Calculation of finite-size corrections for the antiferromagnetic Heisenberg chain

1995 J. Phys. A: Math. Gen. 28 3351

(http://iopscience.iop.org/0305-4470/28/12/009)

J. Phys. A: Math. Gen. 28 (1995) 3351–3361. Printed in the UK

Calculation of finite-size corrections for the antiferromagnetic Heisenberg chain

B-D Dörfel† and S Meißner‡

Institut für Physik, Humboldt-Universität, Theorie der Elementarteilchen
Sitz: Invalidenstraße 110, Unter den Linden 6, 10099 Berlin, Germany

Received 23 December 1994, in final form 5 April 1995

Abstract. The finite-size corrections for the anisotropic Heisenberg model in the gap region are calculated using an exact integral representation based on the Bethe ansatz equations (BAE). The energy corrections are determined by saddle-point approximations for states without complex roots. The case of symmetric states is discussed in greater detail.

1. Introduction

The calculation of finite-size corrections for an exactly integrable model is of interest for a number of reasons. For critical models the energy corrections are closely related to important parameters like central charge or operator dimensions and, besides its intrinsic interest, the treatment of lattice models for finite but large N can give important insights into finite-size studies for both integrable and non-integrable theories.

In this paper we will study the anisotropic Heisenberg chain (XXZ) in its antiferromagnetic (non-critical) region; this is an example of an integrable theory with a gap.

Despite the fact that there is, up to now, no relation between the energy corrections for the lowest states and physically interesting parameters, it is worthwhile examining them in detail. We expect the corrections to be more stable compared to the critical region, which makes use of rather involved techniques like the Wiener–Hopf [1, 2] unnecessary. However, the calculations for excited states using saddle-point approximations meet several technical problems that need to be handled with care.

In section 2 we present our definitions, the BAE and their integral representation. Section 3 deals with the saddle-point approximation for the energy corrections of excited states. In section 4 the results are obtained for states without complex roots and in greater detail for the symmetric states present. Our conclusions are contained in section 5.

2. The XXZ model and its BAE

We use the Hamiltonian

$$H = -\tfrac{1}{2}\sum_{i=1}^{N}(\sigma_i^x\sigma_{i+1}^x + \sigma_i^y\sigma_{i+1}^y + \Delta\sigma_i^z\sigma_{i+1}^z) + \tfrac{1}{2}N\Delta \qquad (2.1)$$

† E-mail: doerfel@ifh.de
‡ E-mail: meissner@qft2.physik.hu-berlin.de

with the parametrization

$$\Delta = -\cosh\gamma \qquad \Delta < -1. \tag{2.2}$$

The BAE then takes the form

$$\left(\frac{\sin(\lambda_j + \frac{1}{2}\mathrm{i}\gamma)}{\sin(\lambda_j - \frac{1}{2}\mathrm{i}\gamma)}\right)^N = -\prod_{k=1}^{p}\frac{\sin(\lambda_j - \lambda_k + \mathrm{i}\gamma)}{\sin(\lambda_j - \lambda_k - \mathrm{i}\gamma)} \qquad j = 1\ldots p. \tag{2.3}$$

$|\mathrm{Re}(\lambda_j)| \leqslant \pi/2$ is limited due to periodicity. The energy per site of a state of p magnons is given by

$$E(N) = -\frac{\sinh^2\gamma}{N}\sum_{j=1}^{p}\frac{2}{\cosh\gamma - \cos 2\lambda_j}. \tag{2.4}$$

Following [3] and [4] we introduce the function

$$\phi(z,\alpha) = \mathrm{i}\log\left(\frac{\sin(z+\mathrm{i}\alpha)}{\sin(z-\mathrm{i}\alpha)}\right) \tag{2.5}$$

with its usual cut structure for non-real z. For a real root λ_j the BAE can be rewritten in the form

$$N\phi(\lambda_j, \tfrac{1}{2}\gamma) = \sum_{k=1}^{M}\phi(\lambda_j - \lambda_k, \gamma) + \sum_{l}[\phi(\lambda_j - \xi_l, \gamma) + \phi(\lambda_j - \bar{\xi}_l, \gamma)] + 2\pi I_j \tag{2.6}$$

where the first sum includes all real roots and the second sum includes all complex pairs. For large N they assemble into two-strings

$$\xi = \sigma_c \pm \mathrm{i}\frac{\gamma}{2}$$

the quartets

$$\xi = \sigma_c \pm \mathrm{i}\tau_c \qquad \sigma_c \pm \mathrm{i}(\gamma - \tau_c) \qquad 0 < \tau_c < \gamma$$

and the wide pairs [3]

$$\xi = \sigma_w \pm \mathrm{i}\tau_w \qquad \tau_w > \gamma.$$

In the thermodynamic limit $N \to \infty$ system (2.6) can be easily solved when the positions of the complex roots and holes (generated by 'unoccupied' I_h) are fixed. The density for the ground state is

$$\sigma(\lambda) = \sigma_\infty^{\mathrm{vac}}(\lambda) + \frac{1}{N}[\sigma_h(\lambda) + \sigma_c(\lambda) + \sigma_w(\lambda)] \tag{2.7}$$

with

$$\sigma_\infty^{\mathrm{vac}}(\lambda_i) = \lim_{N\to\infty}\left(\frac{1}{N}\frac{\mathrm{d}I_i}{\mathrm{d}\lambda_i}\right).$$

$$\sigma_\infty^{\mathrm{vac}}(\lambda) = \frac{1}{2\pi}\sum_{m=-\infty}^{+\infty}\frac{\mathrm{e}^{2\mathrm{i}m\lambda}}{\cosh(m\gamma)} = \frac{K(k)}{\pi^2}\,\mathrm{dn}\left(\frac{2K\lambda}{\pi}, k\right). \tag{2.8}$$

The argument of the elliptic modulus k is given by the relation

$$\frac{K'(k)}{K(k)} = \frac{\gamma}{\pi}. \tag{2.9}$$

The density correction for the holes is

$$\sigma_h(\lambda) = \frac{1}{\pi}\sum_{h=1}^{N_h} p(\lambda - \theta_h) \tag{2.10}$$

with

$$p(\lambda) = \frac{1}{2} + 2\sum_{m=1}^{\infty} \frac{\cos 2m\lambda}{e^{2m\gamma}+1}. \tag{2.11}$$

Using

$$\sigma_N(\lambda) = \frac{1}{N}\frac{dI}{d\lambda} \equiv \frac{dz_N}{d\lambda} \tag{2.12}$$

one can define an analogue of the thermodynamic density on the basis of the counting function

$$z_N(\lambda) = \frac{1}{2\pi}\left[\phi(\lambda, \tfrac{1}{2}\gamma) - \frac{1}{N}\sum_{i=1}^{p}\phi(\lambda - \lambda_i, \gamma)\right] \tag{2.13}$$

for finite N. The appropriate limit is provided by equation (2.6).

In [4], exact integral representations have been derived for this density and the energy $E(N)$:

$$\sigma_N(\lambda) - \sigma_\infty(\lambda) = -\int_{-\pi/2}^{\pi/2} \frac{d\mu}{\pi}\, p(\lambda - \mu)\left\{\frac{1}{N}\sum_{i=1}^{M}\delta(\mu - \lambda_i) + \frac{1}{N}\sum_{h=1}^{N_h}\delta(\mu - \theta_h) - \sigma_N(\mu)\right\} \tag{2.14}$$

$$E(N) - E_\infty = -2\pi \sinh\gamma \int_{-\pi/2}^{\pi/2} d\lambda\, \sigma_\infty^{\text{vac}}(\lambda)\left[\frac{1}{N}\sum_{i=1}^{M}\delta(\lambda - \lambda_i) + \frac{1}{N}\sum_{h=1}^{N_h}\delta(\lambda - \theta_h) - \sigma_N(\lambda)\right] \tag{2.15}$$

where E_∞ denotes, as usual, the energy per site calculated in the limit where all finite-size corrections are disregarded. Also,

$$E_\infty = E_\infty^{\text{vac}} + \frac{1}{N}\sum_{h=1}^{N_h}\varepsilon(\theta_h). \tag{2.16}$$

where

$$\varepsilon(\theta_h) = 2\pi\sigma_\infty^{\text{vac}}(\lambda) \tag{2.17}$$

is the energy contribution of a single hole becoming additive in this limit, and E_∞^{vac} is the bulk contribution to the ground state.

The complex roots have formally dropped out; however, one has to keep in mind that their positions influence the real roots and their holes via BAE.

Formulae (2.14) and (2.15) are the starting point of our analysis.

3. The saddle-point approximation

We now consider integrals of the type emerging in equations (2.14) and (2.15):

$$I_N = \int_{-\pi/2}^{\pi/2} d\lambda\, f(\lambda)\left[\frac{1}{N}\sum_{i=1}^{M}\delta(\lambda - \lambda_i) + \frac{1}{N}\sum_{h=1}^{N_h}\delta(\lambda - \theta_h) - \sigma_N(\lambda)\right] \tag{3.1}$$

with a periodic function $f(\lambda+\pi)=f(\lambda)$. With the new variable $z=z_N(\lambda)$ one obtains

$$I_N=\int_0^P \mathrm{d}z\, f(\lambda(z))\left\{\frac{1}{N}\sum_{k=1}^{M+N_h}\delta(z-z_k)-1\right\} \tag{3.2}$$

with $z_k=(k+\frac{1}{2})/N, k=1,2,\ldots,M+N_h=P$. After the Fourier expansion of the δ-function

$$\frac{1}{N}\sum_{k=1}^{M+N_h}\delta(z-z_k)=\sum_{\alpha=-\infty}^{\infty}(-1)^{\alpha}\mathrm{e}^{2\pi\mathrm{i}Nz\alpha} \tag{3.3}$$

we write

$$\begin{aligned} I_N &= -\int_{-\pi/2}^{\pi/2}\mathrm{d}\lambda\, f(\lambda)\sigma_N(\lambda)\left\{\frac{1}{\mathrm{e}^{2\pi\mathrm{i}Nz_N(\lambda-\mathrm{i}0)}+1}+\frac{1}{\mathrm{e}^{-2\pi\mathrm{i}Nz_N(\lambda+\mathrm{i}0)}+1}\right\} \\ &= \sum_{\substack{\alpha=-\infty\\ \alpha\neq 0}}^{\infty}(-1)^{\alpha}\int_{-\pi/2}^{\pi/2}\mathrm{d}\lambda\, f(\lambda)\sigma_N(\lambda)\mathrm{e}^{2\pi\mathrm{i}N\alpha z_N(\lambda)}. \end{aligned} \tag{3.4}$$

In this sum every term can be calculated using a saddle-point approximation for large N where it is dominated by the solutions of

$$\frac{\mathrm{d}z_N}{\mathrm{d}\lambda}=\sigma_N(\lambda)=0 \tag{3.5}$$

in the complex λ-plane.

It is, therefore, useful to deform the integration contour in representation (3.4) in the following way (see figure 1):

$$I_N=-\int_{C_+}\frac{\mathrm{d}\lambda\, f(\lambda)\sigma_N(\lambda)\mathrm{e}^{2\pi\mathrm{i}Nz_N(\lambda)}}{\mathrm{e}^{2\pi\mathrm{i}Nz_N(\lambda)}+1}-\int_{C_-}\frac{d\lambda\, f(\lambda)\sigma_N(\lambda)\mathrm{e}^{-2\pi\mathrm{i}Nz_N(\lambda)}}{\mathrm{e}^{-2\pi\mathrm{i}Nz_N(\lambda)}+1}+\text{ pole contributions.} \tag{3.6}$$

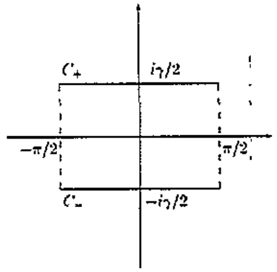

Figure 1. The integration contours C_+ and C_- in the complex λ-plane.

The integrals on the two vertical lines cancel each other and the pole contributions result from possible poles in the upper and lower rectangles respectively (see below).

Returning to the α-expressions

$$I_N=-\sum_{\alpha=1}^{\infty}\int_{C_+}\mathrm{d}\lambda\, f(\lambda)\sigma_N(\lambda)\mathrm{e}^{2\pi\mathrm{i}N\alpha z_N(\lambda)}-\sum_{\alpha=1}^{\infty}\int_{C_-}\mathrm{d}\lambda\, f(\lambda)\sigma_N(\lambda)\mathrm{e}^{-2\pi\mathrm{i}N\alpha z_N(\lambda)}$$

$$+ \text{ pole contributions} \tag{3.7}$$

we see that for real $f(\lambda)$ the second term is the complex conjugate of the first, which we will now consider:

$$\tilde{I}_{N,\alpha} = -\int_{C_+} \mathrm{d}\lambda\, f(\lambda)\sigma_N(\lambda)\mathrm{e}^{2\pi \mathrm{i} N\alpha z_N(\lambda)}. \tag{3.8}$$

We have shown that the replacement of σ_N by σ_∞ and z_N by z_∞ causes an error in $\tilde{I}_{N,\alpha}$ of the order $k_1^{\alpha N}$ with $k_1 = ((1-k')/k)^2$.

In [4], integral (3.6) has been calculated (after the replacement above) for the ground state without further approximation, leading to the energy correction

$$E^{\mathrm{vac}}(N) - E^{\mathrm{vac}}_\infty = -\frac{\sqrt{8k'}}{\pi^{3/2}} K(k) \sinh\gamma \frac{k_1^{N/2}}{N^{3/2}} \left\{1 + \mathrm{O}\left(\frac{1}{N}\right)\right\}. \tag{3.9}$$

We have repeated the calculations for the ground state using a saddle-point approximation and quote the main results. The same method will be used below for excited states where no analytic procedure can be applied.

The solution of $\sigma^{\mathrm{vac}}_\infty(\lambda) = 0$, that is the stationary points, is given by

$$\lambda_0^{\mathrm{vac}} = \tfrac{1}{2}\pi + \tfrac{1}{2}\mathrm{i}\gamma \bmod (\pi, \mathrm{i}\gamma) \tag{3.10}$$

and we introduce $\lambda_0^{\pm} = \mathrm{i}\gamma/2 \pm \pi/2$ for those points on the contour C_+. Also, one has

$$z^{\mathrm{vac}}_\infty(\lambda_0^{\pm}) = \frac{1}{2\pi \mathrm{i}} \ln\sqrt{k_1}. \tag{3.11}$$

After applying the standard saddle-point approximation technique [5] we obtain the asymptotic expansion for $N \to \infty$:

$$\tilde{I}_{N,\alpha} \sim \tfrac{1}{2} k_1^{N\alpha/2} \sum_{\nu=0}^{\infty} \frac{\Gamma(\nu+1)/2}{(2\pi \mathrm{i} N\alpha)^{(\nu+1)/2}} [a_\nu^{(1)} - (-1)^{(\nu+1)/2} a_\nu^{(2)}] \tag{3.12}$$

with the coefficients $a_\nu^{(1)}$ and $a_\nu^{(2)}$ defined as

$$a_\nu^{(1/2)} = \frac{1}{\nu!} \frac{\mathrm{d}^\nu}{\mathrm{d}\lambda^\nu} \left\{ f(\lambda)\sigma^{\mathrm{vac}}_\infty(\lambda) \left(\frac{\lambda - \lambda_0^{\mp}}{\mp\sqrt{\mp(z^{\mathrm{vac}}_\infty(\lambda_0^{\mp}) - z^{\mathrm{vac}}_\infty(\lambda))}} \right)^{\nu+1} \right\} \Bigg|_{\lambda=\lambda_0^{\mp}}. \tag{3.13}$$

The dominant contribution comes from the term with $\alpha = 1$, so we will neglect the other terms with higher α.

For the energy from relation (2.15), the result (3.9) follows where the first non-vanishing correction comes from $\nu = 2$. Up to now the pole contributions from equation (3.6) have been neglected. Using

$$\sigma_N(\lambda)\frac{\mathrm{e}^{2\pi \mathrm{i} N z_N(\lambda)}}{\mathrm{e}^{2\pi \mathrm{i} N z_N(\lambda)} + 1} = \frac{1}{2\pi \mathrm{i} N} \frac{\mathrm{d}}{\mathrm{d}\lambda} \log(1 + \mathrm{e}^{2\pi \mathrm{i} N z_N(\lambda)}) \tag{3.14}$$

and the definition of $z_N(\lambda)$ one obtains the BAE poles for all complex roots with $\mathrm{Im}(\xi_l) < \gamma/2$. Their residuals are given by

$$\begin{aligned} 2\pi \mathrm{i}\, \mathrm{res}_{\xi_l} \left(\sigma_N(\lambda)\frac{\mathrm{e}^{2\pi \mathrm{i} N z_N(\lambda)}}{\mathrm{e}^{2\pi \mathrm{i} N z_N(\lambda)} + 1}\right) &= \oint_{\xi_l} \mathrm{d}\lambda\, \sigma_N(\lambda) \frac{\mathrm{e}^{2\pi \mathrm{i} N z_N(\lambda)}}{\mathrm{e}^{2\pi \mathrm{i} N z_N(\lambda)} + 1} \\ &= \frac{1}{2\pi \mathrm{i} N} \oint_{-1} \mathrm{d}y\, \frac{1}{1+y} \\ &= \frac{1}{N}. \end{aligned} \tag{3.15}$$

From the numerator in equation (3.14) we have another type of pole at $\lambda = \xi_k + i\gamma$ for all complex ξ_k with $\mathrm{Im}(\xi_k + i\gamma) < \gamma/2$, which has residuals $-N^{-1}$. Thus, only the close roots contribute and which for large N group in quartets. The pole contributions in equation (3.6) are, therefore, given by

$$\frac{1}{N}\sum_{l,k}(f(\xi_l) - f(\xi_k + \mathrm{i}\gamma)). \tag{3.16}$$

Taking into account the formation of quartets, we are left with the deviations from an exact quartet structure for finite N. A detailed analysis of those terms can be given only after the corrections to the higher level BAE have been found. This fact motivates us to restrict our analysis to states without complex roots.

We now return to equation (3.8) with $N = \infty$ and consider the first general excited states. $z_\infty(\lambda)$ is no longer equal to $z_\infty^{\mathrm{vac}}(\lambda)$ but has corrections corresponding to

$$\begin{aligned} z_\infty(\lambda) = z_\infty^{\mathrm{vac}} + \frac{1}{2\pi N}\Bigg[\sum_{h=1}^{N_h}\phi(\lambda-\theta_h,\gamma) - \sum_l\{\phi(\lambda-\xi_l,\gamma)+\phi(\lambda-\bar{\xi}_l,\gamma)\} \\ - \int_{-\pi/2}^{\pi/2}(\sigma_h(\mu)+\sigma_{\mathrm{c}}(\mu)+\sigma_{\mathrm{w}}(\mu))\phi(\lambda-\mu,\gamma)\,\mathrm{d}\mu\Bigg]. \end{aligned} \tag{3.17}$$

With the notation

$$\begin{aligned} h(\lambda) = \mathrm{i}\Bigg[\sum_{h=1}^{N_h}\phi(\lambda-\theta_h,\gamma) - \sum_l\{\phi(\lambda-\xi_l,\gamma)+\phi(\lambda-\bar{\xi}_l,\gamma)\} \\ - \int_{-\pi/2}^{\pi/2}(\sigma_h(\mu)+\sigma_{\mathrm{c}}(\mu)+\sigma_{\mathrm{w}}(\mu))\phi(\lambda-\mu,\gamma)\,\mathrm{d}\mu\Bigg] \end{aligned} \tag{3.18}$$

we can rewrite (3.8) as

$$\begin{aligned} \tilde{I}_{N,\alpha} &= -\int_{C_+}\mathrm{d}\lambda\, f(\lambda)\sigma_\infty(\lambda)\mathrm{e}^{2\pi\mathrm{i}N\alpha z_\infty^{\mathrm{vac}}(\lambda)+\alpha h(\lambda)} + \mathrm{O}(k_1^{\alpha N}) \\ &= -\int_{C_+}\mathrm{d}\lambda\, f(\lambda)\mathrm{e}^{\alpha h(\lambda)}\sigma_\infty(\lambda)\mathrm{e}^{2\pi\mathrm{i}N\alpha z_\infty^{\mathrm{vac}}(\lambda)} + \mathrm{O}(k_1^{\alpha N}). \end{aligned} \tag{3.19}$$

Thus, this integral can be treated by our former method based on the saddle points of $z_\infty^{\mathrm{vac}}(\lambda)$ using the replacement $f(\lambda) \to f(\lambda)\mathrm{e}^{h(\lambda)}$ if $\mathrm{e}^{h(\lambda)}$ is holomorphic in a region containing C_+. Furthermore, $\sigma_\infty(\lambda)$ now includes terms depending on N which must be included in the analysis. We have checked that all those requirements are fulfilled.

4. Energy corrections for states with real roots

Motivated by the above analysis, we consider states without complex roots so that holes in the real root distribution are the only excitations left. We analyse the analytical properties of $\sigma_h(\lambda)$ defined through equations (2.10) and (2.11).

With the definitions

$$\begin{aligned} z_1 &= \mathrm{e}^{-2\gamma+2\mathrm{i}\lambda} \\ z_2 &= \mathrm{e}^{-2\gamma-2\mathrm{i}\lambda} \\ q &= \mathrm{e}^{-2\gamma} \qquad 0 < |q| < 1 \end{aligned} \tag{4.1}$$

we derive

$$p(\lambda) = -\tfrac{1}{2} + \tfrac{1}{2}[{}_2\Phi_1(q, -1, -q; q, z_1) + {}_2\Phi_1(q, -1, -q; q, z_2)] \qquad (4.2)$$

where ${}_2\Phi_1(a_1, a_2, b_1; q, z)$ is the q-analogue of the well known hypergeometric function ${}_2\Phi_1(a_1, a_2, b_1; z)$ [6]. We only need the case

$${}_2\Phi_1(q, -1, -q; q, -z) = 1 + 2\sum_{m=1}^{\infty} \frac{z^m}{1+q^m}. \qquad (4.3)$$

The analytic properties of these basic hypergeometric series are found in [7]. It now follows that $\sigma_h(\lambda)$ is a holomorphic function in the region of integration.

Now, we can write down the energy correction

$$\begin{aligned} E(N) - E_\infty &= 2\pi \sinh\gamma \int_{C_+} \mathrm{d}\lambda\, (\sigma_\infty^{\mathrm{vac}}(\lambda))^2 \mathrm{e}^{h(\lambda)} \mathrm{e}^{2\pi \mathrm{i} N z_\infty^{\mathrm{vac}}(\lambda)} \\ &\quad + \frac{2\pi \sinh\gamma}{N} \int_{C_+} \mathrm{d}\lambda\, \sigma_\infty^{\mathrm{vac}}(\lambda)\sigma_h(\lambda) \mathrm{e}^{h(\lambda)} \mathrm{e}^{2\pi \mathrm{i} N z_\infty^{\mathrm{vac}}(\lambda)} + \mathrm{cc} + \mathrm{O}(k_1^N). \end{aligned} \qquad (4.4)$$

To produce an expression like (3.12) we use (3.13) for the general coefficients. For the coefficients of the first term in equation (4.4) we obtain

$$\begin{aligned} \tilde{a}_\nu^{(1/2)} &= \frac{1}{\nu!} \frac{\mathrm{d}^\nu}{\mathrm{d}\lambda^\nu} \left\{ (\sigma_\infty^{\mathrm{vac}}(\lambda))^2 \mathrm{e}^{h(\lambda)} \left(\frac{\lambda - \lambda_0^\mp}{\mp\sqrt{\mp(z_\infty^{\mathrm{vac}}(\lambda_0^\mp) - z_\infty^{\mathrm{vac}}(\lambda))}} \right)^{\nu+1} \right\} \Bigg|_{\lambda=\lambda_0^\mp} \\ &= \frac{1}{\nu!} \sum_{i=0}^{\nu} a_\nu^{(1/2)} \frac{\mathrm{d}^{\nu-i}}{\mathrm{d}\lambda^{\nu-i}} \left\{ \mathrm{e}^{h(\lambda)} \left(\frac{\lambda - \lambda_0^\mp}{\mp\sqrt{\mp(z_\infty^{\mathrm{vac}}(\lambda_0^\mp) - z_\infty^{\mathrm{vac}}(\lambda))}} \right)^{\nu-i} \right\} \Bigg|_{\lambda=\lambda_0^\mp} \end{aligned} \qquad (4.5)$$

where in the last line $a_\nu^{(1/2)}$ are the coefficients for the ground state which have been calculated previously. The leading contribution is given by $\nu = 2$ with $\tilde{a}_2^{(1/2)} = \mathrm{e}^{h(\lambda_0^\mp)} a_2^{(1/2)}$ and causes a term of order $k_1^{N/2} N^{-3/2}$. The analysis of the second term in equation (4.4) gives a leading behaviour of order $k_1^{N/2} N^{-5/2}$ confirming the superficial analysis that these terms are suppressed by $1/N$. Hence,

$$\begin{aligned} E(N) - E_\infty &= 2\pi \sinh\gamma\, \tfrac{1}{2}(a_2^{(1)} \mathrm{e}^{h(\lambda_0^-)} + a_2^{(2)} \mathrm{e}^{h(\lambda_0^+)}) \frac{k_1^{N/2}}{(2\pi \mathrm{i} N)^{3/2}} + \mathrm{cc} + \mathrm{O}\left(\frac{k_1^N}{N^{5/2}}\right) \\ &= -\frac{\sqrt{8k'}}{\pi^{3/2}} K(k) \sinh\gamma \frac{k_1^{N/2}}{N^{3/2}} \left\{ \mathrm{e}^{h(\lambda_0^-)} + \overline{\mathrm{e}^{h(\lambda_0^-)}} + \mathrm{O}\left(\frac{1}{N}\right) \right\}. \end{aligned} \qquad (4.6)$$

Finally, we calculate $\mathrm{e}^{h(\lambda_0^-)}$. Recalling equation (3.18) we have

$$\exp(h(\lambda)) = \prod_{h=1}^{N_h} \exp(\tilde{h}(\lambda, \theta_h)) \qquad (4.7)$$

$$\tilde{h}(\lambda, \theta_h) = \mathrm{i}\left[\phi(\lambda - \theta_h) - \frac{1}{\pi} \int_{-\pi/2}^{\pi/2} p(\mu - \theta_h)\phi(\lambda - \mu)\, \mathrm{d}\mu \right]. \qquad (4.8)$$

It is straightforward to use a Fourier series expansion:

$$\tilde{h}(\lambda, \theta_h) = \mathrm{i} \sum_{m=-\infty}^{\infty} c_m(y, \gamma) \frac{\mathrm{e}^{2|m|\gamma}}{\mathrm{e}^{2|m|\gamma}+1} \mathrm{e}^{2\mathrm{i}m(x-\theta_h)}$$

$$c_m(y, \gamma) = \begin{cases} \frac{\mathrm{i}}{m}\left((-1)^m - \mathrm{e}^{-2my}\mathrm{e}^{-2|m|\gamma}\right) & m \neq 0 \\ \pi + 2\mathrm{i}y & m = 0 \end{cases} \tag{4.9}$$

for $\lambda = x + \mathrm{i}y$. Further, for $\lambda = \lambda_0^- = -\pi/2 + \mathrm{i}\gamma/2$ one has

$$\tilde{h}(\lambda_0^-, \theta_h) = 2F_3(\theta_h) - \frac{\gamma}{2} + \mathrm{i}\left[\frac{\pi}{2} + 2F_1(\theta_h) + 2F_2(\theta_h)\right] \tag{4.10}$$

with the new functions

$$F_1(\theta_h) = \sum_{m=1}^{\infty} \frac{1}{m} \frac{\mathrm{e}^{2m\gamma}}{\mathrm{e}^{2m\gamma}+1} \sin 2m\theta_h$$

$$F_2(\theta_h) = \sum_{m=1}^{\infty} \frac{(-1)^m}{m} \frac{\cosh m\gamma}{\mathrm{e}^{2m\gamma}+1} \sin 2m\theta_h$$

$$F_3(\theta_h) = \sum_{m=1}^{\infty} \frac{(-1)^m}{m} \frac{\sinh m\gamma}{\mathrm{e}^{2m\gamma}+1} \cos 2m\theta_h. \tag{4.11}$$

To our knowledge only F_2 is related to any known functions [8]:

$$F_2(x) = -\tfrac{1}{2} \arctan\left(\frac{\mathrm{e}^{-\gamma}\sin 2x}{1+\mathrm{e}^{-\gamma}\cos 2x}\right). \tag{4.12}$$

Thus,

$$\exp(h(\lambda_0^-)) + \overline{\exp(h(\lambda_0^-))} = 2(-1)^{N_h/2} \exp\left(-\frac{N_h}{2}\gamma\right) \exp\left(2\sum_{h=1}^{N_h} F_3(\theta_h)\right) \times \cos\left(\sum_{h=1}^{N_h}[F_1(\theta_h) + F_2(\theta_h)]\right). \tag{4.13}$$

Together with equation (4.6) this gives the final answer to our problem: the leading energy correction for states with an arbitrary distribution of holes.

Making the result more evident, we consider low excitations ($N_h = 2$) and symmetric states ($\theta_1 = -\theta_2$). The odd functions F_1 and F_2 drop out and we are left with the even function $F_3(\theta), 0 \leqslant \theta \leqslant \pi/2$, which will be analysed below. For these states we have obtained

$$E(N) - E_\infty = \frac{\sqrt{8k'}}{\pi^{3/2}} K(k) \sinh\gamma \frac{k_1^{N/2}}{N^{3/2}} \left\{2\mathrm{e}^{-\gamma}\exp(4F_3(\theta)) + \mathrm{O}\left(\frac{1}{N}\right)\right\}. \tag{4.14}$$

With the help of formula (4.3), $F_3(\theta)$ can be defined using integrals of basic hypergeometric series as

$$F_3(\theta) = \frac{1}{8z_1}\int_0^{z_1} {}_2\Phi_1(q, -1, -q; q, z)\,\mathrm{d}z - \frac{1}{8z_2}\int_0^{z_2} {}_2\Phi_1(q, -1, -q; q, z)\,\mathrm{d}z + \frac{1}{8z_3}\int_0^{z_3} {}_2\Phi_1(q, -1, -q; q, z)\,\mathrm{d}z - \frac{1}{8z_4}\int_0^{z_4} {}_2\Phi_1(q, -1, -q; q, z)\,\mathrm{d}z$$

$$z_1 = -\mathrm{e}^{-\gamma+2\mathrm{i}\theta}$$

$$z_2 = -\mathrm{e}^{-3\gamma+2\mathrm{i}\theta}$$

$$z_3 = -e^{-\gamma-2i\theta}$$
$$z_4 = -e^{-3\gamma-2i\theta}$$
$$q = e^{-2\gamma} \qquad 0 < |q| < 1. \tag{4.15}$$

F_3 is, therefore, analytic as long as $|z_i| < 1$ and $\gamma > 0$.

For its asymptotic behaviour with respect to γ it is easier to use formula (4.11). For large γ one can state that

$$F_3(\theta) = -\tfrac{1}{2}e^{-\gamma}\cos 2\theta + O(e^{-2\gamma}). \tag{4.16}$$

As $\gamma \to 0$ we expect singularities near the phase transition point because of the vanishing gap; this is where our method of calculation breaks down. We propose the regularization $m\gamma \to m\gamma e^{-\epsilon m} = \beta$ and to expand in a series of β. This yields an asymptotic expansion of the form

$$F_3(\theta) = \sum_{k=1}^{\infty} a_k \gamma^k \lim_{\epsilon\to 0} \sum_{m=1}^{\infty} (-1)^m m^{k-1} e^{-\epsilon m k} \cos 2m\theta. \tag{4.17}$$

For small k the coefficients a_k can be determined explicitly [9] and

$$F_3(\theta) = -\tfrac{1}{4}\gamma + \frac{1}{4}\left(\frac{1}{1+\cos 2\theta}\right)\gamma^2 + O(\gamma^3). \tag{4.18}$$

We have numerically calculated the values of the functions $F_3(\theta)$ for different γ. The results are shown in figures 2–4.

From figures 3 and 4 one can see that F_3 is close to its asymptotics except, of course, for the region $\gamma \sim 1$. In general, the whole function becomes flatter with increasing γ. Both effects can also be seen from figure 5, where we show F_3 as a function of γ for fixed θ. Figure 5 also shows that the general structure in the (γ–θ) plane is rather involved.

With the asymptotics of $F_3(\theta)$ it is a straightforward task to look at the behaviour of the energy correction in equation (4.14) for both limits:

$$E(N) - E_\infty = \sqrt{\frac{2}{\pi}}\,(2e^{-\gamma/2})^N \frac{1}{N^{3/2}}\{1 - 2e^{-\gamma}\cos 2\theta + \text{hoc}\} \qquad \text{for } \gamma \to \infty \tag{4.19}$$

and

$$E(N) - E_\infty = 4\sqrt{2\pi}\, e^{-\pi^2/\gamma} \frac{1}{N^{3/2}}\left\{1 - \gamma + \frac{1}{1+\cos 2\theta}\gamma^2 + \text{hoc}\right\} \qquad \text{for } \gamma \to 0. \tag{4.20}$$

Formula (4.20) is only valid for $N \to \infty$ so that $k_1^{N/2}$ can still be neglected. That is just what we expect for smaller γ; one needs larger and larger N to select the leading term.

Formulae (4.6) and (4.14) can be compared with direct numerical diagonalization of short chains. To identify the states it is useful to recall the relation between the rapidity of a hole θ and its momentum contribution [3]:

$$p_h(\theta) = \text{am}\left[\frac{2K\theta}{\pi}, k\right] - \frac{\pi}{2} \tag{4.21}$$

$$P_\infty = P_\infty^{\text{vac}} + \frac{1}{N}\sum_{h=1}^{N_h} p_h(\theta_h) \tag{4.22}$$

which are completely analogous to equations (2.16) and (2.17).

The easiest way to proceed is to use equation (4.14) with $\theta = \pi/2$; this gives the energy correction for the lowest state with $S_z = 1$.

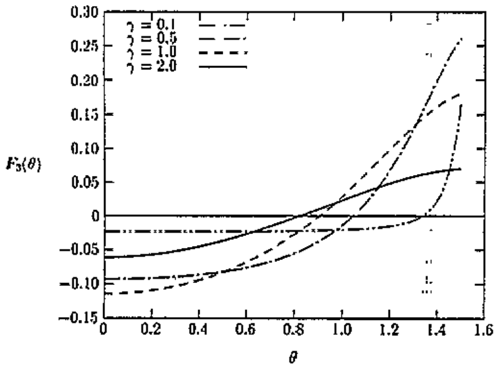

Figure 2. The function $F_3(\theta)$ for $0 \leqslant \theta \leqslant \pi/2$ and different γ.

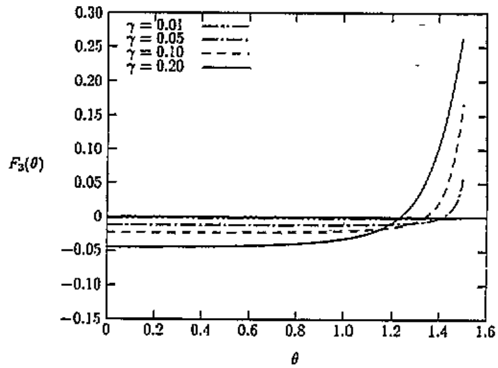

Figure 3. As for figure 2 but for small γ.

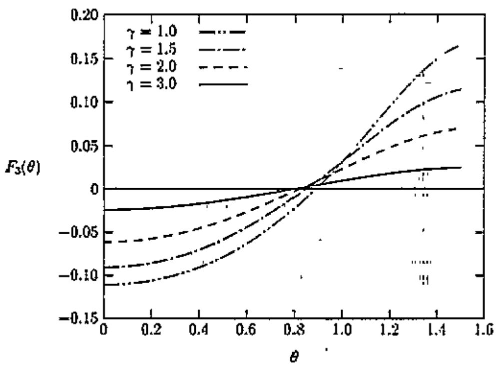

Figure 4. As for figure 2 but for large γ.

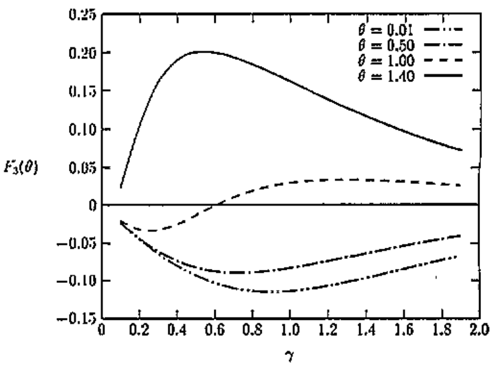

Figure 5. The function $F_3(\theta)$ as function of γ for $\gamma > 0$ and fixed values of θ.

5. Conclusions

We have calculated the finite-size energy corrections for the anisotropic Heisenberg chain (XXZ) in the antiferromagnetic (non-critical) region for weakly excited states. The main result is that this correction is qualitatively of the same value in order of N as for the ground state. The dependence on the hole parameters can be factorized (formulae (4.6) and (4.13)) and includes an oscillating and an exponential factor, as well as a general factor (depending on N_h). Both factors are defined using non-elementary functions described by Fourier series.

We have demonstrated that in the gap region the saddle-point approximation works well but has to be treated with care. For states with complex roots we cannot exclude the influence of pole terms; these can be handled only after the corrections to higher level BAE are calculated.

The corrections arising from the fact that, for finite N, the hole parameters θ_h cannot be fixed arbitrarily but are discrete numbers separated by $O(1/N)$ have not been taken into account. Due to analycity with respect to θ_h they produce next-to-leading corrections to those calculated above.

References

[1] Woynarovich F and Eckle H P 1987 *J. Phys. A: Math. Gen.* **20** 97

[2] Hamer C J, Quispel G R W and Batchelor M T 1987 *J. Phys. A: Math. Gen.* **20** 5677

[3] Babelon O, de Vega H J and Viallet C M 1983 *Nucl. Phys.* B **220** 13

[4] de Vega H J and Woynarovich F 1985 *Nucl. Phys.* B **251** 439

[5] Doetsch G 1971 *Handbuch der Laplace Transformation* vol 1–3 (Basel: Birkhäuser)

[6] Bateman H and Erdelyi A 1955 *Higher Transcendental Functions* (New York: McGraw-Hill)

[7] Gasper G and Rahman M 1990 *Basic Hypergeometric Series* (Cambridge: Cambridge University Press)

[8] Gradstein I S and Ryshik I M 1981 *Summen-, Produkt-, und Integraltafeln* (Frankfurt: Harri Deutsch)

[9] Meißner S 1994 Finite-Size-Korrekturen zu schwach angeregten Zuständen des antiferromagnetischen Heisenberg-Modells *Diploma Thesis* Humboldt-Universität zu Berlin