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LETTER TO THE EDITOR

Finite-size corrections for the *XXX* antiferromagnet

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Abstract. We present a method of calculating finite-size corrections for the isotropic (XXX) Heisenberg chain in the antiferromagnetic case. The leading corrections to the energy and the root density of the ground state are compared with the numerical data up to $N=256$ sites in the chain.

Integrable models such as the one-dimensional isotropic (XXX) Heisenberg model (HM) with the Hamiltonian

$$H=(J/4)\sum_{n=1}^{N}(\boldsymbol{\sigma}_n\cdot\boldsymbol{\sigma}_{n+1}-1)\qquad(\boldsymbol{\sigma}_{N+1}\equiv\boldsymbol{\sigma}_1)\tag{1}$$

are solved by applying the Bethe ansatz technique (Bethe 1931). The explicit solution requires the knowledge of the roots λ_j of the so-called Bethe ansatz equations (BAE)

$$\left(\frac{\lambda_j+\mathrm{i}/2}{\lambda_j-\mathrm{i}/2}\right)^N=-\prod_{k=1}^{M}\frac{\lambda_j-\lambda_k+\mathrm{i}}{\lambda_j-\lambda_k-\mathrm{i}}\qquad(j=1\ldots M).\tag{2}$$

For the vacuum state in the case of N even, $J>0$ (antiferromagnetic HM), the solution includes $M=N/2$ real roots. In the infinite-size limit, $N\to\infty$, the number of equations as well as the number of roots tend to infinity. Then the BAE are reduced to a linear integral equation for a density function (Hulthén 1938), which can easily be solved (for a survey, see Faddeev and Takhtajan 1981).

Recently, de Vega and Woynarovich (1985) have suggested a method of calculating finite-size corrections for models with a non-zero mass gap. This restriction played a crucial role in their calculations. Therefore, the method cannot be directly applied to the XXX HM where the mass gap vanishes.

However, using a similar starting point idea, we were able to derive an analytic expression for the leading correction to the vacuum energy which is in good agreement with our numerical results. Furthermore, we present an iteration procedure, based directly on the BAE, for evaluating the root density and demonstrating the relation of the first approximation to the exact density calculated numerically.

In our case the BAE (2) can be transformed to the following system of equations:

$$Q_j/N=(1/\pi)\tan^{-1}(2\lambda_j)-(1/\pi N)\sum_{k=1}^{M}\tan^{-1}(\lambda_j-\lambda_k)\tag{3}$$

where the Q_j, $|Q_j|\leq Q_{\max}$ are (half)-integers according to $Q_{\max}=N/4-\frac{1}{2}$. For large

N, it is useful to consider $z(\lambda_j) = Q_j/N$

$$z(\lambda) = (1/\pi)\tan^{-1}(2\lambda) - (1/\pi N)\sum_{k=1}^{M}\tan^{-1}(\lambda - \lambda_k) \tag{4}$$

and the derivative of this function, $dz(\lambda)/d\lambda = \sigma_N(\lambda)$

$$\sigma_N(\lambda) = (1/\pi)\frac{\frac{1}{2}}{\frac{1}{4}+\lambda^2} - \frac{1}{\pi N}\sum_{k=1}^{M}\frac{1}{1+(\lambda-\lambda_k)^2} \tag{5}$$

which plays the role of a root density. The energy is given by

$$E_N = -J\sum_{j=1}^{M}\frac{\frac{1}{2}}{\frac{1}{4}+\lambda_j^2}. \tag{6}$$

Using the technique of de Vega and Woynarovich (1985), we present the finite-size corrections in the form

$$\Delta\sigma_N(\lambda) = \sigma_N(\lambda) - \sigma_\infty(\lambda) = -\int_{-\infty}^{\infty} d\mu\, P(\lambda-\mu)\left((1/N)\sum_{k=1}^{M}\delta(\mu-\lambda_k) - \sigma_N(\mu)\right) \tag{7}$$

$$\Delta E_N = E_N - E_\infty = -\pi JN\int_{-\infty}^{\infty} d\lambda\, \sigma_\infty(\lambda)\left((1/N)\sum_{k=1}^{M}\delta(\lambda-\lambda_k) - \sigma_N(\mu)\right). \tag{8}$$

Here

$$P(\lambda) = \int_{-\infty}^{\infty}\frac{d\rho}{2\pi}\frac{e^{i\lambda\rho}}{1+e^{|\rho|}} = (1/\pi)\,\mathrm{Re}\,\beta(1-i\lambda) \tag{9}$$

and the infinite-size expressions are

$$\sigma_\infty(\lambda) = [2\cosh(\pi\lambda)]^{-1} \qquad E_\infty = -JN\ln 2. \tag{10}$$

We now compute the leading-order contribution to ΔE_N. Solving equation (4) with respect to λ defines a function $\lambda_N[z]$ for continuous z. Changing the integration variables in equation (8), we obtain

$$\Delta E_N = -\pi JN\int_{-1/4}^{1/4} dz\,\sigma_\infty(\lambda_N[z])\left((1/N)\sum_{k=1}^{M}\delta(z-z_k) - 1\right) \tag{11}$$

with $z_k = -\frac{1}{4} + (k-\frac{1}{2})/N$. The problem is that as long as the exact values of $\sigma_N(\lambda)$ is unknown, $\lambda_N[z]$ is not available, either. Below we will argue that, for the leading energy correction, one can substitute

$$\lambda_\infty[z] = (1/\pi)\ln\tan[\pi(z+\tfrac{1}{4})] \tag{12}$$

instead. Then, the correction is evaluated to

$$\begin{aligned}\Delta E_N^{(1)} &= -\pi JN\{[2N\sin(\pi/N)]^{-1} - (1/2\pi)\}\\ &= -(J/N)(\pi^2/12) + O(N^{-3}).\end{aligned} \tag{13}$$

The coefficient $\pi^2/12 \approx 0.8225$ agrees with our 'experimental' value ≈ 0.823 calculated by equation (6) using the numerical solutions of equation (2) up to $N = 256$ (table 1). The finite-size corrections to the ground state energy had been first computed for relatively small N by Hulthén (1938); later, the N dependence ($N \leqslant 12$) was plotted by Bonner and Fisher (1964), and for $N \leqslant 16$ calculated by Grieger (1984); but up to now, no analytic expression was obtained.

Table 1. The finite-size corrections $\Delta E_N = E_N - E_\infty$ to the ground state energy, multiplied by $-N/J$ (numerical results).

N	$-(N/J)\,\Delta E_N$	N	$-(N/J)\,\Delta E_N$	N	$-(N/J)\,\Delta E_N$
4	0.909 645	10	0.839 745	64	0.824 437
6	0.863 355	16	0.831 064	130	0.823 687
8	0.847 328	32	0.826 165	256	0.823 318

We now wish to estimate the error caused by using $\lambda_\infty[z]$ instead of $\lambda_N[z]$ in equation (11):

$$\Delta E_N^{(2)} = -2\pi JN \int_0^{1/4} dz\{\sigma_\infty(\lambda_N[z]) - \sigma_\infty(\lambda_\infty[z])\}\left((1/N)\sum_{k=1}^{M}\delta(z-z_k) - 1\right). \tag{14}$$

We split the integration interval into two parts. In the first region, $0 \leqslant z \leqslant \frac{1}{4} - 1/N$, $\Delta\lambda_N[z] = \lambda_N[z] - \lambda_\infty[z]$ is small and

$$\Delta\lambda_N[z] \approx -[\sigma_\infty(\lambda_\infty[z])]^{-1}\int_0^{\lambda_\infty[z]} d\lambda\, \Delta\sigma_N(\lambda). \tag{15}$$

Then, expanding σ_∞, we obtain

$$\Delta E_N^{(2)} \approx -2\pi^2 JN \int_0^{1/4-1/N} dz\,\sin(2\pi z)\int_0^{\lambda_\infty[z]} d\lambda\,\Delta\sigma_N(\lambda)\left((1/N)\sum_{k=1}^{M}\delta(z-z_k) - 1\right)$$
$$-2\pi JN\int_{1/4-1/N}^{1/4} dz\, e^{-\pi\lambda_\infty[z]}(e^{-\pi\Delta\lambda_N[z]} - 1)\left((1/N)\sum_{k=1}^{M}\delta(z-z_k) - 1\right). \tag{16}$$

The difference between the sum and the integral in equation (16) yields a $1/N^2$ factor, and another $1/N$ factor results from $\int d\lambda\,\Delta\sigma_N$ (see below). In the second region, $\frac{1}{4} - 1/N \leqslant z \leqslant \frac{1}{4}$, $\Delta\lambda_N[z]$ remains no longer small, but the fast decrease in $\sigma_\infty(\lambda)$ causes an additional damping. Combining these arguments, we have $\Delta E_N^{(2)} = O(1/N^2)$. Thus, equations (11) and (13) can be effectively used for computing the energy corrections in the *XXX* HM.

Let us now proceed to the root-density correction. The difference between the sum and the integral in equation (7) can be estimated as

$$\Delta\sigma_N(\lambda) = -(1/2N)[P(\lambda - \lambda_{\max}) + P(\lambda + \lambda_{\max})]$$
$$+\int_{z_{\max}}^{1/4} dz[P(\lambda - \lambda_N[z]) + P(\lambda + \lambda_N[z])]$$
$$-(1/12N^3)\sum_{k=2}^{M}\frac{\partial}{\partial z}\left[\frac{1}{\sigma_N(\lambda_N[z])}\frac{\partial P(\lambda - \lambda_N[z])}{\partial\lambda_N[z]}\right]\Bigg|_{z=z_k^*} \tag{17}$$

where $\lambda_{\max} = \lambda_N[z_{\max}]$, $z_{\max} = \frac{1}{4} - (1/2N)$ and $z_{k-1} \leqslant z_k^* \leqslant z_k$. We see that, after converting the latter sum into an integral, one should be able to estimate $1/\sigma_N(\lambda_{\max})$. From our numerical results we can conclude that $1/\sigma_N(\lambda_{\max}) = O(N)$ for $N \to \infty$. Then, it is not difficult to derive the following relations from equation (17):

$$|\Delta\sigma_N(\lambda)| \leq A/N \qquad \left|\int_0^{\lambda_\infty[z]} d\lambda\ \Delta\sigma_N(\lambda)\right| \leq B/N \tag{18}$$

where A and B are constants.

Unfortunately, $\Delta\sigma_N(\lambda)$ cannot be calculated simply by iterating equation (7). Owing to the slow decrease in the β function (9), the error caused by replacing $\lambda_N[z]$ by $\lambda_\infty[z]$ cannot be controlled, and the results obtained in this way would be incorrect. This is confirmed by numerical calculations; even for $\Delta\sigma_N(0)$, the estimate then has the wrong sign and does not tend to zero as $N\to\infty$.

Therefore, we apply another iteration scheme for $\sigma_N(\lambda)$, based on equations (4) and (5). Independently, a similar method has been used by Grieger (1984) for solving BAE. To obtain $\sigma_N^{(1)}$, on the RHS we use $\lambda_k = \lambda_\infty[z_k]$ from equation (12). Then, each root is corrected through equation (4), and thereafter $\sigma_N^{(2)}$ can be found, etc. To illustrate the efficiency of the scheme, in table 2 and figure 1 we compare the first iteration $\Delta\sigma_N^{(1)}(\lambda) = \sigma_N^{(1)}(\lambda) - \sigma_\infty(\lambda)$ with the exact $\Delta\sigma_N(\lambda)$ calculated via the direct numerical solution of the BAE (2).

Finally, in table 3 and figure 2 we show the N dependence of the density correction by comparing the cases of $N=10$ ($\lambda_{max}=0.598\,087$) and $N=256$ ($\lambda_{max}=1.635\,314$).

Table 2. The exact finite-size root-density correction $\Delta\sigma_N = \sigma_N - \sigma_\infty$ and its first approximation $\Delta\sigma_N^{(1)} = \sigma_N^{(1)} - \sigma_\infty$ at $N=10$.

λ	$\Delta\sigma_{10}(\lambda)$	$\Delta\sigma_{10}^{(1)}(\lambda)$	λ	$\Delta\sigma_{10}(\lambda)$	$\Delta\sigma_{10}^{(1)}(\lambda)$
0	-2.92×10^{-13}	-3.44×10^{-3}	1.6	1.47×10^{-3}	1.61×10^{-3}
0.2	-2.96×10^{-3}	-3.43×10^{-3}	1.8	1.50×10^{-3}	1.61×10^{-3}
0.4	-2.98×10^{-3}	-3.31×10^{-3}	2	1.38×10^{-3}	1.47×10^{-3}
0.6	-2.66×10^{-3}	-2.80×10^{-3}	2.2	1.19×10^{-3}	1.25×10^{-3}
0.8	-1.81×10^{-3}	-1.79×10^{-3}	2.4	9.84×10^{-4}	1.04×10^{-3}
1	-6.43×10^{-4}	-5.06×10^{-4}	2.6	8.00×10^{-4}	8.41×10^{-4}
1.2	4.36×10^{-4}	6.10×10^{-4}	6	3.39×10^{-5}	3.58×10^{-5}
1.4	1.15×10^{-3}	1.31×10^{-3}	16	6.47×10^{-7}	6.88×10^{-7}

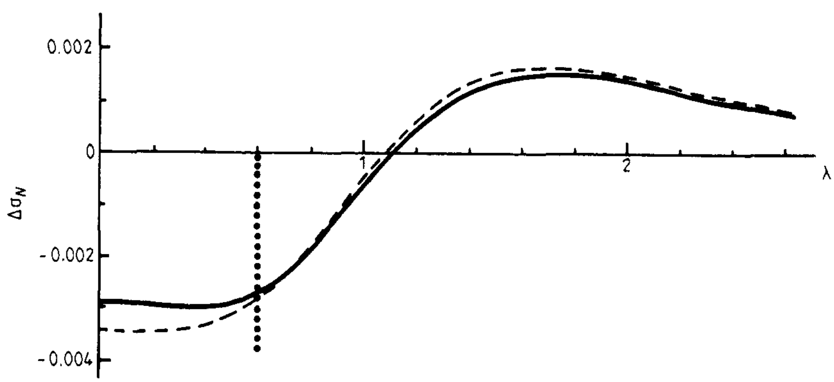

Figure 1. The exact $\Delta\sigma_N$ (full curve) and its first approximation $\Delta\sigma_N^{(1)}$ (broken curve) as functions of λ for $N=10$. The λ_{max} position is marked by dots.

Table 3. The relative correction $\delta\sigma_N(\lambda)=\Delta\sigma_N(\lambda)/\sigma_N(\lambda)$ to the root density for $N=10$ and $N=256$.

λ	$\delta\sigma_{10}(\lambda)$	$\delta\sigma_{256}(\lambda)$	λ	$\delta\sigma_{10}(\lambda)$	$\delta\sigma_{256}(\lambda)$
0	-5.87×10^{-3}	-4.50×10^{-5}	1.8	0.300	-1.85×10^{-2}
0.2	-7.19×10^{-3}	-5.70×10^{-5}	2	0.424	-1.26×10^{-2}
0.4	-1.14×10^{-2}	-1.04×10^{-4}	2.2	0.543	1.76×10^{-2}
0.6	-1.82×10^{-2}	-2.29×10^{-4}	2.4	0.649	8.06×10^{-2}
0.8	-2.31×10^{-2}	-5.47×10^{-4}	2.6	0.738	0.175
1	-1.51×10^{-2}	-1.34×10^{-3}	3	0.864	0.417
1.2	1.86×10^{-2}	-3.23×10^{-3}	5	$1-1.95\times10^{-2}$	0.865
1.4	8.54×10^{-2}	-7.17×10^{-3}	6	$1-1.92\times10^{-4}$	$1-1.96\times10^{-3}$
1.6	0.183	-1.34×10^{-2}	16	$1-2.29\times10^{-16}$	$1-3.08\times10^{-15}$

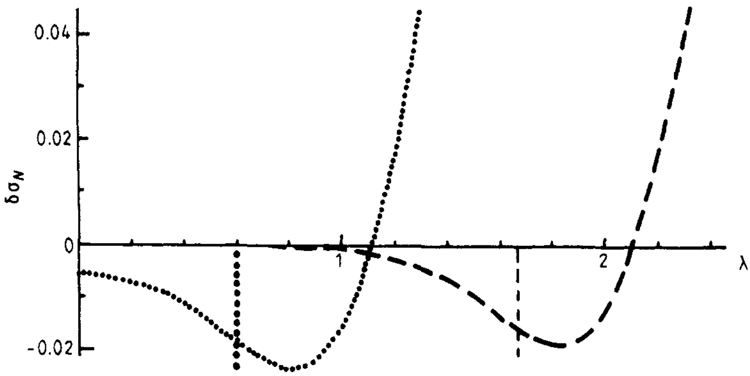

Figure 2. The relative density corrections $\delta\sigma_N=\Delta\sigma_N/\sigma_N$ as functions of λ for $N=10$ (dotted curve) and $N=256$ (broken curve). The λ_{max} positions are marked by vertical lines.

One sees that, with the increase in N, the region where the relative correction is small widens, while the correction itself decreases inside this region and remains practically unchanged on its boundary.

Our numerical data agree in domains of overlap with the results of other authors, particularly those of Grieger (1984) up to $N=16$.

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