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LETTER TO THE EDITOR

Ground-state energy corrections for antiferromagnetic $s=\frac{1}{2}$ chains with short-range interaction

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Abstract. The leading finite-size effects in the description of the antiferromagnetic ground state of 1D quantum $s=\frac{1}{2}$ chains with non-nearest-neighbour short-range exchange are calculated in the framework of the asymptotic Bethe-ansatz method under a few general assumptions on the properties of scattering phases and energies of magnons.

The one-dimensional lattice spin chains have proven to be very useful objects for studying the critical phenomena in quantum statistics [1, 2]. The restriction to nearest-neighbour exchange allows one to transform the $s=\frac{1}{2}$ spin systems to the fermionic ones with local quartic interaction [3] and to establish their connection with 2D conformal field theories [2, 4, 5]. The critical behaviour of these chains is given by the $k=1$ SU(2) invariant Wess–Zumino model [2]. However, much less is known about the general spin systems described by the Hamiltonians

$$\mathscr{H}^{(N)}=\frac{1}{2}\sum_{j\neq k}^{N} h_N(j-k)\,\frac{\sigma_j\sigma_k-1}{2} \qquad h_N(j)=h_N(N-j) \tag{1}$$

with an arbitrary short-range exchange $h_N(j)$. Its behaviour with respect to criticality is definitely non-universal. So, it was strictly shown recently [6] that the model with next-nearest-neighbour exchange $h_N(j)=\delta_{j,1}+\lambda\delta_{j,2}+\{j\to N-j\}$ has a gap at $\lambda=\frac{1}{2}$.

For critical spin chains, besides well classified systems with $0<c<1$ there is a large variety of cases with $c=1$ and $c>1$. While the usual XXX model belongs to the first class, its integrable generalizations to higher spins belong to the second one [7]. An important fact was established by de Vega [8], who showed that c equals the number of nested Bethe-ansatz systems of equations if the ground state is determined by their real roots. However, the proof relies on the nearest-neighbour case only. It is therefore of interest to look for the confirmation of this result for more general form of the spin exchange.

For conformally invariant one-dimensional quantum systems with periodic boundary conditions and an even number of sites N the leading finite-size correction to the antiferromagnetic ground-state energy per site is related to the central charge via [4, 5]

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$$\Delta\varepsilon_N = \frac{E^{(N)}}{N} - \lim_{N'\to\infty} \frac{E^{(N')}}{N'} = -\frac{\pi c}{6N^2}\xi \tag{2}$$

where ξ is the velocity of the lowest-lying elementary excitations. This relation will be used below to determine the central charge for the integrable model with non-nearest-neighbour spin interaction of short range [9]. The exchange integrals of [9] for infinite chains are of inverse square hyperbolic form

$$h_\kappa(j) = J\frac{\sinh^2(\pi/\kappa)}{\sinh^2(j\pi/\kappa)} \qquad \kappa \in R_+$$

and the nearest-neighbour case treated by Bethe is recovered as $\kappa\to 0$. The solution to the diagonalization problem for the Hamiltonians with this type of exchange has been completely described in [9] for the infinite chains in the ferromagnetic regime $J<0$. It was shown that for arbitrary $M\in \boldsymbol{Z}_+$ the M-magnon wavefunction $\psi(n_1 \ldots n_M)$ reduces to the Bethe-like form in the asymptotic region $|n_\lambda - n_\nu| \gg \kappa$, i.e. the scattering of magnons is factorizable. The two-magnon phase shift $\phi(k_1, k_2)$ is expressed through their quasimomenta $k_1, k_2 \in \boldsymbol{R} \bmod 2\pi$ as

$$\cot\frac{\phi(k_1,k_2)}{2} = f(k_1) - f(k_2) \tag{3}$$

with $f(k)$ containing the elliptic Weierstrass ζ function [9]. The energy of the M-magnon state is

$$E_M(k) = \sum_{j=1}^{M} \varepsilon(k_j) \tag{4}$$

where $\varepsilon(k)$ is determined through $f(k)$ and its derivative.

To find an appropriate description of the antiferromagnetic ground state at $J>0$, one has to consider large but finite N. The exact solution to this problem is still not available. Nevertheless one can use the asymptotic method of Sutherland which has been claimed to be valid for all integrable models [10]. It consists in considering the wavefunctions of the *infinite* many-body systems only in the asymptotic region $|n_\lambda - n_\nu| \to \infty$ instead of their exact values, and imposing periodic b.c. as was done by Bethe. In this way, one arrives, for this model, at the asymptotic equations of the Bethe ansatz (ABA)

$$\exp(\mathrm{i}Nk_j) = \prod_{l\neq j}^{M} \exp[\mathrm{i}\phi(k_j, k_l)] \qquad j = 1, \ldots, M \tag{5}$$

where the phase shift ϕ is expressed through the parameters $\{k\}$ as in (3) and the corresponding energy is given by (4).

We shall show later that all the quantities referred to antiferromagnetic ground state can be found explicitly even in more general case, i.e. under very few assumptions about the properties of one-magnon energy $\varepsilon(k)$ and the function $f(k)$ in the formula (3) for the phase shift. Namely, hereafter it will be assumed that the derivatives of both these functions are continuous on $k\in(0, 2\pi)$ and $f(k)$ decreases monotonically on this interval:

$$f'(k) < 0 \qquad \lim_{k\to 0} kf(k) = 1. \tag{6}$$

As a consequence of the time-reversal invariance $f(k)$ should be antisymmetric with respect to $k=\pi$:

$$f(k)=-f(2\pi-k). \tag{7}$$

The function $\varepsilon(k)$ should be symmetric, $\varepsilon(k)=\varepsilon(2\pi-k)$. The magnon dispersion is assumed to be soft as it would be for all the models with short-range interaction:

$$\varepsilon(k)|_{k\to 0}\sim-\varepsilon_0 k^2 \tag{8}$$

where $\mathrm{sign}(\varepsilon_0)=\mathrm{sign}(J)$.

With appropriate choice of the branch of the logarithms one can represent (5) as

$$\frac{Q_j}{N}=\frac{\mu_j}{2\pi}-\frac{1}{\pi N}\sum_{l=1}^{M}\tan^{-1}[f(k_j)-f(k_l)] \qquad j=1,\ldots,M \tag{9}$$

where $\mu_j=\pi-k_j$ and the (half)integers $\{Q_j\}$ run over the interval $[-Q_{\max}, Q_{\max}]$, $Q_{\max}=(N-M-1)/2$.

Let us introduce the odd function $\mu(\lambda)$ through the relation

$$\lambda=f(\pi-\mu). \tag{10}$$

It is determined by (10) uniquely on the real axis and increases from $-\pi$ to π, $\mu'(\lambda)=-[f'(k(\lambda))]^{-1}>0$. As $\lambda\to\pm\infty$, the first two terms in the μ asymptotics are given by

$$\mu(\lambda)\sim\pm(\pi\mp\lambda^{-1}). \tag{11}$$

The ABA equations now can be written as

$$z_{2M}(\lambda_j)=N^{-1}Q_j \qquad j=1,\ldots,M \tag{12}$$

where $z_{2M}(\lambda)$ has continuous first derivative on the real axis

$$z_{2M}(\lambda)=(2\pi)^{-1}\mu(\lambda)-\frac{1}{\pi N}\sum_{l=1}^{M}\tan^{-1}(\lambda-\lambda_l). \tag{13}$$

We adopt the usual hypothesis [11–13] about the structure of antiferromagnetic vacuum state, i.e. that it is formed by real roots of (12) at $M=N/2$ and the corresponding ascending sequence of $\{Q\}$ does not contain holes. Note that the existence of at least one real solution to (12) at $M=N/2$ can be proven for an arbitrary monotonically increasing function $\mu(\lambda)$ by using an argument similar to Griffiths [14]. The root density $\sigma_N(\lambda)=\mathrm{d}z_N(\lambda)/\mathrm{d}\lambda$ is normalized as

$$\int_{-\infty}^{\infty}\sigma_N(\lambda)\,\mathrm{d}\lambda=\tfrac{1}{2}.$$

This can be seen directly from (13) since the asymptotics (11) gives $z_N(\pm\infty)=\pm\frac{1}{4}$. The equation for $\sigma_N(\lambda)$ reads

$$\sigma_N(\lambda)=(2\pi)^{-1}\mu'(\lambda)-\int_{-\infty}^{\infty}A(\lambda-\lambda')\sigma_N(\lambda')\,\mathrm{d}\lambda'$$
$$-\int_{-\infty}^{\infty}A(\lambda-\lambda')\left[\frac{1}{N}\sum_{l=1}^{N/2}\delta(\lambda'-\lambda_l)-\sigma_N(\lambda')\right]\mathrm{d}\lambda' \tag{14}$$

where $A(\lambda)=[\pi(1+\lambda^2)]^{-1}$. At $N\to\infty$ it reduces to the Húlthén-like form

$$\sigma_\infty(\lambda)+\int_{-\infty}^{\infty}\sigma_\infty(\lambda')A(\lambda-\lambda')\,\mathrm{d}\lambda'=(2\pi)^{-1}\mu'(\lambda). \tag{15}$$

The solution to (15) is found by Fourier transform:

$$\sigma_\infty(\lambda)=(2\pi)^{-2}\int_{-\infty}^{\infty}\frac{\exp(\mathrm{i}p\lambda)}{1+\exp(-|p|)}\int_{-\infty}^{\infty}\mu'(\tau)\exp(-\mathrm{i}p\tau)\,\mathrm{d}\tau. \tag{16}$$

Inserting (16) into (4) gives the asymptotic energy per site:

$$\varepsilon_\infty=\lim_{N\to\infty}N^{-1}E_{N/2}=\int_{-\infty}^{\infty}\varepsilon(k(\lambda))\sigma_\infty(\lambda)\,\mathrm{d}\lambda$$
$$=-(2\pi)^{-2}\int_0^{2\pi}\mathrm{d}k\;\varepsilon(k)f'(k)\int_{-\infty}^{\infty}\frac{\exp(\mathrm{i}pf(k))}{1+\exp(-|p|)}\int_0^{2\pi}\mathrm{d}k'\exp[-\mathrm{i}pf(k')]. \tag{17}$$

Now let us calculate the leading finite-size correction to (17). Following [15], one can transform (14) to an inhomogeneous linear integral equation for $\Delta\sigma_N(\lambda)=\sigma_N(\lambda)-\sigma_\infty(\lambda)$ with the solution

$$\Delta\sigma_N(\lambda)=\int_{-\infty}^{\infty}\mathrm{d}\lambda'\,P(\lambda-\lambda')\left[\frac{1}{N}\sum_{l=1}^{N/2}\delta(\lambda'-\lambda_l)-\sigma_N(\lambda')\right]\mathrm{d}\lambda' \tag{18}$$

where

$$P(\lambda)=\frac{1}{2\pi}\int_{-\infty}^{\infty}\frac{\exp(\mathrm{i}p\lambda)}{1+\exp(|p|)}\,\mathrm{d}p=(2\pi)^{-1}\,\Re\mathrm{e}\left[\psi\left(1+\frac{\mathrm{i}\lambda}{2}\right)-\psi\left(\frac{1+\mathrm{i}\lambda}{2}\right)\right] \tag{19}$$

$\psi(x)$ being the logarithmic derivative of the Euler gamma function. The correction to the energy per site ε_∞ can be written in the form

$$\Delta\varepsilon_N=N^{-1}E_{N/2}-\varepsilon_\infty=\int_{-\infty}^{\infty}\mathrm{d}\lambda'\,\Phi(\lambda')\left[\frac{1}{N}\sum_{l=1}^{N/2}\delta(\lambda'-\lambda_l)-\sigma_N(\lambda')\right]$$

where

$$\Phi(\lambda)=(2\pi)^{-1}\int_{-\infty}^{\infty}\mathrm{d}p\,\frac{\exp(\mathrm{i}p\lambda)}{1+\exp(-|p|)}\int_{-\infty}^{\infty}\exp(-\mathrm{i}p\lambda')\varepsilon(k(\lambda'))\,\mathrm{d}\lambda'. \tag{20}$$

The change of variables $\lambda\to z_N(\lambda)$ in combination with the definition of the root density $\sigma_N(\lambda)$ now gives

$$\Delta\varepsilon_N=\int_{-1/4}^{1/4}\mathrm{d}z_N\,\tilde{\Phi}(z_N)\left[\frac{1}{N}\sum_{l=0}^{N/2-1}\delta(z_N-\tilde{z}_l)+1\right]. \tag{21}$$

Here $\tilde{\Phi}(z_N)=\Phi(\lambda(z_N))$ has a continuous first derivative as follows from (7), (13) and (20). The sequence of numbers $\{\tilde{z}\}$ is defined by the ABA equations (12):

$$\tilde{z}_l=z_N(\lambda_{l+1})=-\frac{1}{4}+\frac{1}{2N}+\frac{l}{N}.$$

This enables one to apply the Euler–Maclaurin formula on the interval $(-1/4+1/2N, 1/4-1/2N)$ for simplifying (21). The result reads

$$\Delta\varepsilon_N = -(12N^2)^{-1}\varphi_N + \mathrm{O}(N^{-3}) \qquad \varphi_N = \frac{1}{2}\left[\frac{\mathrm{d}\tilde{\Phi}}{\mathrm{d}z_N}\left(\frac{1}{4}\right) - \frac{\mathrm{d}\tilde{\Phi}}{\mathrm{d}z_N}\left(-\frac{1}{4}\right)\right]. \tag{22}$$

It should be noted that any explicit expression for the function $z_N(\lambda)$ and its inverse $\lambda(z_N)$ has not been used up to this stage. Their explicit values are determined according to (13) by unknown roots of (12) at $M=N/2$. To evaluate the object of our interest, the constant in leading term of (22), it is sufficient, as in the Bethe case [16], to replace $\mathrm{d}\lambda/\mathrm{d}z_N$ by its asymptotics as $N\to\infty$, $[\sigma_\infty(\lambda(z_N))]^{-1}$. In this limit $\tilde{\Phi}(z_N)$ becomes even. The final expression of its derivative at $z_N=\frac{1}{4}$ after returning to the k variable in the integrands of (15) and (20) yields

$$\varphi_\infty = 2\pi\mathrm{i}\lim_{\lambda\to+\infty}\frac{\displaystyle\int_{-\infty}^{\infty} p\,\mathrm{d}p\,\frac{\exp(\mathrm{i}p\lambda)}{1+\exp(-|p|)}\int_0^{2\pi}\mathrm{d}k\;\varepsilon(k)f'(k)\exp[-\mathrm{i}pf(k)]}{\displaystyle\int_{-\infty}^{\infty}\frac{\exp(\mathrm{i}p\lambda)}{1+\exp(-|p|)}\int_0^{2\pi}\mathrm{d}k\exp[-\mathrm{i}pf(k)]}. \tag{23}$$

The elementary excitations over the antiferromagnetic vacuum in the limit $N\to\infty$ are the $s=\frac{1}{2}$ spin waves of Faddeev–Takhtajan type [17]. To evaluate the energy and momentum of such an elementary excitation, one has to make the usual assumption about the structure of the corresponding set of numbers $\{Q\}$. Let Q_s be the position of the hole in this set determined by the 'rapidity' $\lambda_h=s$. The linear integral equation of des Cloizeaux–Pearson type for the root density in the presence of a spin wave reads

$$\tilde{\sigma}_\infty(\lambda)+\pi^{-1}\int_{-\infty}^{\infty}\frac{\tilde{\sigma}_\infty(\lambda')\,\mathrm{d}\lambda'}{1+(\lambda-\lambda')^2} = (2\pi)^{-1}\mu'(\lambda) - N^{-1}\delta(\lambda-s).$$

The density distortion $\Delta\sigma_\infty(\lambda)=\tilde{\sigma}_\infty(\lambda)-\sigma_\infty(\lambda)$ does not depend on μ: it is given by

$$\Delta\sigma_\infty(\lambda) = N^{-1}[P(\lambda-s)-\delta(\lambda-s)]$$

with $P(\lambda)$ defined by (17). By using this formula one immediately obtains explicit expressions for the energy and momentum of this excitation:

$$\varepsilon_h(s) = -(2\pi)^{-1}\int_{-\infty}^{\infty}\mathrm{d}p\,\frac{\exp(\mathrm{i}ps)}{1+\exp(-|p|)}\int_{-\infty}^{\infty}\varepsilon(k(\lambda))\exp(-\mathrm{i}p\lambda)\,\mathrm{d}\lambda$$

$$k_h(s) = N\int_{-\infty}^{\infty} k(\lambda)\Delta\sigma_\infty(\lambda)\,\mathrm{d}\lambda = -k(s)+\int_{-\infty}^{\infty}P(\lambda-s)k(\lambda)\,\mathrm{d}\lambda. \tag{24}$$

As can be seen from (7) and (24), the zero-momentum limit corresponds to large positive s. The expression for the sound velocity ξ reads

$$\xi = \lim_{s\to\infty} -\frac{\mathrm{d}\varepsilon_h(s)/\mathrm{d}s}{\mathrm{d}k_h(s)/\mathrm{d}s}. \tag{25}$$

The denominator in (25) can be transformed as follows. The result of differentiation of $k_h(s)$ with respect to s reads

$$\frac{\mathrm{d}k_h(s)}{\mathrm{d}s} = -k'(s) + \int_{-\infty}^{\infty} \mathrm{d}\lambda \left\{ \frac{\mathrm{d}}{\mathrm{d}\lambda} [-k(\lambda)P(\lambda - s)] + k'(\lambda)P(\lambda - s) \right\}.$$

The contribution of the first term in curly brackets vanishes since $P(\lambda)$ is proportional to λ^{-2} as $\lambda \to \infty$. The transition to the variable k in the integrands of (25) now yields

$$\xi = (2\pi)^{-1}\varphi_\infty. \tag{26}$$

Comparing (22), (23) and (26) with (2), we conclude that $c=1$ for all the models described by the BA-type equations (5).

After having determined the central charge it is now straightforward to try to calculate the anomalous dimensions of the primary operators. Conformal invariance implies for the energies of the lowest-lying excitations

$$E_{l,nm}^{(N)} - E_0^{(N)} = \xi \frac{2\pi}{N} [x_l + n + m] + \mathrm{o}(N^{-1}) \tag{27}$$

where $\{x_l\}$ are the dimensions and $n, m = 0, 1 \ldots$ The excitation energies $E_{l,nm}^{(N)}$ can be calculated in the leading order in N^{-1} if one considers, besides the vacuum distribution of the real roots, a finite number of holes in it near the ends. The calculations follow the lines of [18] and [19]. This is possible if one assumes that the asymptotics of $\sigma_\infty(\lambda)$ and $\Phi(\lambda)$ for large λ are determined by a single pair of poles of their Fourier transforms, lying symmetrically on the imaginary p-axis. Using now the fact $c=1$ it follows that both pairs must coincide. Their actual position does not enter into the final result

$$x_j = \frac{1}{2}\left(\frac{H^+ + H^-}{2}\right)^2 + \frac{1}{2}\left(\frac{H^+ - H^-}{2}\right)^2$$

where H^+ and H^- are the numbers of holes near the right and left ends of the root distribution.

Thus, one obtains the same dimensions as in the case of the standard XXX Heisenberg chain. This illustrates the fact that different models may have an identical set of conformal parameters.

To conclude, one should stress that the result for the central charge does not depend on the concrete form of the functions $\varepsilon(k)$ and $f(k)$ when the restrictions (6)–(8) are obeyed. On the other hand, it turned out to be crucial that the ground state is formed by a sea of real roots fulfilling the Bethe-type system of equations and the low-lying excitations over the antiferromagnetic vacuum are described by holes in the sequence of quantum numbers $\{Q\}$. Both these statements are supported mainly by numerical analysis for the usual XXX chain [19]. It would be of interest to find an analytic method of confirmation extended to the more general form of the magnon energies and phase shifts given by (3).

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