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Solution of the Bethe ansatz equations with complex roots for finite size: the spin $S \geqslant 1$ isotropic and anisotropic chains

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Abstract. The Bethe ansatz equations for spin-S ($S \geqslant 1$) integrable vertex models (and magnetic chains) where the ground state is formed by complex roots are investigated for finite-size N. It is shown that the finite-size corrections to the imaginary parts of the roots (Bethe strings) for $N \gg 1$ are given by $\alpha_m/[N\sigma(\eta)]$ where η is the real part of the roots, $\sigma(\eta)$ is the density of the real parts, and m is the index of a root within a string. The constants α_m are determined by a set of algebraic equations, and are given explicitly by

$$\alpha_m = \frac{1}{\pi} \ln\left(\frac{\cos[\frac{1}{2}\pi(S-m-1)/(S+1)]}{\cos[\frac{1}{2}\pi(S-m)/(S+1)]}\right).$$

For the best known, $S=1$, case $\alpha_0 = \ln 2/(2\pi)$.

These results are found through a generalisation of the Euler-Maclaurin formula including non-analytic contributions in N^{-1} which turn out to be essential in the solution of the present problem.

1. Introduction

The Bethe ansatz provides through the solution of a system of coupled algebraic equations the exact eigenvalues and eigenvectors of an integrable model. (For a recent review see de Vega (1989).)

For antiferromagnetic regimes the explicit solution of the Bethe ansatz equations (BAE) is straightforward in the thermodynamic limit only. The analytic resolution of the BAE for a finite number of sites is a formidable task as soon as the number of sites N is not very small. A systematic procedure to solve the BAE for large but finite N and to analytically compute asymptotic expansions for the physical quantities has been proposed by de Vega and Woynarovich (1985). This method has been elaborated and generalised for different cases by Woynarovich and Eckle (1987), Batchelor *et al* (1987), de Vega and Karowski (1987), Woynarovich (1987) and de Vega (1987, 1988). In all the cases treated in the above works the ground state is formed by a set of *real* roots.

In the spin-S integrable models with $S \geqslant 1$ (Takhtadzhyan 1982, Kulish and Reshetikhin 1981, Babujan 1983) the ground-state solution of the BAE is given by a set of *complex* roots. Therefore, these models are outside the scope of the analytic methods developed so far. The present paper is a first step to the analytic solution of the BAE for large N when the ground state is formed by complex roots. We formulate

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our method for those models for which in the thermodynamic limit the roots form Bethe strings, i.e. sets of roots with common real parts and imaginary parts differing from each other by a constant. For an isotropic model

$$\eta_j + \mathrm{i}(S - \tfrac{1}{2} - m) \qquad j = 1, 2, \ldots, N/2 \quad m = 0, 1, \ldots, 2S-1. \tag{1.1}$$

For finite size both the real and imaginary parts of the roots are modified by finite-N effects

$$\eta_j^m + \mathrm{i}(S - \tfrac{1}{2} - m) + \mathrm{i}\delta_j^m. \tag{1.2}$$

Neglecting the finite-size effects in the imaginary parts (δ_j^m) the finite-size corrections for the real parts can be treated by standard methods (see the references above). This approximation is, however, not sufficient, as clearly indicated by the fact that calculating the central charge in this way yields $c = 1$ for all spins, which is clearly a wrong result (Alcaraz and Martins 1988, Avdeev and Dörfel 1987, de Vega 1987).

We present here a method for analytically calculating the finite-size effects on δ_j^m. We find that unlike the case where strings like (1.2) appear as excitations (Bethe 1931, Takahashi 1971) the δ_j^m are not exponentially small in N but much larger, $\delta_j^m = \mathrm{O}(1/N)$.

The basic step in calculating finite-size corrections is to approximate the sums over the roots of the BAE by integrals plus correction terms. These correction terms are given by the Euler-Maclaurin formula or related formulae. These formulae assume analytic behaviour of the summand as a function of the summation variable. In the case of strings of type (1.2), these analyticity requirements do not hold: in the summands there are branch points or poles at distances $\mathrm{O}(\delta)$ from the real axis, and so these terms need special care. In appendix 1 we give a generalisation of the Euler-Maclaurin formula including the effects (non-analytic in $1/N$) of these singularities (equations (A1.10) with (A1.9) and (A1.15)).

With the help of this generalised Euler-Maclaurin formula we calculate the first correction in $1/N$ to the $N = \infty$ form of the BAE. The solution of these equations yields the correction to the imaginary parts of the Bethe strings

$$\delta^m(\eta) \underset{N \gg 1}{=} \alpha_m / [2N\sigma(\eta)] \tag{1.3}$$

where η stands for the real part of the root and $\sigma(\eta)$ is the density of real parts. The constants α_m follow as solutions of a set of algebraic equations

$$\alpha_m = \frac{1}{\pi} \ln\left(\frac{\cos[\frac{1}{2}\pi(S - m - 1)/(S+1)]}{\cos[\frac{1}{2}\pi(S-m)/(S+1)]} \right). \tag{1.4}$$

A formula like (1.3) was proposed by Avdeev and Dörfel (1987) on grounds of numerical calculations. The numerical values for α_0 in the $S = 1$ and $S = \frac{3}{2}$ cases given by them are in agreement with our exact analytic results.

Throughout the calculation we concentrate on the finite-size corrections to the imaginary parts of the BAE roots, i.e. on $\delta^m(\eta)$. Therefore we neglect the finite-size corrections to all other quantities which do not contribute to order $1/N$ in $\delta^m(\eta)$.

Our results hold for roots where the real part is not too close to the ends of the distribution (that is, $\eta \leqslant (1/\pi) \ln N$, i.e. $\sigma(\eta) \geqslant 1/N$). Nevertheless (1.3) yields good results even when $\eta \approx (\ln N)$!

In section 2 we treat the $S = 1$ case, both the isotropic (rational) and the anisotropic (trigonometric) one. Section 3 is devoted to the general case of arbitrary spin $S > 1$ (isotropic). The generalisation of the Euler-Maclaurin formula to include the non-analytic corrections in $1/N$ is derived in appendix 1. Appendix 2 contains the general solution of the algebraic equations yielding α_m.

2. The $S=1$ Bethe ansatz equations

2.1. *The isotropic case*

The BAE for the $S=1$ integrable rational model as well as for the $S=1$ integrable XXX chain (Takhtadzhyan 1982) can be written as

$$\left(\frac{\lambda_j - \mathrm{i}}{\lambda_j + \mathrm{i}}\right)^N = -\prod_{k=1}^{r} \frac{\lambda_j - \lambda_k - \mathrm{i}}{\lambda_j - \lambda_k + \mathrm{i}} \tag{2.1}$$

where the number of roots r for the ground state is $r=N$. The roots of (2.1) appear in complex conjugate pairs

$$\lambda_j^{\mp} = \eta_j \pm \mathrm{i}(\tfrac{1}{2} + \delta_j). \tag{2.2}$$

Here we singled out the imaginary part $\pm\frac{1}{2}$ that corresponds to the string hypothesis (Takhtadzhyan 1982, Kulish and Reshetikhin 1981, Babujan 1983) valid for the $N=\infty$ limit. For finite size we allow for a correction δ_j. This correction is expected to be small except for roots with η_j near the end of the distribution ($|\mathrm{Re}\,\eta_j| \leqslant \ln N$). We also assume $\delta_j > 0$. The consistency of these assumptions is verified in the course of the derivation and in the final results.

Inserting (2.2) into (2.1) yields

$$\left(\frac{\eta_j + \mathrm{i}\delta_j - \mathrm{i}/2}{\eta_j + \mathrm{i}\delta_j + \mathrm{i}/2}\right)^N \left(\frac{\eta_j + \mathrm{i}\delta_j + \mathrm{i} - \mathrm{i}/2}{\eta_j + \mathrm{i}\delta_j + \mathrm{i} + \mathrm{i}/2}\right)^N$$
$$= -\prod_{k=1}^{N/2} \frac{\eta_j - \eta_k + \mathrm{i}(\delta_j - \delta_k) - \mathrm{i}}{\eta_j - \eta_k + \mathrm{i}(\delta_j - \delta_k) + \mathrm{i}} \, \frac{\eta_j - \eta_k + \mathrm{i}(\delta_j + \delta_k + 1) - \mathrm{i}}{\eta_j - \eta_k + \mathrm{i}(\delta_j + \delta_k + 1) + \mathrm{i}} \tag{2.3}$$

where we used the result

$$\frac{\eta_j + \mathrm{i}/2 - \mathrm{i}}{\eta_j + \mathrm{i}/2 + \mathrm{i}} = \frac{\eta_j - \mathrm{i}/2}{\eta_j + \mathrm{i}/2} \, \frac{\eta_j + \mathrm{i} - \mathrm{i}/2}{\eta_j + \mathrm{i} + \mathrm{i}/2}. \tag{2.4}$$

Taking the logarithm of (2.3) yields

$$N\Psi_{1/2}(\eta_j + \delta_j) - \sum_{k=1}^{N/2} \Psi_1(\eta_j - \eta_k + \mathrm{i}(\delta_j - \delta_k)) + N\Phi_{1/2}(\eta_j + \delta_j + \mathrm{i})$$
$$- \sum_{k=1}^{N/2} \Phi_1(\eta_j - \eta_k + \mathrm{i}(\delta_j + \delta_k) + \mathrm{i}) = 2\pi I_j \tag{2.5}$$

where $I_j = \frac{1}{2}(N/2 + 1) \pmod 1$ and

$$\Psi_a(x) = \frac{1}{\mathrm{i}} \ln \frac{1 + \mathrm{i}x/a}{1 - \mathrm{i}x/a} = 2\tan^{-1}\frac{x}{a}$$
$$\Phi_a(x) = \frac{1}{\mathrm{i}} \ln \frac{x - \mathrm{i}a}{x + \mathrm{i}a}. \tag{2.6}$$

(Note that $\Psi_a(z)$ and $\Phi_a(z)$ differ merely in the cut structure: for $\Phi_a(z)$ the cut runs between the two branch points $z = \pm\mathrm{i}a$ while for $\Psi_a(z)$ the cuts run from the branch points $z=\pm ia$ to $\mathrm{Im}\, z=\pm\infty$.) For $N\to\infty$ in the usual procedure all the summands in (2.5) are replaced by integrals. To approximate, however, the second sum in (2.5)

$$X(\eta_j)=\sum_{k=1}^{N/2}\Phi_1(\eta_j-\eta_k+\mathrm{i}(\delta_j+\delta_k)+\mathrm{i}) \tag{2.7}$$

by an integral is a delicate matter. For $N\to\infty$, $\delta\to 0$ and the terms $k\approx j$ diverge due to the branch point of Φ_1 at i. The naive $N\to\infty$ approximation of (2.7) is

$$N\int_{-\infty}^{\infty}\Phi_1(\eta_1-\eta'+\mathrm{i}+\mathrm{i}0)\sigma(\eta')\,\mathrm{d}\eta' \tag{2.8}$$

with $\sigma(\eta)$ being the density of the η_j. This approximation is sufficient in the $N=\infty$ limit, but to establish the N dependence of δ as $N\to\infty$ we also have to correctly calculate the contributions of the $k\approx j$ terms diverging at $\delta=0$.

As one can see from (2.6) and (2.7), the most important (nearest to the real axis) singularity of the summand in (2.7) is situated at

$$\eta_j-\eta_k+\mathrm{i}(\delta_j+\delta_k)=0. \tag{2.9}$$

Since δ_j and δ_k are small (of order $1/N$ as we shall see) those terms are indeed dangerous when $|\eta_j-\eta_k|\ll 1$. In these terms we can approximate

$$\eta_j-\eta_k\approx(j-k)/[N\sigma(\eta_j)] \qquad \delta_j\approx\delta_k. \tag{2.10}$$

This implies that in the variable k (the summation variable) the singularity (a logarithmic branch point) is at

$$k=j+\mathrm{i}\alpha \qquad \alpha\equiv 2N\sigma(\eta_j)\delta_j. \tag{2.11}$$

In evaluating the contribution of this singularity it will be also important to know (appendix 1) that the jump when crossing the cut starting from $k=j+\mathrm{i}\alpha$ is

$$\Delta=-2\pi\mathrm{i}. \tag{2.12}$$

The presence of such a branch point in the summands of (2.7) as a function of k yields contributions non-analytic in $1/N$, which are outside the scope of the standard Euler-Maclaurin formula. In appendix 1 we derive a generalisation of the Euler-Maclaurin formula which correctly takes account of such singularities (equation (A1.10)).

Inserting (A1.10), including the non-analytic term (A1.9), into (2.7) yields

$$X(\eta)=N\int_{-\infty}^{\infty}\mathrm{d}\eta'\,\sigma(\eta')\Phi_1(\eta-\eta'+\mathrm{i}+\mathrm{i}(\delta(\eta)+\delta(\eta')))$$
$$-\mathrm{i}\ln[1-\exp(-2\pi\alpha(\eta))]+\mathrm{O}(1/N). \tag{2.13}$$

We have used the result that $u+\mathrm{i}v$ in (A1.9) equals $j+\mathrm{i}\alpha$ (equation (2.11)) with j being an integer. It has also been supposed that there exists a continuous function $\delta(\eta)$ for which $\delta(\eta_j)=\delta_j$. By this, $\alpha(\eta)$ is given by

$$\alpha(\eta)=2N\sigma(\eta)\delta(\eta).$$

The $\mathrm{O}(1/N)$ term in (2.13) includes all the analytic finite-size corrections. (Note that the second term on the RHS is explicitly non-analytic in $1/N$; there is a significant singularity of the type $\exp(A/z)$ with $z=1/N$.)

Inserting (2.13) into (2.5) and approximating the first term in (2.5) by the appropriate integral (in this sum the singularities are far enough from the real axis to give negligible contributions), we arrive at

$$\Psi_{1/2}[\eta_j+\mathrm{i}\delta(\eta_j)]-\int_{-\infty}^{\infty}\mathrm{d}\eta'\,\sigma(\eta')\Psi_1[\eta_j-\eta'+\mathrm{i}\delta(\eta_j)-\mathrm{i}\delta(\eta')]$$
$$+\Phi_{1/2}[\eta_j+\mathrm{i}+\mathrm{i}\delta(\eta_j)]-\int_{-\infty}^{\infty}\mathrm{d}\eta'\,\sigma(\eta')\Phi_1(\eta_j-\eta'+\mathrm{i}\delta(\eta_j)+\mathrm{i}\delta(\eta')+\mathrm{i})$$
$$+(\mathrm{i}/N)\ln[1-\exp(-2\pi\alpha(\eta_j))]=2\pi I_j/N. \tag{2.14}$$

Expanding (2.14) in powers of δ yields

$$\Psi_{1/2}(\eta_j)-\int_{-\infty}^{\infty}\mathrm{d}\eta'\,\sigma(\eta')\Psi_1(\eta_j-\eta')+\Phi_{1/2}(\eta_j+\mathrm{i})-\int_{-\infty}^{\infty}\mathrm{d}\eta'\,\sigma(\eta')\Phi_1(\eta_j-\eta'+\mathrm{i}+\mathrm{i}0)$$
$$+\Bigg[\Psi'_{1/2}(\eta_j)-\int_{-\infty}^{\infty}\mathrm{d}\eta'\,\sigma(\eta')\Psi'_1(\eta_j-\eta')$$
$$+\Phi'_{1/2}(\eta_j+\mathrm{i})-\int_{-\infty}^{\infty}\mathrm{d}\eta'\,\sigma(\eta')\Phi'_1(\eta_j-\eta'+\mathrm{i}+\mathrm{i}0)\Bigg]\mathrm{i}\delta(\eta_j)$$
$$+\int_{-\infty}^{\infty}\mathrm{d}\eta'\,\sigma(\eta')[\Psi'_1(\eta_j-\eta')+\Phi'_1(\eta_j-\eta'+\mathrm{i}+\mathrm{i}0)]\mathrm{i}\delta(\eta')$$
$$+(\mathrm{i}/N)\ln[1-\exp(-2\pi\alpha(\eta_j))]=2\pi I_j/N. \tag{2.15}$$

This equation can be solved in two steps.

(i) For $N\to\infty$ those terms proportional to δ or $1/N$ vanish. The remaining equation becomes

$$\Psi_{1/2}(\eta_j)+\Phi_{1/2}(\eta_j+\mathrm{i})-\int_{-\infty}^{\infty}\mathrm{d}\eta'\,\sigma(\eta')[\Psi_1(\eta_j-\eta')+\Phi_1(\eta_j-\eta'+\mathrm{i}+\mathrm{i}0)]$$
$$=2\pi z(\eta_j)$$
$$=2\pi I_j/N. \tag{2.16}$$

Then, realising that $\sigma(\eta)=z'(\eta)$ yields

$$\sigma(\eta)=\frac{1}{2\cosh(\pi\eta)}\qquad z(\eta)=(1/\pi)\tan^{-1}(\mathrm{e}^{\pi\eta})-\tfrac{1}{4}. \tag{2.17}$$

(ii) Substituting this back in (2.15), we find

$$\pi\alpha(\eta_j)+\frac{1}{2}\int_{-\infty}^{\infty}\mathrm{d}\eta'\,\alpha(\eta')[\psi'_1(\eta_j-\eta')+\Phi'_1(\eta_j-\eta'+\mathrm{i}+\mathrm{i}0)]$$
$$+\ln[1-\exp(-2\pi\alpha(\eta_j))]=0. \tag{2.18}$$

This equation admits a constant solution $\alpha(\eta)=\alpha_0$. Integrating with respect to η', we find that

$$-2\pi\alpha_0=\ln[1-\exp(-2\pi\alpha_0)]. \tag{2.19}$$

Hence

$$\alpha_0=\ln 2/(2\pi)=0.110\,3178\ldots. \tag{2.20}$$

That is,

$$\delta(\eta)=\frac{\ln 2}{4\pi}\frac{1}{N\sigma(\eta)}=\frac{\ln 2}{2\pi N}\cosh(\pi\eta). \tag{2.21}$$

Numerical calculations performed by Avdeev and Dörfel (1987) suggested an expression for $\delta(\eta)$ similar to (2.21). The numerical value then found for α_0 is in perfect agreement with our exact result (2.20).

The formula (2.21) holds for the bulk, i.e. for $\delta(\eta)\ll 1$, which means $N\sigma(\eta)\gg 1$ or $\pi\eta<\ln N$. (Near the ends of the distribution $\pi\eta\approx\ln N$, and the derivation of (2.20) ceases to be valid.) Comparison with numerical results shows, however, that (2.21) gives the correct order of magnitude even for the largest roots. Let us apply (2.21) to the worse case, that is for the last root $\eta_j=\Lambda$ (the root associated with $I_{max}=\frac{1}{2}(N/2-1)$). We find from (2.16) and (2.17) that

$$\Lambda=(1/\pi)\ln(2N/\pi)+O(1). \tag{2.22}$$

Therefore (2.31) yields

$$\lim_{\Lambda\to\infty}\delta(\Lambda)=\frac{\ln 2}{2\pi^2}=0.035\,115\ldots. \tag{2.23}$$

This value underestimates the numerical value of $\delta_{max}=0.046\,65$ found by Avdeev and Dörfel (1987) by about 30%.

2.2. *The anisotropic case*

The anisotropic case can be treated in complete analogy with the isotropic one. The BAE are

$$\left(\frac{\sinh(\lambda_j+i\gamma)}{\sinh(\lambda_j-i\gamma)}\right)^N=-\prod_{k=1}^{r}\frac{\sinh(\lambda_j+\lambda_k-i\gamma)}{\sinh(\lambda_j-\lambda_k-i\gamma)}. \tag{2.24}$$

We note that the properties of these equations are different for $\gamma<\pi/2$ and $\gamma>\pi/2$. Our subsequent treatment holds for $\gamma<\pi/2$. The number of roots of (2.24) for the ground state, just as in the isotropic case, is $r=N$ and the roots form complex conjugate pairs

$$\lambda_j^{\pm}=\eta_j\pm i(\gamma/2+\delta_j). \tag{2.25}$$

Here $\pm i\gamma/2$ are the imaginary parts for the roots in the $N=\infty$ limit (string hypothesis). The δ_j are of order $1/N$ except for the roots near the ends of the distribution ($\eta_j\approx(\gamma/\pi)\ln N$). Taking the logarithm of (2.24) in analogy with (2.5) we get

$$\begin{aligned} N\Psi(\eta_j+i\delta_j;\gamma/2) &\\ &=2\pi I_j+\sum_{k=1}^{N/2}\Psi(\eta_j-\eta_k+i(\delta_j-\delta_k);\gamma)\\ &\quad-N\Phi(\eta_j+i\gamma+i\delta_j;\gamma/2)\\ &\quad+\sum_{k=1}^{N/2}\Phi(\eta_j-\eta_k+i\gamma+i(\delta_j+\delta_k);\gamma) \end{aligned} \tag{2.26}$$

with $I_j = \frac{1}{2}(N/2+1) (\mathrm{mod}\ 1)$, and

$$\Psi(x;\gamma) \equiv \frac{1}{\mathrm{i}} \ln \frac{\sin(\gamma+\mathrm{i}x)}{\sin(\gamma-\mathrm{i}x)} = 2\tan^{-1}\left(\frac{\tanh x}{\tan\gamma}\right)$$
$$\Phi(x;\gamma) \equiv \frac{1}{\mathrm{i}} \ln\left(\frac{\sinh(x-\mathrm{i}\gamma)}{\sinh(x+\mathrm{i}\gamma)}\right). \tag{2.27}$$

Also here $\Psi(z;\gamma)$ and $\Phi(z;\gamma)$ differ in the choice of cuts only. As in the isotropic case, the second sum must be treated with care. As in (2.7), we define

$$X(\eta_j) = \sum_{k=1}^{N/2} \Phi(\eta_j - \eta_k + \mathrm{i}\gamma + \mathrm{i}\delta_j + \mathrm{i}\delta_k;\gamma). \tag{2.28}$$

The location of the relevant branch points is again given by (2.9) and around this point (2.10) holds, i.e. the summands in (2.28) near the branch point, as functions of the summation variable $k \equiv z$, have the form

$$f(z) = \frac{1}{\mathrm{i}} \ln\left\{ \sinh\left(\frac{j+\mathrm{i}\alpha - z}{N\sigma(\eta)}\right)\left[\sinh\left(\frac{j+\mathrm{i}\alpha-z}{N\sigma(\eta)} + 2\mathrm{i}\gamma\right)\right]^{-1}\right\} \tag{2.29}$$

with α given by (2.11). Also for this function $\Delta = -2\pi\mathrm{i}$ as in (2.12). The other branch point where the cut terminates is sufficiently far away, thus (A1.10) with (A1.9) apply, leading to

$$X(\eta) = -\mathrm{i}\ln[1-\exp(-2\pi\alpha(\eta))]$$
$$+N\int_{-\infty}^{\infty} \mathrm{d}\eta'\,\sigma(\eta')\Phi(\eta-\eta'+\mathrm{i}\delta(\eta)+\mathrm{i}\delta(\eta')+\mathrm{i}\gamma;\gamma) + O(1/N). \tag{2.30}$$

Through a completely analogous calculation to (2.14)-(2.21), we find

$$\delta(\eta) = \frac{\ln 2}{4\pi} \frac{1}{N\sigma(\eta)} \tag{2.31}$$

where now

$$\sigma(\eta) = 1/[2\gamma\cosh(\pi\eta/\gamma)]. \tag{2.32}$$

Finally, for the anisotropic model we have

$$\delta(\eta) = \frac{\ln 2}{2\pi N}\gamma\cosh\left(\frac{\pi\eta}{\gamma}\right). \tag{2.33}$$

This formula is identical to (2.21) up to the rescaling of the variable $\lambda_j^{\pm} = \eta_j \pm \mathrm{i}(\gamma/2+\delta_j)$ by a factor γ^{-1}. As before, (2.33) holds in the bulk, which for this case means $|\eta| < (\gamma/\pi)\ln N$.

3. The spin-S Bethe ansatz equations

The BAE in the spin-S case read

$$\left(\frac{\lambda_\alpha - \mathrm{i}S}{\lambda_\alpha + \mathrm{i}S}\right)^N = -\prod_{\beta=1}^{r} \frac{\lambda_\alpha - \lambda_\beta - \mathrm{i}}{\lambda_\alpha - \lambda_\beta + \mathrm{i}} \tag{3.1}$$

where $r = NS$ for the ground state. We parametrise the roots as

$$\lambda_\alpha \equiv \lambda_j^m = \eta_j^m + \mathrm{i}(S - \tfrac{1}{2} - m) + \mathrm{i}\delta_j^m \qquad m = 0, 1, 2, \ldots, 2S-1 \tag{3.2}$$

where η_j^m is real, and we have singled out the imaginary part $(S-\frac{1}{2}-m)$ proposed by the string hypothesis. Therefore we expect δ_j^m to vanish in the bulk when $N\to\infty$.

Since the roots λ_α appear in complex conjugated pairs

$$\delta_j^{2S-1-m} = -\delta_j^m . \tag{3.3}$$

Therefore, we have only S $(S-\frac{1}{2})$ independent and real unknowns δ_j^m for a given j when S is an integer (half-integer):

$$\begin{aligned} &\delta_j^m \quad \text{with } m=0,1,\dots,S-1 && \text{for } S=\text{integer} \\ &\delta_j^m \quad \text{with } m=0,1,\dots,S-\tfrac{1}{2} && \text{for } S=\text{half-odd integer.} \end{aligned} \tag{3.4}$$

Notice that $\delta_j^{S-1/2}=0$ in the second case.

It is convenient to rewrite the LHS of (3.1) with the help of the identity

$$\frac{\lambda_j^m - \mathrm{i}S}{\lambda_j^m+\mathrm{i}S} = \frac{\mu_j^m+\mathrm{i}(S-\frac{1}{2}-m)-\mathrm{i}S}{\mu_j^m+\mathrm{i}(S-\frac{1}{2}-m)+\mathrm{i}S} = \prod_{l=-m}^{2S-1-m} \frac{\mu_j^m+\mathrm{i}l-\mathrm{i}/2}{\mu_j^m+\mathrm{i}l+\mathrm{i}/2} \tag{3.5}$$

where

$$\mu_j^m \equiv \eta_j^m + \mathrm{i}\delta_j^m . \tag{3.6}$$

Then the BAE (3.1) can be recast as

$$\prod_{l=-m}^{2S-1-m}\left(\frac{\mu_j^m+\mathrm{i}(l-\frac{1}{2})}{\mu_j^m+\mathrm{i}(l+\frac{1}{2})}\right)^N = -\prod_{k=1}^{N/2}\prod_{l=-m}^{2S-1-m}\frac{\mu_j^m-\mu_k^{m+l}+\mathrm{i}(l-1)}{\mu_j^m-\mu_k^{m+l}+\mathrm{i}(l+1)}. \tag{3.7}$$

Taking the logarithm yields

$$\begin{aligned} &N\Psi_{1/2}(\mu_j^m)-\sum_k \Psi_1(\mu_j^m-\mu_k^m)-2\pi I_j^m \\ &\quad+\sum_{\substack{l=-m\\ l\neq 0}}^{2S-1-m}\Big(N\Phi_{1/2}(\mu_j^m+\mathrm{i}l)-\sum_k \Phi_1(\mu_j^m-\mu_k^{m+l}+\mathrm{i}l)\Big)=0 \end{aligned} \tag{3.8}$$

where Ψ_λ and Φ_λ are defined by (2.6) and $I_j^m=\frac{1}{2}(N/2+1)$ (mod 1). Since the δ_j^m vanish for $N\to\infty$, the terms $l=\pm1$ are to be treated with care. For this we single out the piece

$$\begin{aligned} X^m(\mu_j^m) &= \sum_k [\Phi_1(\mu_j^m-\mu_k^{m+1}+\mathrm{i})+\Phi_1(\mu_j^m-\mu_k^{m-1}-\mathrm{i})] \\ &= \sum_k [\Phi_1(\eta_j^m-\eta_k^{m+1}+\mathrm{i}+\mathrm{i}\delta_j^m-\mathrm{i}\delta_k^{m+1})+\Phi_1(\eta_j^m-\eta_k^{m-1}-\mathrm{i}+\mathrm{i}\delta_j^m-\mathrm{i}\delta_k^{m-1})]. \end{aligned} \tag{3.9}$$

(The finite-size corrections due to the branch points in the terms with $l\neq\pm1$ are exponentially small in N). We evaluate (3.9) by once again using (A1.10) with (A1.9) and (A1.15). We find

$$\begin{aligned} X^m_{(\eta)} &= -\mathrm{i}\ln[1-\exp(-2\pi\alpha_m^+(\eta))]+\mathrm{i}\log[1-\exp(2\pi\alpha_m^-(\eta))] \\ &\quad + N\int_{-\infty}^{\infty}\mathrm{d}\eta'\,\sigma^{m+1}(\eta')\Phi_1(\eta-\eta'+\mathrm{i}+\mathrm{i}\delta^m(\eta)-\mathrm{i}\delta^{m+1}(\eta')) \\ &\quad + N\int_{-\infty}^{\infty}\mathrm{d}\eta'\,\sigma^{m-1}(\eta')\Phi_1(\eta-\eta'-\mathrm{i}+\mathrm{i}\delta^m(\eta)-\mathrm{i}\delta^{m-1}(\eta')) \\ &\quad + \mathrm{O}(1/N) \end{aligned} \tag{3.10}$$

with

$$\alpha_m^{\pm}(\eta)=N\sigma^{m\pm1}(\eta)(\delta^m(\eta)-\delta^{m\pm1}(\eta)) \tag{3.11}$$

and we have assumed $\delta_j^m>\delta_j^{m+1}$ (this will be confirmed by the final result). Inserting (3.10) back in (3.8) and expanding to first order in δ yields, in analogy with (2.15),

$$\begin{aligned}
&N\Psi_{1/2}(\eta_j^m)-\int_{-\infty}^{\infty}\mathrm{d}\eta'\,\sigma^m(\eta')\Psi_1(\eta_j^m-\eta')-2\pi Nz^m(\eta_j^m)\\
&\quad+N\sum_{\substack{l=-m\\ l\neq0}}^{2S-1-m}\bigg(\Phi_{1/2}(\eta_j^m+\mathrm{i}l)\\
&\quad-\int_{-\infty}^{\infty}\mathrm{d}\eta'\,\sigma^{m+l}(\eta')\Phi_1(\eta_j^m-\eta'+\mathrm{i}l+\mathrm{i}0\,\mathrm{sgn}(l)\bigg)\\
&\quad+\mathrm{i}N\bigg(\delta^m(\eta_j)\Psi'_{1/2}(\eta_j^m)\\
&\quad-\int_{-\infty}^{\infty}\mathrm{d}\eta'\,\sigma^m(\eta')\Psi'_1(\eta_j^m-\eta')(\delta^m(\eta_j)-\delta^m(\eta'))\bigg)\\
&\quad+\mathrm{i}N\sum_{\substack{l=-m\\ l\neq0}}^{2S-1-m}\bigg(\delta^m(\eta_j)\Phi'_{1/2}(\eta_j^m+\mathrm{i}l)\\
&\quad-\int_{-\infty}^{\infty}\mathrm{d}\eta'\,\sigma^{m+l}(\eta')\Phi'_1(\eta_j^m-\eta'+\mathrm{i}l+\mathrm{i}0\,\mathrm{sg}(l))(\delta^m(\eta_j)-\delta^{m+l}(\eta'))\bigg)\\
&\quad+\mathrm{i}\ln\left(\frac{1-\exp(-2\pi\alpha_m^+(\eta_j))}{1-\exp(2\pi\alpha_m^-(\eta_j))}\right)=0.
\end{aligned} \tag{3.12}$$

Here we denoted $I_j^m/N=z^m(\eta_j)$. As we did for (2.15), we first solve (3.12) for $N=\infty$. This gives

$$\begin{aligned}
\sigma^m(\eta)&=\sigma(\eta)=\frac{1}{2\cosh\pi\eta}\\
z^m(\eta)&=z(\eta)=(1/\pi)\tan^{-1}(\mathrm{e}^{\pi\eta})-\tfrac14.
\end{aligned} \tag{3.13}$$

Notice that the fact that the $N=\infty$ limit of (3.12) gives m-independent densities $\sigma(\eta)$ and counting functions $z(\eta)$ justifies the Bethe-string hypothesis at $N=\infty$.

Now inserting (3.13) into (3.12) yields

$$\begin{aligned}
&\pi\alpha_m(\eta)+\frac12\int_{-\infty}^{\infty}\mathrm{d}\eta'\,\Psi'_1(\eta-\eta')\alpha_m(\eta')\\
&\quad+\frac12\sum_{\substack{l=-m\\ l\neq0}}^{2S-1-m}\int_{-\infty}^{\infty}\mathrm{d}\eta'\,\alpha_{m+l}(\eta')\Phi'_1(\eta-\eta'+\mathrm{i}l+\mathrm{i}0\,\mathrm{sg}(l))\\
&=-\ln\left(\frac{1-\exp[\pi(\alpha_m-\alpha_{m-1})]}{1-\exp[\pi(\alpha_{m+1}-\alpha_m)]}\right)
\end{aligned} \tag{3.14}$$

where

$$\alpha_m(\eta)=2N\sigma(\eta)\delta^m(\eta). \tag{3.15}$$

This equation has a set of η-independent solutions $\alpha_m(\eta)=\alpha_m$. Setting

$$x_m=\exp(-\pi\alpha_m) \tag{3.16}$$

we find for the constants x_m the set of algebraic equations

$$(x_0)^2 = 1 - x_0/x_1 \tag{3.17a}$$

$$(x_m)^2 = (1 - x_m/x_{m+1})/(1 - x_{m-1}/x_m) \qquad m = 1, 2, 3, \ldots, 2S-2 \tag{3.17b}$$

$$(x_{2S-1})^2 = 1/(1 - x_{2S-2}/x_{2S-1}). \tag{3.17c}$$

Due to (3.3), an acceptable solution of this system must satisfy

$$x_m = 1/x_{2S-1-m}. \tag{3.18}$$

This condition is compatible with (3.17) since (3.17) are invariant under the transformation (3.18).

Equations (3.17) can be solved in closed form (see appendix 2) to give

$$x_m = \frac{\cos[\frac{1}{2}\pi(S-m)/(S+1)]}{\cos[\frac{1}{2}\pi(S-m-1)/(S+1)]} \tag{3.19}$$

thus, according to (3.16)

$$\alpha_m = \frac{1}{\pi} \ln\left(\frac{\cos[\frac{1}{2}\pi(S-m-1)/(S+1)]}{\cos[\frac{1}{2}\pi(S-m)/(S+1)]}\right) \tag{3.20}$$

i.e.

$$\delta^m(\eta) = \frac{1}{2\pi N\sigma(\eta)} \ln\left(\frac{\cos[\frac{1}{2}\pi(S-m-1)/(S+1)]}{\cos[\frac{1}{2}\pi(S-m)/(S+1)]}\right). \tag{3.21}$$

It is not hard to see that (3.21) satisfies (3.3) and that

$$\delta^m(\eta) > \delta^{m+1}(\eta) \tag{3.22}$$

as was assumed above.

Equations (3.20) and (3.21) for $S = 1$ ($m = 0$) coincide with (2.20) and (2.21). For $S = \frac{3}{2}$ (3.20) yields

$$\alpha_0 = (1/\pi) \ln[\cos(3\pi/10)/\cos(\pi/10)] = 0.153\,174\,48 \ldots. \tag{3.23}$$

The numerical value found by Avdeev and Dörfel (1987) agrees within its error with (3.23). When $S = 2$ (3.20) yields

$$\begin{aligned} \alpha_0 &= (1/\pi) \ln[\cos(\pi/6)/\cos(\pi/3)] = 0.174\,849\,58 \ldots \\ \alpha_1 &= (1/\pi) \ln[1/\cos(\pi/6)] = 0.045\,786\,024 \ldots \end{aligned} \tag{3.24}$$

The numerical results obtained by Alcaraz and Martins (1988) for chains with $N = 16$ are consistent with our exact results, since they are about 10% larger than (3.24).

Appendix 1. Generalisation of the Euler–Maclaurin formula including non-analytic terms in $1/N$

The Euler–Maclaurin formula expresses a finite sum

$$\sum_{k=n_1}^{n_2} f(k) \tag{A1.1}$$

as an integral of $f(x)$ over x plus a sum of odd derivatives of $f(x)$ at the end points. It holds when $f(z)$ is holomorphic in the strip $n_1 \leqslant \operatorname{Re} z \leqslant n_2$ (Olver 1974). Here we generalise this formula for the case when $f(z)$ has a branch point at

$$z = u + \mathrm{i}v \qquad n_1 < u < n_2 \qquad v > 0. \tag{A1.2}$$

The interesting case for the Bethe ansatz equations is when $f(z)$ has a logarithmic cut with a constant discontinuity. First we treat the simplest case, when the cut runs to infinity. We choose the cut so that

$$f(u+\mathrm{i}y+0)-f(u+\mathrm{i}y-0)=\mathrm{i}\Theta(y-v)\Delta \tag{A1.3}$$

where $\Theta(t)$ stands for the step function. This equation defines Δ. We shall also assume that $f(z)$ does not grow too fast as $|\mathrm{Im}\ z|\to\infty$, i.e.

$$\lim_{|y_{\mathrm{Im}\,z}|\to\infty} \exp(-2\pi|\mathrm{Im}\ z|)f(z)=0. \tag{A1.4}$$

Since the residue of the function $\cot(\pi z)$ at any integer k is $1/\pi$, we have

$$\sum_{k=n_1+1}^{n_2-1} f(k)=\frac{1}{2\mathrm{i}}\int_{\mathbf{C}} \mathrm{d}z\ \cot(\pi z)f(z) \tag{A1.5}$$

where $\mathbf{C}$ is the contour depicted in figure 1. Let us denote the parts of $\mathbf{C}$ lying in the half planes $\pm\mathrm{Im}\ z>0$ by $\mathbf{C}_\pm$ respectively. Then we have

$$\int_{n_1+\delta}^{n_2-\delta} f(x)\,\mathrm{d}x=-\frac{1}{2}\int_{\mathbf{C}_+} f(z)\,\mathrm{d}z+\frac{1}{2}\int_{\mathbf{C}_-} f(z)\,\mathrm{d}z. \tag{A1.6}$$

Combining (A1.5) and (A1.6) yields

$$\sum_{k=n_1+1}^{n_2-1} f(k)-\int_{n_1+\delta}^{n_2-\delta} f(x)\,\mathrm{d}x$$
$$=\int_{\mathbf{C}'_+}\frac{f(z)\,\mathrm{d}z}{1-\exp(-2\pi\mathrm{i}z)}+\int_{\mathbf{C}'_-}\frac{f(z)\,\mathrm{d}z}{\exp(2\pi\mathrm{i}z)-1}$$
$$-\mathrm{i}\int_v \frac{\mathrm{d}y}{1-\exp[-2\pi\mathrm{i}(u+\mathrm{i}y)]}[f(\mu+\mathrm{i}y+0)-f(u+\mathrm{i}y-0)]. \tag{A1.7}$$

The contours $\mathbf{C}'_\pm$ are depicted in figure 2, and the last term takes into account the contributions of the cut. This term, using (A1.3), yields

$$G=\frac{\Delta}{2\pi}\log\frac{1-\exp[2\pi\mathrm{i}(u+\mathrm{i}v)]}{1-\exp[2\pi\mathrm{i}(u+\mathrm{i}k)]} \tag{A1.8}$$

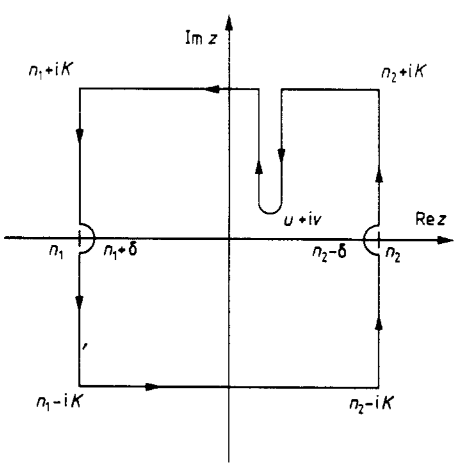

Figure 1. The integration contour **C** in (A1.5).

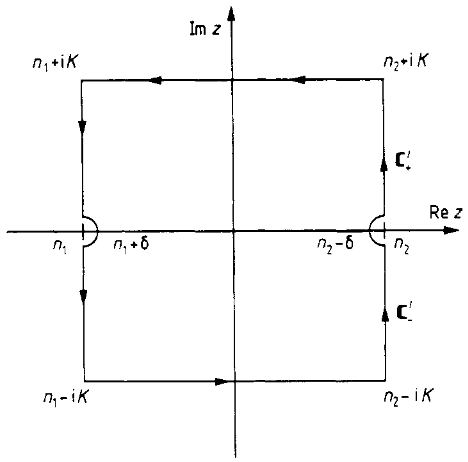

Figure 2. The integration contour $\mathbf{C}'_+$ ($\operatorname{Im} z>0$) and $\mathbf{C}'_-$ ($\operatorname{Im} z<0$) in (A1.7).

which, by letting $K\to\infty$, gives

$$G=\frac{\Delta}{2\pi}\log\{1-\exp[2\pi i(u+iv)]\}. \tag{A1.9}$$

This is the contribution which is absent in the standard Euler–Maclaurin formula and which is non-analytic in $1/N$. The usual terms in the Euler–Maclaurin formula follow from the integral over $\mathbf{C}'_+$ and $\mathbf{C}'_-$ with the final result

$$\sum_{k=n_1}^{n_2} f(k)=\int_{n_1}^{n_2} f(x)\,dx+\tfrac{1}{2}[f(n_1)+f(n_2)]$$
$$+\sum_{s=1}^{m-1}\frac{B_{2s}}{(2s)!}\left(f^{(2s-1)}(n_2)-f^{(2s-1)}(n_1)\right)+G+R_m(n_1,n_2) \tag{A1.10}$$

with G given by (A1.9). (Both the derivation of the usual terms and the rest $R_m(n_1, n_2)$ can be found in Olver (1974).)

A modified version of (A1.10) can be obtained by slightly deforming the integration contours as given in figure 3:

$$\sum_{k=n_1}^{n_2} f(k)=\int_{n_1-1/2}^{n_2+1/2} f(x)\,dx$$
$$-\sum_{s=1}^{m-1}\frac{1-2^{1-2s}}{(2s)!}B_{2s}\left(f^{(2s-1)}(n_2+\tfrac{1}{2})-f^{(2s-1)}(n_1-\tfrac{1}{2})\right)+G'+R'_m(n_1,n_2). \tag{A1.11}$$

In the case when the cut terminates at a finite point $u'+iv'$ the non-analytic contribution G is

$$G'=\frac{\Delta}{2\pi}\ln\frac{1-\exp[2\pi i(u+iv)]}{1-\exp[2\pi i(u'+iv'')]}. \tag{A1.12}$$

Even in this case, however, if $v'\gg 1$ (as it is in the BAE case) the denominator is ≈ 1, and the correction G is given by (A1.9).

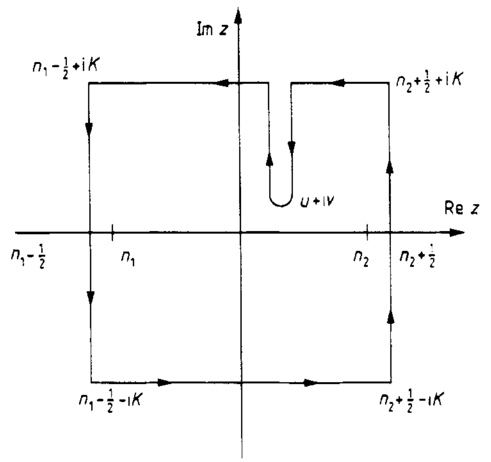

Figure 3. The integration contour which leads to (A1.11).

The generalisation of (A1.9)-(A1.11) to the case when the cut is in the lower half-plane is straightforward. When a branch point is at

$$z'' = u'' + iv'' \qquad v'' < 0 \qquad n_1 < u'' < n_2 \tag{A1.13}$$

and the discontinuity is

$$f(u'' + iy + 0) - f(u'' + iy - 0) = i\Delta\Theta(-y - v'') \tag{A1.14}$$

an analogous derivation leads to

$$G'' = -\frac{\Delta}{2\pi}\log\{1 - \exp[-2\pi i(u'' + iv'')]\} \tag{A1.15}$$

with the usual terms in (A1.10) and (A1.11) unchanged. Equation (A1.15) can also be used in the case when the cut terminates at a finite value, but far enough from the real axis.

Appendix 2. The solution of equations (3.17)

Starting with (3.17*a*) and then applying (3.17*b*) for increasing *m*, we find the following recursion:

$$x_m = (1/x_0) - (1/x_{m+1}) \qquad m = 0, 1, \ldots, 2S-2. \tag{A2.1}$$

This recurrence is closed by (3.17*c*). Equation (A2.1) for $m = 2S-2$ together with (3.17*c*) gives

$$x_{2S-1} = 1/x_0 \tag{A2.2}$$

(see (3.18)). Substituting (A2.2) into (A2.1) successively, we express x_m as a function of x_0

$$\begin{aligned} x_{2S-2} &= (1/x_0) - x_0 \\ x_{2S-3} &= (1/x_0) - 1/[(1/x_0) - x_0] \\ x_{2S-4} &= (1/x_0) - 1/\{(1/x_0) - 1/[(1/x_0) - x_0]\} \\ &\vdots \end{aligned} \tag{A2.3}$$

It is convenient to introduce $F_n(x_0)$ such that

$$x_{2S-n} = F_n(x_0)/F_{n-1}(x_0). \tag{A2.4}$$

Then (A2.1) yields

$$F_n(x_0) = F_{n-1}(x_0)/x_0 - F_{n-2}(x_0) \tag{A2.5}$$

with

$$F_0(x_0) = 1 \qquad F_1(x_0) = 1/x_0. \tag{A2.6}$$

Introducing

$$2y \equiv 1/x_0 \qquad u_n(y) \equiv F_n(x_0) \tag{A2.7}$$

(A2.4) gives

$$x_{2S-n} = u_n(y)/u_{n-1}(y) \tag{A2.8}$$

and (A2.5) together with (A2.6) yields

$$u_n(y) = 2yu_{n-1}(y) - u_{n-2}(y) \tag{A2.9}$$

with

$$u_0 = 1 \qquad u_1 = 2y. \tag{A2.10}$$

Equations (A2.9) with (A2.10) are the recursion relations for the Chebyshev polynomials of second kind

$$u_n(y) = \sin[(n+1)\cos^{-1}(y)]/\sin[\cos^{-1}(y)]. \tag{A2.11}$$

Inserting (A2.8) into (A2.1) for $m = 0$ ($n = 2S$) leads to the equation

$$u_{2S+1}(y) = 0 \tag{A2.12}$$

which by (A2.11) has the solution

$$y = \cos[\tfrac{1}{2}l\pi/(S+1)] \qquad l = 0, 1, \ldots. \tag{A2.13}$$

The solution which generates all x_m positive is given by $l = 1$. Thus

$$x_{2S-n} = \sin[\tfrac{1}{2}\pi(n+1)/(S+1)]/\sin[\tfrac{1}{2}n\pi/(S+1)] \tag{A2.14}$$

i.e.

$$x_m = \cos[\tfrac{1}{2}\pi(S-m)/(S+1)]/\cos[\tfrac{1}{2}\pi(S-m-1)/(S+1)]. \tag{A2.15}$$

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