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LETTER TO THE EDITOR

Finite-size corrections for ground states of the XXZ Heisenberg chain in the critical region

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Abstract. The methods of de Vega and Woynarovitch are used to calculate finite-size corrections to the ground state energy in different sectors for the XXZ Heisenberg chain, in the critical region $-1 < \Delta < 1$. The finite-size scaling amplitude for the mass gap between the lowest lying sectors is derived. Using conformal invariance, the scaling dimension is extracted for an associated operator, corresponding to the electric field operator in the 8-vertex model. The conjecture of Baxter and Kelland for the electric field exponent is confirmed.

Recently, a method was given by de Vega and Woynarovitch (1985) for calculating the leading-order finite-size corrections to the ground state energy of any model which is soluble by the Bethe ansatz. They considered only cases where the mass gap was non-zero. Here we apply the treatment to a case where the bulk mass gap is zero, i.e. the system is at a critical point.

Let us consider the XXZ Heisenberg chain, with Hamiltonian

$$H = -\frac{1}{2} \sum_{n=1}^N (\sigma_n^X \sigma_{n+1}^X + \sigma_n^Y \sigma_{n+1}^Y + \Delta \sigma_n^Z \sigma_{n+1}^Z) \tag{1}$$

and periodic boundary conditions. The total number of sites N will be assumed even, for convenience. The Bethe ansatz for this system was discussed by Yang and Yang (1966). The total number of down spins m is conserved, so we may label each sector of states by $y = 1 - 2m/N$. The Bethe ansatz for the eigenvectors involves a momentum p_j for each down spin, and phase factors which involve pairs of p_j , given by

$$\theta(p, q) = 2 \tan^{-1} \left(\frac{\Delta \sin[(p - q)/2]}{\cos[(p + q)/2] - \Delta \cos[(p - q)/2]} \right). \tag{2}$$

The periodic boundary conditions are satisfied if

$$Np_j = 2\pi I_j - \sum_{l=1}^m \theta(p_j, p_l) \tag{3}$$

where the I_j are integers or half-odd integers given by

$$I_1, I_2, \dots, I_m = -\left(\frac{m-1}{2}\right), -\left(\frac{m-1}{2}\right) + 1, \dots, +\left(\frac{m-1}{2}\right) \tag{4}$$

for the ground state in each sector. The energy is given by

$$E = -\frac{1}{2}N\Delta + 2 \sum_{j=1}^m (\Delta - \cos p_j). \tag{5}$$

Let us now restrict our consideration to the case $-1 < \Delta < 1, y = 0$. A convenient change of variables is then

$$\Delta = -\cos \gamma \quad 0 < \gamma < \pi \tag{6}$$

and

$$p = 2 \tan^{-1}[(\cot \frac{1}{2}\gamma) \tanh \lambda]. \tag{7}$$

Let

$$\phi(\lambda, \gamma) = 2 \tan^{-1}\left(\frac{\tanh \lambda}{\tan \gamma}\right) \tag{8}$$

then (3) becomes

$$N\phi(\lambda_j, \gamma/2) = 2\pi I_j + \sum_{i=1}^m \phi(\lambda_j - \lambda_i, \gamma) \tag{9}$$

and the energy is

$$E = \frac{1}{2}N \cos \gamma - \sin \gamma \sum_{j=1}^m \phi'(\lambda_j, \frac{1}{2}\gamma) \tag{10}$$

where the prime denotes differentiation with respect to λ .

At this point, de Vega and Woyrnarovitch (1985) define the function

$$Z_N(\lambda) = \frac{1}{2\pi} \left[\phi(\lambda, \frac{1}{2}\gamma) - \frac{1}{N} \sum_{j=1}^m \phi(\lambda - \lambda_j, \gamma) \right]. \tag{11}$$

This function is continuous and monotonically increasing for real λ , and at the roots of (9)

$$Z_N(\lambda_i) = I_i / N. \tag{12}$$

Its derivative will be denoted

$$\sigma_N(\lambda) = dZ_N / d\lambda. \tag{13}$$

When N goes to infinity the λ_i tend to a continuous distribution with density $N\sigma_N(\lambda)$, and equation (9) gives rise to a linear integral equation with difference kernel

$$\sigma_\infty(\lambda) = \frac{1}{2\pi} \phi'(\lambda, \frac{1}{2}\gamma) - \int_{-\infty}^{\infty} \frac{d\mu}{2\pi} \sigma_\infty(\mu) \phi'(\lambda - \mu, \gamma). \tag{14}$$

This may be solved by Fourier transformation to give

$$\sigma_\infty(\lambda) = \frac{1}{2\gamma \cosh(\pi\lambda/\gamma)}. \tag{15}$$

The energy per site in this limit reduces to

$$f_\infty = \lim_{N \rightarrow \infty} \left(\frac{E}{N} \right) = \frac{1}{2} \cos \gamma - \sin^2 \gamma \int_{-\infty}^{\infty} \frac{d\mu}{\cosh(\pi\mu)} \frac{1}{[\cosh(2\gamma\mu) - \cos \gamma]}. \tag{16}$$

Now de Vega and Woynarovitch (1985) show that one can derive similar integral equations valid for any N . The definitions (11) and (13) give

$$\sigma_N(\lambda) = \frac{1}{2\pi} \phi'(\lambda, \frac{1}{2}\gamma) - \int_{-\infty}^{\infty} \frac{d\mu}{2\pi} \sigma_N(\mu) \phi'(\lambda - \mu, \gamma) - \int_{-\infty}^{\infty} \frac{d\mu}{2\pi} \phi'(\lambda - \mu, \gamma) \left(\frac{1}{N} \sum_{i=1}^m \delta(\mu - \lambda_i) - \delta_N(\mu) \right) \quad (17)$$

whence one obtains a linear integral equation for $\sigma_N(\lambda) - \sigma_{\infty}(\lambda)$ leading to the result

$$\sigma_N(\lambda) - \sigma_{\infty}(\lambda) = - \int_{-\infty}^{\infty} \frac{d\mu}{\pi} p(\lambda - \mu) \left(\frac{1}{N} \sum_{i=1}^m \delta(\mu - \lambda_i) - \sigma_N(\mu) \right) \quad (18)$$

with

$$p(\lambda - \mu) = \frac{1}{2} \int_{-\infty}^{\infty} dX e^{i(\lambda - \mu)X} \frac{\sinh[(\pi - 2\gamma)X/2]}{\{\sinh(\pi X/2) + \sinh[(\pi - 2\gamma)X/2]\}} \quad (19)$$

For the energy per site $f_N = E/N$, one obtains similarly

$$f_N - f_{\infty} = -2\pi \sin \gamma \int_{-\infty}^{\infty} d\lambda \sigma_{\infty}(\lambda) \left(\frac{1}{N} \sum_{i=1}^m \delta(\lambda - \lambda_i) - \sigma_N(\lambda) \right). \quad (20)$$

Our objective now is to obtain the leading order behaviour of equation (20) for large N . For the case with a non-zero mass gap, de Vega and Woynarovitch (1985) proceeded to perform a Poisson resummation, and evaluate the leading Fourier coefficient by saddle-point methods. In the present case, we can proceed more directly. Equation (20) can be rewritten in terms of the variable $Z_N(\lambda)$:

$$f_N - f_{\infty} = -\frac{\pi}{\gamma} \sin \gamma \int_{-1/4}^{1/4} dZ \frac{1}{\cosh[(\pi/\gamma)\lambda_N(Z)]} \left(\frac{1}{N} \sum_{i=1}^m \delta(Z - Z_N(\lambda_i)) - 1 \right) \quad (21)$$

where $\lambda_N(Z)$ is the function inverse to $Z_N(\lambda)$. Use the relationship valid as N goes to infinity, from (13) and (15),

$$\cosh\left(\frac{\pi\lambda}{\gamma}\right) = \frac{1}{\cos(2\pi Z)} \quad (22)$$

then equation (21) can easily be evaluated to give

$$f_N - f_{\infty} \underset{N \rightarrow \infty}{\sim} -\frac{\pi^2}{6\gamma} \sin \gamma \frac{1}{N^2}. \quad (23)$$

This is the required leading order finite-size correction to the ground state energy.

The discussion given above can be generalised to the case with y non-zero but small. One finds that to leading order the finite-size correction is constant in y . It follows that the mass gap between the two lowest lying eigenvalues is

$$F_N = N(f_N(2/N) - f_N(0)) \underset{N \rightarrow \infty}{\sim} N(f_{\infty}(2/N) - f_{\infty}(0)) \quad (24)$$

where $f_N(y)$ is the energy per site in sector y . But the right-hand side of this expression has already been evaluated[†] by Yang and Yang (1966).

[†] Our variable $f_N(y)$ differs by a factor of 2 from $f(\Delta, y)$ as defined by Yang and Yang.

Hence one finds

$$F_N \underset{N \rightarrow \infty}{\sim} \frac{\pi}{N\gamma} (\pi - \gamma) \sin \gamma. \quad (25)$$

The finite-size scaling amplitudes predicted by equations (23) and (25) have been checked against numerical results for this model.

Now Cardy (1984) has shown by conformal invariance that the finite-size scaling amplitude of the mass gap for a system at its critical point is related to a critical exponent. If the mass gap scales as

$$F_N \underset{N \rightarrow \infty}{\sim} A/N \quad (26)$$

where N is the size of the system, then

$$A = 2\pi X \quad (27)$$

where X is the scaling dimension of the associated operator. In the Hamiltonian field theory framework, there is a problem in choosing the 'correct' normalisation for the Hamiltonian operator; however von Gehlen *et al* (1985) have pointed out that this may be fixed by looking at the energy-momentum dispersion relation. For the present case, Johnson *et al* (1973) showed that the excitation energy is

$$\Delta E = (\pi/\gamma) \sin \gamma (\sin q_1 + \sin q_2) \quad (28)$$

for a two-'particle' excitation with momenta q_1 and q_2 ; so the Hamiltonian (1) should be divided by a factor $(\pi/\gamma) \sin \gamma$ to give the correct dispersion relation for massless particles in the continuum limit. Hence the scaling dimension corresponding to the amplitude (25) is

$$X = \left(\frac{\pi - \gamma}{2\pi} \right). \quad (29)$$

The operator to which this dimension belongs will be one which produces a transition between the two states involved, e.g. a 'transverse field' $h \sum_{n=1}^N \sigma_n^x$ added to the Hamiltonian (1). Such a Hamiltonian would correspond† to the 8-vertex model in an 'electric' field (Baxter 1982). A strong conjecture for its critical exponent was put forward by Baxter and Kelland (1974):

$$\beta_c = \frac{1}{4}(\pi/\gamma - 1). \quad (30)$$

Using scaling relations between the exponents, our result (29) is found to confirm this conjecture.

A more detailed account of these calculations will be given in a later work.

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† I am indebted to Professor Rodney Baxter for this remark.

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