{d}v \tag{14}$$

where $-\theta < b < 0 < a < \theta$. Using (8) this last equation is equivalent to

$$\begin{aligned} &\hat{P}(k) + (1 - \mathrm{e}^{-\pi k})\hat{Q}(k) \\ &\quad = \frac{1}{2\pi} \int_{-\infty+a\mathrm{i}}^{\infty+a\mathrm{i}} \ln \frac{1 + p(v)}{2} \mathrm{e}^{-\mathrm{i}kv}\, \mathrm{d}v - \frac{1}{2\pi} \int_{-\infty+b\mathrm{i}}^{\infty+b\mathrm{i}} \ln \frac{1 + 1/p(v)}{2} \mathrm{e}^{-\mathrm{i}kv}\, \mathrm{d}v \\ &\qquad - \frac{1}{2\pi} \int_{-\infty+b\mathrm{i}}^{\infty+b\mathrm{i}} \ln\left\{ \mathrm{i} \tanh\left[\frac{\pi}{2\theta}\left(v - \frac{\theta}{2}\mathrm{i}\right)\right] \frac{\cosh[(v - \mathrm{i}\pi/2)/2]}{\cosh[(v + \mathrm{i}\pi/2)/2]} \right\}^N \mathrm{e}^{-\mathrm{i}kv}\, \mathrm{d}v. \end{aligned} \tag{15}$$

From (13) and (15) the functions $\hat{Q}(k)$ and $\hat{P}(k)$ can be determined in terms of $p(v)$. From $\hat{P}(k)$ we calculate $P(v)$ using $p(-v) = 1/p(v)$, with the result

$$\ln P(v) = \frac{1}{2\pi} \int_{-\infty+b\mathrm{i}}^{\infty+b\mathrm{i}} \ln \frac{1 + 1/p(w)}{2} (F(v + w) - F(v - w))\, \mathrm{d}w \tag{16}$$

where

$$F(v) := \int_{-\infty}^{\infty} \frac{\sinh(\pi - 2\theta)k}{\cosh\theta k \, \sinh(\pi - \theta)k} \, \mathrm{e}^{\mathrm{i}2kv} \, \mathrm{d}k. \tag{17}$$

Choosing $b = -\theta/2$ and respecting the pole of $F(v)$ at $v = -\theta\mathrm{i}$ we find

$$P(v - \mathrm{i}\theta/2) = \exp\left(\frac{1}{2}R(v)^* + \frac{1}{2\pi}\int_{-\infty+b\mathrm{i}}^{\infty+b\mathrm{i}} (R(v-w)^* F(w - \mathrm{i}\theta) - R(v-w)F(w)) \, \mathrm{d}w\right) \tag{18}$$

where we have used the abbreviation

$$R(v) := \ln\frac{1 + 1/p(v - \mathrm{i}\theta/2)}{2} = \ln\frac{1 + [\tanh(\pi v/2\theta)]^N/P(v - \mathrm{i}\theta/2)}{2}.$$

This is a nonlinear integral equation for $P(v)$ where N enters simply as a (real) parameter but no longer plays the role of the number of unknown variables.

The ground state energy of the spin-$\frac{1}{2}$ XXZ chain is calculated from

$$E_0 = -\mathrm{i}(\theta/\pi)(\ln\Lambda)'(-\mathrm{i}\theta/2) \tag{19}$$

where an appropriate normalisation factor [18] was introduced to render the sound velocity as $\zeta = 1$. Now writing $E_0 = Ne_0 + \Delta E_N$, the finite-size correction ΔE_N can be expressed in terms of $p(v)$:

$$\Delta E_N = -\frac{2}{\pi}\int_0^{\infty} \frac{(\mathrm{Re}\, R(v))'}{\sinh(\pi v/\theta)} \, \mathrm{d}v. \tag{20}$$

To find a closed-form expression for the central charge c via (1), we introduce a new variable x by

$$v = \frac{2\theta}{\pi}\left(\frac{1}{2}\ln N + x\right) \tag{21}$$

and the limiting functions

$$\begin{aligned} \alpha(x) &:= \lim_{N\to\infty} P(v - \mathrm{i}\theta/2) \\ \gamma(x) &:= \lim_{N\to\infty} R(v) = \ln\frac{1 + \exp[-2\exp(-2x)]/\alpha(x)}{2}. \end{aligned} \tag{22}$$

Equations (18), (21) and (22) then yield an integral equation for $\alpha(x)$,

$$\begin{aligned} \alpha(x) = \exp\Bigg\{\frac{1}{2}\gamma(x)^* + \frac{1}{2\pi}\int_{-\infty}^{\infty}\Bigg[&\gamma(x-y)^* F\left(\frac{2\theta}{\pi}y - \theta\mathrm{i}\right)\frac{2\theta}{\pi} \\ &- \gamma(x-y)F\left(\frac{2\theta}{\pi}y\right)\frac{2\theta}{\pi}\Bigg]\mathrm{d}y\Bigg\}. \end{aligned} \tag{23}$$

The central charge can be calculated from the solution $\alpha(x)$ after performing the appropriate limit in (20). We find

$$c = \frac{48}{\pi^2} \int_{-\infty}^{\infty} \mathrm{Re}\,(\gamma(x) + \ln 2) \mathrm{e}^{-2x}\, \mathrm{d}x. \tag{24}$$

Up to now we have not solved (23) analytically. The solution, however, can be found numerically by iteration. This yields the known value of $c = 1$ within an error of order 10^{-6}.

Our alternative method for the spin-$\frac{1}{2}$ XXZ chain may look rather complicated. However, one should take into consideration that even for spin-$\frac{1}{2}$, a thorough treatment of the finite-size corrections within the standard method is still involved [6]. By inspection, we have $\lim_{x\to\pm\infty} \alpha(x) = 1$ as the asymptotic behaviour of $\alpha(x)$. Here the crude approximation $\alpha(x) \equiv 1$, corresponding to Hamer's procedure [18], does not solve (23), but fortunately (24) gives $c = 1$. (A comparable approximation for the spin-1 chain below does not work.)

We turn now to the spin-1 antiferromagnetic XXZ chain, i.e. to the model of Zamolodchikov and Fateev [19]. Here the eigenvalues of the transfer matrix of the corresponding 19-vertex model are given by [15, 16]

$$\Lambda(v) = L(v)L(v + \theta\mathrm{i}) - \sinh(v - \theta\mathrm{i})^N \sinh(v + 2\theta\mathrm{i})^N \tag{25}$$

and

$$L(v)q(v) = \Phi(v - \theta\mathrm{i})q(v + \theta\mathrm{i}) + \Phi(v + \theta\mathrm{i})q(v - \theta\mathrm{i}) \tag{26}$$

where $q(v)$ and $\Phi(v)$ are as defined in (6). The numbers v_j are determined by the Bethe ansatz equations $p(v_j) = -1$ where $p(v)$ is now defined by

$$p(v) := \frac{\Phi(v - \theta\mathrm{i})q(v + \theta\mathrm{i})}{\Phi(v + \theta\mathrm{i})q(v - \theta\mathrm{i})}. \tag{27}$$

For the ground state, the $N_- = N$ roots v_j are distributed symmetrically about 0 and are close to the lines $\mathrm{Im}\,(v) = \pm\theta/2$, but do not lie on them exactly. We assume N even and $0 < \theta < \pi/3$.

In order to proceed, we define some functions $Q_1(v)$, $Q_2(v)$, $P_1(v)$ and $P_2(v)$ for which the strips of the complex plane where the ANZZ property holds are

$$\begin{aligned}
Q_1(v) &:= \frac{q(v)}{(\sinh v)^N} && -\pi + \theta/2 < \mathrm{Im}\,(v) < -\theta/2 \\
Q_2(v) &:= \frac{q(v)}{(\cosh v)^N} && -\theta/2 < \mathrm{Im}\,(v) < \theta/2 \\
P_1(v) &:= \left[\coth\left(\frac{\pi}{2\theta}v\right)\right]^N p(v) && -3\theta/2 < \mathrm{Im}\,(v) < -\theta/2 \\
P_2(v) &:= p(v) && -\theta/2 < \mathrm{Im}\,(v) < \theta/2.
\end{aligned} \tag{28}$$

On similar lines as above using the ANZZ property of $h_1(v) := (1 + p(v))/2Q_2(v)$ and $h_2(v) := (1 + p(v))Q_2(v - \theta\mathrm{i})/2Q_1(v)$ in $-\theta < \mathrm{Im}\,(v) < 0$ and $0 < \mathrm{Im}\,(v) < \theta$, respectively, four equations can be derived for $\hat{Q}_1(k)$, $\hat{Q}_2(k)$, $\hat{P}_1(k)$ and $\hat{P}_2(k)$. They finally yield two coupled nonlinear integral equations for $P_1(v)$ and $P_2(v)$:

$$P_1(v-\theta \mathrm{i}) = \left(\frac{R_2(v)}{R_1(v)P_2(v)}\right)^{1/2} \exp\left[\mathrm{i} \fint_{-\infty}^{\infty} \frac{R(v-w)}{2\theta \sinh \pi w/\theta}\,\mathrm{d}w \right. \\ \left. + \frac{\mathrm{i}}{2(\pi-2\theta)} \int_{-\infty}^{\infty} \ln P_2(v-w) \left(\coth \frac{\pi w}{\pi - 2\theta} + \coth \frac{\pi(\theta \mathrm{i} - w)}{\pi - 2\theta}\right) \mathrm{d}w\right] \tag{29}$$

$$P_2(v) = \frac{R_1(-v)}{R_1(v)} \exp\left(\mathrm{i} \fint_{-\infty}^{\infty} \frac{R(v-w)+R(w-v)}{\theta \sinh \pi w/\theta}\,\mathrm{d}w\right)$$

where

$$R_1(v) := 1 + [\tanh(\pi v/2\theta)]^N / P_1(v-\theta\mathrm{i}) \qquad R_2(v) := 1 + P_2(v)$$
$$R(v) := \ln\left(\frac{R_1(v)}{2}\,\frac{R_2(v)}{2}\right). \tag{30}$$

The ground state energy of the spin-1 XXZ chain is calculated from

$$E_0 = -\mathrm{i}(\theta/\pi)(\ln\Lambda)'(-\theta\mathrm{i}) = Ne_0 - \mathrm{i}(\theta/\pi)(\ln P_2)'(0). \tag{31}$$

We introduce the variable x as in (21) and the limiting functions

$$\alpha(x) := \lim_{N\to\infty} P_1(v-\theta\mathrm{i}) \qquad \beta(x) := \lim_{N\to\infty} P_2(v)$$
$$\gamma(x) := \lim_{N\to\infty} R(v) = \ln\left(\frac{1+\exp[-2\exp(-2x)]/\alpha(x)}{2}\,\frac{1+\beta(x)}{2}\right). \tag{32}$$

Then in this limit (29) and (32) yield

$$\alpha(x) = \left(\frac{1+1/\beta(x)}{1+\exp[-2\exp(-2x)]/\alpha(x)}\right)^{1/2} \exp\left[\frac{\mathrm{i}}{\pi} \fint_{-\infty}^{\infty} \frac{\gamma(x-y)}{\sinh 2y}\,\mathrm{d}y \right. \\ + \frac{\theta\mathrm{i}}{\pi(\pi-2\theta)} \int_{-\infty}^{\infty} \ln\beta(x-y) \left(\coth\frac{\theta}{\pi-2\theta}2y \right. \\ \left.\left. + \coth\frac{\theta}{\pi-2\theta}(\pi\mathrm{i}-2y)\right)\mathrm{d}y\right] \tag{33}$$

$$\beta(x) = \frac{1+\exp[-2\exp(-2x)]/\alpha(x)^*}{1+\exp[-2\exp(-2x)]/\alpha(x)} \exp\left(\frac{4\mathrm{i}}{\pi} \fint_{-\infty}^{\infty} \frac{\mathrm{Re}\,\gamma(x-y)}{\sinh 2y}\,\mathrm{d}y\right).$$

The solution of these integral equations gives the central charge as

$$c = \frac{96}{\pi^2} \int_{-\infty}^{\infty} \mathrm{Re}\,(\gamma(x) + \ln 2)\mathrm{e}^{-2x}\,\mathrm{d}x. \tag{34}$$

We have not yet solved (33) analytically. The limiting behaviour, however,

$$\lim_{x\to\pm\infty} \alpha(x) = \begin{cases} 1 \\ \sqrt{2} \end{cases} \qquad \lim_{x\to\pm\infty} \beta(x) = \begin{cases} 1 \\ 1 \end{cases} \tag{35}$$

is derived easily. From this the deviation of the Bethe ansatz roots v_j from the lines $\mathrm{Im}\,(v) = \pm\theta/2$ can be derived as

$$\Delta v_j = \pm\frac{\ln 2}{4\pi}\,\frac{\mathrm{i}}{N\sigma(v)} \tag{36}$$

where $\sigma(v)$ is the root density. This result is in agreement with the findings of [14].

The integral equations (33) can be solved numerically by iteration. In this way we have obtained the result $c = \frac{3}{2}$ for $\theta = 0, 0.1\pi, \pi/6, 0.2\pi$ and 0.3π with an error of order 10^{-6}. In fact the spin-1 result is expected to hold in the wider range $0 < \theta < \pi/2$ [20], as is borne out by the numerical results [21, 22]. A detailed derivation of our results, along with their extension to spin-s, will be published elsewhere.

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