The finite size spectrum of the 2-dimensional O(3) nonlinear $\sigma$-model

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Abstract

Nonlinear integral equations are proposed for the description of the full finite size spectrum of the 2-dimensional O(3) nonlinear $\sigma$-model in a periodic box. Numerical results for the energy eigenvalues are compared to the rotator spectrum and perturbation theory for small volumes and with the recently proposed generalized Lüscher formulas at large volumes.
1 Introduction

The study of finite size (FS) effects in quantum field theories has recently been received a lot of attention. While understanding the structure of FS effects has always been an important part of the theory of quantum fields (in particular in the numerical simulation of lattice field theories), this renewed interest is due to the important role FS effects are playing in the verification of the AdS/CFT correspondence [1]. Partially motivated by similarity to the AdS/CFT problem, nonlinear integral equations (NLIE) have been proposed [2] to describe the spectrum of excited states in the 2-dimensional O(4) nonlinear $\sigma$-model confined to a finite, periodic box. Motivated also by a problem in the AdS/CFT correspondence, a generalization of Lüscher’s formulas [3], giving the leading large volume dependence for all excited states were proposed [4]. This result was successfully applied for calculating the 4-loop [4] and 5-loop [5] anomalous dimension of an important operator in the AdS/CFT correspondence.

In this paper we propose a set of nonlinear integral equations and corresponding quantization conditions for the description of the full finite size spectrum of the O(3) NLS model. Based on the proposal that the O(3) NLS model can be represented as a limit of appropriately perturbed $Z_N$ parafermion conformal field theories (CFT), the Thermodynamic Bethe Ansatz (TBA) equations for the ground state of the O(3) NLS model were proposed first [7] and [1]. The equations could be formulated in a rather elegant form in terms of the incidence matrix $I_{jk}$ of an infinite Dynkin diagram of type $\mathcal{D}$ depicted in Figure 1:

$$\log y_k(\theta) = -\ell \delta_{k0} \cosh \theta + \sum_{j=0}^{\infty} I_{kj} (K \ast \ln Y_j)(\theta), \quad Y_k(\theta) = 1 + y_k(\theta), \quad k = 0, 1, 2, ... \quad (1.1)$$

where $\ell$ is the volume $^2$, $K(\theta)$ denotes the TBA kernel $K(\theta) = \frac{1}{2\pi \cosh(\theta)}$ and $\ast$ denotes convolution: $(f \ast g)(x) = \int_{-\infty}^{\infty} dy f(x-y)g(y)$. The energy of the ground state can

\footnote{Later a generalization to a more general class of $G/H$ coset models were given in [6].}

\footnote{We measure all energies and lengths in units defined by the infinite volume mass gap of the model.}
be expressed in terms of the solution of (1.1) by a simple integral expression:

$$E = - \int_{-\infty}^{\infty} \frac{d\theta}{2\pi} \cosh \theta \ln Y_0(\theta).$$  \hspace{1cm} (1.2)

It was also shown that the solutions of the ground state TBA equations satisfy certain functional equations, the so-called Y-system equations, which take the following form for the $O(3)$ NLS model:

$$y_k(\theta + iq) y_k(\theta - iq) = \prod_{j=0}^{\infty} Y_j(\theta)^{I_{kj}}, \quad q = \frac{\pi}{2}, \quad k = 0, 1, ....$$  \hspace{1cm} (1.3)

Detailed studies of analogous problems for integrable lattice models [8] indicated that the Y-system is universal in the sense that different solutions of the same Y-system describe all excited states of the model. The difference between the solutions is encoded into their analytic structure. Thus the excited states can also be described by TBA equations, which are similar to the ground state TBA equations but are supplemented by additional source terms and quantization conditions.

For relativistic quantum field theories (QFT) this phenomenon was first observed in [9], where for certain perturbed CFTs it was demonstrated that excited state TBA equations can be obtained by the analytic continuation of some parameters of the ground state equations. Later, based on an integrable lattice regularization, universality of the Y-system for all excited states was demonstrated and excited state TBA equations were derived in the sine-Gordon model [10]. In this model it was also shown that the source terms for excitations can be determined by studying the large volume asymptotics of the Y-functions.

The above examples suggested that it is true in general also for relativistic QFTs that the same Y-system describes all excited states of the model and the TBA equations for the ground state and excited states differ only by source terms and
additional quantization conditions, which can be determined from the knowledge of the infrared (IR) asymptotics of the \( Y \)-functions. Accepting the above hypothesis 1-particle TBA equations were proposed for the \( O(3) \) and \( O(4) \) NLS models by an appropriate modification of the analytic properties of the vacuum \( Y \)-functions \[11\].

The disadvantage of the TBA approach to sigma models is that the number of unknown functions is infinite. It is desirable to find an equivalent nonlinear integral equation (NLIE) description of the problem, with only a few unknown functions. Although such a set of NLIEs is equivalent to the \( Y \)-system and TBA, it is a very useful technical tool that makes the analysis of finite size effects more efficient. In the cases of interest a \( Y \)-system is equivalent to a \( T \)-system and the latter can be solved by an auxiliary linear problem called TQ-relations. As it was shown in a series of papers the TQ-relations are the basic tool for the derivation of an NLIE \[12\]. In \[13, 14, 15\] integrable lattice regularizations were used to derive NLIEs for certain QFTs, while in the case of the \( O(4) \) NLS model \[2\] started directly from the TQ-relations of the continuum theory.

In a series of integrable lattice models \[12\] and relativistic QFTs \[13, 14, 15\] it has also been demonstrated that similarly to the TBA case the NLIE for the ground state and excited states differ only in source terms and quantization conditions, which can be determined from the IR analysis of the unknown functions. Using this hypothesis and starting from the ground state equations \[16, 17\] 1-particle NLIEs were proposed for the \( O(3) \) and \( O(4) \) NLS models \[18\].

The organization of the paper is as follows. In the next section we propose a set of nonlinear integral equations and quantization conditions for the full spectrum of the periodic \( O(3) \) NLS model. In Section 3 we study the large volume limit and give a detailed analysis of the spectrum of 2-particle states in this limit using the solution of the asymptotic Bethe Ansatz. In Section 4 we discuss our numerical results, both for small volumes, where comparison to the rotator spectrum and perturbation theory, and for large volumes, where comparison with the Bajnok-Janik formulas, are presented. Technical details are explained in Appendices A and B.
The nonlinear integral equations

Our starting point in this paper is the hypothesis that the same Y-system describes all excited states of the $O(3)$ NLS model. We generalize the NLIE technique to describe the complete finite size spectrum of the model. The generalization is based on the equivalent formulations of the Y-system [13] through a T-system and TQ-relations. With the help of the TQ-relations we can define appropriate auxiliary functions in terms of which the infinite set of TBA equations can be reduced to a finite set of equations, containing only a few unknown functions.

In the large $\ell$ limit eigenstates of the model are multi-particle states satisfying the Bethe-Yang equations, which provide quantization conditions on the set of particle rapidities, $X = \{\theta_k\}$, $k = 1, 2, \ldots, N$. This is constructed as follows. We take an $M$-magnon solution of the asymptotic Bethe equations:

$$\frac{\varphi_0(u_j + i \pi)}{\varphi_0(u_j - i \pi)} = -\frac{Q_0(u_j + i \pi)}{Q_0(u_j - i \pi)}, \quad j = 1, \ldots, M, \quad (2.1)$$

where

$$\varphi_0(\theta) = \prod_{k=1}^{N} (\theta - \theta_k), \quad Q_0(\theta) = \prod_{j=1}^{M} (\theta - u_j), \quad (2.2)$$

and the $u_j$s are the magnon rapidities and their number $M \leq N$ determines the isospin of the $N$-particle state through the formula $J = N - M$.

Next we construct the T-system elements for $k = 0, 1, \ldots$

$$T_k(\theta) = Q_0(\theta + i(k + 1)q)Q_0(\theta - i(k + 1)q) \sum_{j=0}^{k} \xi(\theta + i(k - 2j)q), \quad (2.3)$$

where

$$\xi(\theta) = \frac{\varphi_0(\theta + iq)\varphi_0(\theta - iq)}{Q_0(\theta + iq)Q_0(\theta - iq)}. \quad (2.4)$$

In particular,

$$T_0(\theta) = \varphi_0(\theta + iq) \varphi_0(\theta - iq), \quad T_1(\theta) = \varphi_0(\theta) \tilde{T}_1(\theta), \quad (2.5)$$

where

$$\tilde{T}_1(\theta) = \frac{1}{Q_0(\theta)} \{ \varphi_0(\theta + i\pi)Q_0(\theta - i\pi) + \varphi_0(\theta - i\pi)Q_0(\theta + i\pi) \}, \quad (2.6)$$
which is a polynomial of degree $N$ as a consequence of the Bethe Ansatz equations \(2.1\). It can be shown also that all $T_k$ are polynomials of degree $2N$.

Using the definition

$$\phi(\theta) = \varphi_0(\theta) \varphi_0(\theta + 2iq)$$

(2.7)

it is possible to verify that the functions $\phi, T_0, T_1, \ldots$ form a semi-infinite T-system

$$T_k(\theta + iq) T_k(\theta - iq) - T_{k-1}(\theta) T_{k+1}(\theta) = \phi(\theta + ikq) \bar{\phi}(\theta - ikq),$$

(2.8)

where $\bar{\phi}$ is the complex conjugate of $\phi$. The system is semi-infinite because it can be consistently truncated putting $T_{-1}(\theta) \equiv 0$.

Next one constructs the Y-system elements

$$y_k(\theta) = \frac{T_k(\theta + iq) T_{k+1}(\theta)}{\phi(\theta + ikq) \phi(x - ikq)},$$

(2.9)

$$Y_k(\theta) = \frac{T_k(\theta + iq) T_k(\theta - iq)}{\phi(\theta + ikq) \phi(x - ikq)},$$

(2.10)

which satisfy the Y-system equations

$$y_k(\theta + iq) y_k(\theta - iq) = Y_{k+1}(\theta) Y_{k-1}(\theta)$$

(2.11)

for $k = 2, 3, \ldots$ and

$$y_1(\theta + iq) y_1(\theta - iq) = Y_2(\theta).$$

(2.12)

The main result in this construction is that

$$y_1(\theta) = \Lambda(\theta + iq|\theta),$$

(2.13)

where $\Lambda(\theta, \theta)$ denotes the eigenvalue of the transfer matrix made out of the two-particle S-matrix $\hat{S}_{ij}(\theta)$ of the $O(3)$ NLS model:

$$T(\theta, \theta) = \text{Tr}_0(\hat{S}_{01}(\theta - \theta_1) \hat{S}_{02}(\theta - \theta_2) \ldots \hat{S}_{0N}(\theta - \theta_N)).$$

(2.14)

More precisely, here we deal with the spin-1 transfer matrix, where both in the auxiliary space and in the “quantum” spaces we take the spin-1 representation of SU(2).

\[a\text{Throughout this paper } f \text{ denotes the complex conjugate of the function } f.\]
It is a common experience in the theory of Bethe Ansatz equations that the polynomials $T_k$ have only real roots inside the physical strip $|\text{Im} \theta| < q$ (see, for example, [19]). We denote the set of real roots of $T_k$ (which may be empty) by $t_k$ for $k = 1, 2, \ldots$. From (2.5) we see that

$$t_1 = X \cup \tilde{t}_1,$$

where $\tilde{t}_1$ is the set of real roots of $\tilde{T}_1$ and from (2.9) we see that, denoting the set of roots of $y_k$ inside the physical strip by $\eta_k$,

$$\eta_k = t_{k-1} \cup t_{k+1}, \quad k = 2, 3, \ldots \quad \eta_1 = t_2.$$  

Furthermore, we see that the quantization conditions

$$Y_k(z - iq) = 0, \quad z \in t_k, \quad k = 2, 3, \ldots \quad Y_1(z - iq) = 0, \quad z \in \tilde{t}_1$$

are satisfied by (2.10).

We need one more equation to quantize the rapidities of the physical particles. They are determined from $y_0(\theta)$ by the equation:

$$Y_0(\theta_k - iq) = 0, \quad k = 1, 2, \ldots N$$

For large $\ell$ this equation is equivalent to the Bethe-Yang equations

$$e^{i \ell \sinh \theta} \Lambda(\theta_k, \theta) = -1,$$

if $y_0(\theta) = e^{-\ell \cosh \theta} y_1(\theta)$. This relation is consistent with the Y-system equations (1.3) independently of the value of $\ell$. In this paper we will assume that this relation holds exactly.

For finite $\ell$ the Y-system equations (2.11) for $k = 3, 4, \ldots$ and (2.12) are unchanged and only the $k = 2$ equation is modified to

$$y_2(\theta + iq) y_2(\theta - iq) = Y_3(\theta) Y_1(\theta) Y_0(\theta).$$

Since the only change is the inclusion of the multiplier $Y_0$, which is very close to unity for large $\ell$, we will assume that the finite $\ell$ solution is a smooth deformation of the Bethe Ansatz construction, i.e. both the functions $y_k(\theta)$ and the sets $t_k$ are
smooth deformations of the ones determined by the above explicit construction at large $\ell$. (2.15) still holds, but with $X$ containing the modified particle rapidities $\theta_k$.

Now it would be possible to rewrite the Y-system equations for excited states as a set of TBA integral equations similar to (1.1), by adding source terms corresponding to the $y_k$ roots. This would be supplemented by quantization conditions of the form (2.17) and (2.18). In this paper we leave out this step and proceed directly to the NLIE description.

Assuming that the solution of the excited state Y-system (1.3) is found, we first build a T-system, which is equivalent to it. Since the semi-infinite Y-system (2.11) for $k = 3, 4, \ldots$ is of the form of the standard $A_1$ Y-system, we can find suitable T-system functions $\phi, T_k$ satisfying (2.8) so that (2.9) and (2.10) hold for $k = 2, 3, \ldots$. The $k = 2$ relation (2.20) corresponds to the modified relations

$$Y_1(\theta) Y_0(\theta) - 1 = y_1(\theta) \left[ Y_0(\theta) + e^{-\ell \cosh \theta} \right] = \frac{T_0(\theta) T_2(\theta)}{\phi(\theta + i q) \phi(x - i q)}, \quad (2.21)$$

$$Y_1(\theta) Y_0(\theta) = \frac{T_1(\theta + i q) T_1(\theta - i q)}{\phi(\theta + i q) \phi(x - i q)}. \quad (2.22)$$

In Appendix A it is shown explicitly that it is always possible to find T-system functions $T_k$ for $k = 0, 1, \ldots$ such that (2.21), (2.22) are satisfied, (2.9) and (2.10) hold for $k = 2, 3, \ldots$ Furthermore the T-system equations (2.8) are satisfied for $k = 1, 2, \ldots$ with $\phi$ given by (2.7) (with the modified $\theta_k$ rapidities). The T-system functions obtained this way are smooth deformations of the corresponding ones constructed in the large $\ell$ limit.

Next we construct the TQ system. This is based on the fact that the T-system equations (2.8) are integrable and have a Lax representation [2] through the auxiliary problem (TQ-relations)

$$T_{k+1}(\theta)Q(\theta + ikq) - T_k(\theta - ikq)Q(\theta + i(k+2)q) = \phi(\theta + ikq)\tilde{Q}(\theta - i(k+2)q),$$

$$T_{k-1}(\theta)\tilde{Q}(\theta - i(k+2)q) - T_k(\theta - ikq)\tilde{Q}(\theta - ikq) = -\tilde{\phi}(\theta - ikq)Q(\theta + ikq). \quad (2.23)$$

It can be shown that in the Bethe Ansatz limit $Q(\theta) = \tilde{Q}(\theta) = Q_0(\theta)$ satisfies the TQ system (2.23). In Appendix A we show how to find a $Q(\theta)$ solution which is a smooth deformation of $Q_0(\theta)$. 

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Both equations (2.28) and (2.23) are invariant under the gauge transformation

\[
T_k(\theta) \to g(\theta + i k q) \bar{g}(\theta - i k q) T_k(\theta),
\]

\[
\phi(\theta) \to g(\theta + i q) g(\theta - i q) \phi(\theta),
\]

\[
Q(\theta) \to g(\theta - i q) Q(\theta).
\]  

(2.24)

The Y-functions \(y_k\) are gauge invariant.

We will use for the NLIE the following gauge invariant auxiliary functions:

\[
b_k(\theta) = \frac{Q(\theta + i (k + 2) q)}{Q(\theta - i (k + 2) q)} T_k(\theta - i q), \quad k \geq 0,
\]  

(2.25)

\[
B_k(\theta) = \frac{Q(\theta + i k q)}{Q(\theta - i (k + 2) q)} \frac{T_{k+1}(\theta)}{\phi(\theta + i k q)}, \quad k \geq 0.
\]  

(2.26)

where

\[
B_k(\theta) = 1 + b_k(\theta).
\]  

(2.27)

Furthermore the auxiliary functions (2.25, 2.26) satisfy the functional equations

\[
b_k(\theta) \bar{b}_k(\theta) = Y_k(\theta) [1 + \delta_{k1} y_0(\theta)], \quad k \geq 1,
\]  

(2.28)

\[
B_k(\theta + i q) \bar{B}_k(\theta - i q) = Y_{k+1}(\theta), \quad k \geq 1.
\]  

(2.29)

(2.27), (2.28) and (2.29), together with the analytic properties that can be read off the representation (2.25, 2.26) are the key to find a set of NLIEs that effectively truncate the TBA equations at the \(k\)th node.

The complete set of unknown functions of our NLIE we discuss below are the functions: \(b_1(\theta)\), which will be denoted by \(b(\theta - i \gamma)\) for short, \(y_1(\theta)\) and \(y_0(\theta)\). For the quantization conditions the function \(b_0(\theta)\) will be used as well.

The derivation of the NLIE is given in Appendix B, for an important subset of multiparticle states. Here we present the equations and quantization conditions for the most general excited state of the model precisely. The NLIEs take the form:

\[
\log b(\theta) = i \pi \delta_b + i D^{\gamma+}(\theta) + i g_1^{\gamma+}(\theta) + i g_0^{\gamma+}(\theta) + (G \ast \ln B)(\theta) - (G^{2+\gamma} \ast \ln \bar{B})(\theta)
\]

\[+ \ (K^{-2+\gamma} \ast \ln Y_1)(\theta) + (K^{-2+\gamma} \ast \ln Y_0)(\theta), \quad \delta_b \in \{0, 1\}, \]

\[
\log y_1(\theta) = i \pi \delta_y + i g_1(\theta) + (K^{+2-\gamma} \ast \ln B)(\theta) + (K^{+2-\gamma} \ast \ln \bar{B})(\theta), \quad \delta_y \in \{0, 1\}
\]

\[
\log y_0(\theta) = -\ell \cosh \theta + \log y_1(\theta),
\]

\[
B(\theta) = 1 + b(\theta), \quad Y_1(\theta) = 1 + y_1(\theta), \quad Y_0(\theta) = 1 + y_0(\theta).
\]  

(2.30)
where $\gamma$ is a contour shifting parameter restricted into the interval $0 < \gamma < \frac{\pi}{2}$, \ln denotes the "fundamental" logarithm function having its branch cut on the negative real axis and we introduced the notation for any function $f$:

$$f^{\pm \eta}(\theta) = f(\theta \pm i\eta).$$

The kernel function $G$ of (2.30) reads as

$$G(\theta) = \int_{-\infty}^{\infty} \frac{dq}{2\pi} e^{iq\theta} \frac{e^{-\frac{|q|}{2}}}{2 \cosh \frac{\pi q}{2}},$$

while $K(\theta)$ is the kernel of the TBA equations. The source terms of (2.30) read as:

$$g_b(\theta) = \sum_{j=1}^{N_2} \chi(\theta - h_j) + \sum_{j=1}^{N_S} \left( \chi(\theta - v_j) + \chi(\theta - \bar{v}_j) \right) - \sum_{j=1}^{N_P} \left( \chi(\theta - s_j) + \chi(\theta - \bar{s}_j) \right) - \sum_{j=1}^{M_C} \chi(\theta - c_j) - \sum_{j=1}^{M_W} \chi(\theta - w_j),$$

$$g_1(\theta) = \sum_{j=1}^{N_1} \chi_K(\theta - h_j^{(1)}),$$

$$g_y(\theta) = \lim_{\eta \to 0^+} \tilde{g}_y \left( \theta + i\frac{\pi}{2} - i\eta \right),$$

$$\tilde{g}_y(\theta) = \sum_{j=1}^{N_2} \chi_K(\theta - h_j) + \sum_{j=1}^{N_S} \left( \chi_K(\theta - v_j) + \chi_K(\theta - \bar{v}_j) \right) - \sum_{j=1}^{M_P} \left( \chi_K(\theta - s_j) + \chi_K(\theta - \bar{s}_j) \right) - \sum_{j=1}^{M_C} \chi_K(\theta - c_j) - \sum_{j=1}^{M_W} \chi_K(\theta - w_j),$$

where $\chi(\theta)$ and $\chi_K(\theta)$ are proportional to the odd primitives of the kernel functions

$$\chi(\theta) = 2\pi \int_0^{\theta} dx \ G(x), \quad \chi_K(\theta) = 2\pi \int_0^{\theta} dx \ K(x),$$

and the second determination of any function $f_{II}(\theta)$ is defined by:

$$f_{II}(\theta) = f(\theta) + f(\theta - i\pi \text{sign(Im } \theta)).$$
The function $\chi_K(\theta)$ is given by the formula:

$$\chi_K(\theta) = i \ln \frac{\sinh \left( i \frac{\pi}{4} + \frac{\theta}{2} \right)}{\sinh \left( i \frac{\pi}{4} - \frac{\theta}{2} \right)}, \quad \chi_K(\theta) = -\chi_K(-\theta) \quad \forall \theta \in \mathbb{C}. \quad (2.37)$$

The branch cuts are chosen to run parallel to the real axis so that $\chi_K(\theta)$ is an odd real analytic function on the entire complex plane and continuous along the real axis. In this case $\chi_K(\theta)$ is not periodic anymore with respect to $2\pi i$. It is periodic only modulo $2\pi$, i.e. the following identity holds:

$$\chi_K(\theta + 2\pi i) = \chi_K(\theta) - 2\pi.$$

It follows that the distance between the consecutive cuts is $2\pi i$ and the jump of $\chi_K(\theta)$ is equal to $-2\pi$ at each branch cut crossed from below. The choice of branch cuts is depicted in Figure 2.

![Figure 2: Locations of the branch cuts of $\chi_K(\theta)$.](image)

Although all physical quantities should be gauge-invariant, i.e. invariant under (2.24), the description of the source objects is nevertheless more transparent in a particular gauge fixed by the condition (2.7). In this gauge it is possible to show (see Appendix A) that $T_1(\theta_j) = 0$ for all physical rapidity $\theta_j$, $j = 1, 2, \ldots, N$ and we can define $\tilde{T}_1(\theta)$ by

$$T_1(\theta) = \tilde{T}_1(\theta)\varphi_0(\theta). \quad (2.38)$$
In what follows we will work in this fixed gauge.

The objects appearing in the source terms of (2.30) are as follows.

1. **Type I holes**: \( \{h_j^{(1)}\}, \ j = 1, \ldots, N_1 \) which are zeroes of \( \tilde{T}_1(x) \) satisfying the condition: \( 0 \leq |\text{Im} \ h_j^{(1)}| < \frac{\pi}{2} \).

2. **Holes**: \( \{h_j\}, \ j = 1, \ldots, N_2 \) corresponding to zeroes of \( T_2(x) \), with \( 0 \leq |\text{Im} \ h_j| < \gamma \).

3. "Close objects": \( \{c_j\}, \ j = 1, \ldots, M_C \) which are "source objects" satisfying the condition: \( \gamma < |\text{Im} \ c_j| < \pi \).

4. "Wide objects": \( \{w_j\}, \ j = 1, \ldots, M_W \), with \( \pi < |\text{Im} \ w_j| \).

Close and wide objects appear in complex conjugate pairs and they are related to the zeroes of the \( Q \) function in the same manner as in the spin-1 XXX chains \([19, 20]\).

There are also two types of special objects in the source terms of the equations. They are defined by the relations:

\[
\text{Im} \log b^{-\gamma}(s_j) = 2\pi I_{s_j}, \quad |b^{-\gamma}(s_j)| > 1, \quad (\text{Im} \log b^{-\gamma})'(s_j) < 0, \quad j = 1, \ldots, N_S, \tag{2.39}
\]
\[
\text{Im} \log b^{-\gamma}(v_j) = 2\pi I_{v_j}, \quad |b^{-\gamma}(v_j)| > 1, \quad (\text{Im} \log b^{-\gamma})'(v_j) > 0, \quad j = 1, \ldots, N_V \tag{2.40}
\]

and they are called ordinary and virtual special objects respectively \([20]\). The function \( D(\theta) \) of (2.30) is expressed by the asymptotic rapidities of the \( N \) particle state:

\[
D(\theta) = \sum_{k=1}^{N} \chi_K(\theta - \theta_k).
\]

The values of the constants of the NLIE (2.30) depend on the number of different

\[\text{The term "type I hole" comes from the fact that in the thermodynamic limit of the equations the real zeroes of } \tilde{T}_1(\theta) \text{ correspond to holes in the distribution of real Bethe roots.}\]

\[\text{The term "hole" comes from the fact that in the thermodynamic limit of the equations the real zeroes of } T_2(\theta) \text{ correspond to holes in the distribution of 2-strings.}\]
source objects:

\[ \delta_b \equiv \frac{N + N_1}{2} + J \,(\text{mod } 2), \quad \text{and} \quad \delta_y \equiv J + M_W \,(\text{mod } 2), \quad (2.41) \]

where \( J \) denotes the isospin of the state. In addition to (2.30) we need two other equations for the determination of type I holes and wide objects. For the determination of type I holes, a counting function can be defined:

\[ Z_1(\theta) = \hat{g}_y(\theta) + \frac{1}{i} (K^{-\gamma} \ln B)(\theta) - \frac{1}{i} (K^{+\gamma} \ln \bar{B})(\theta) - \delta_y, \quad 0 \leq |\text{Im } \theta| < \frac{\pi}{2}, \quad (2.42) \]

where \( Z_1(\theta) = -i \log b_0(\theta) \). The function necessary for the determination of wide objects is

\[ \log b_0(\theta + iq) = i g_{II}(\theta) + (G_{II}^{-\gamma} \ln B)(\theta) - (G_{II}^{+\gamma} \ln \bar{B})(\theta), \quad \pi < \text{Im } (\theta). \quad (2.43) \]

Taking into account the fact that \( K_{II}(\theta) \) and \( \chi_{II}(\theta) \) are zero, this equation looks as if it were the second determination of the first equation in (2.30).

The source objects appearing in the NLIE are not arbitrary parameters, they have to satisfy certain quantization conditions dictated by the analytic properties of the unknown functions of the NLIE. The quantization conditions for ”magnonic” degrees of freedom read as:

- For holes:
  \[ \frac{1}{i} \log b^{-\gamma}(h_j) = 2\pi I_{h_j}, \quad j = 1, ..., N_2. \quad (2.44) \]

- For close source objects (only for the upper part of the close pair):
  \[ \frac{1}{i} \log b^{-\gamma}(c_j) = 2\pi I_{c_j}, \quad j = 1, ..., M_C/2. \quad (2.45) \]

- For wide objects (upper part of the wide pair):
  \[ -i \log b_0(w_j^1 + iq) = 2\pi I_{w_j^1}, \quad j = 1, ..., M_W/2. \quad (2.46) \]

(We have determined only the upper parts of the complex pairs, the lower parts are simply given by complex conjugation.)

For ordinary and virtual special objects the defining relations (2.39) and (2.40) themselves play the role of quantization conditions.
Finally for type I holes:

$$Z_1(h_j^{(1)}) = 2\pi I_{h_j^{(1)}}, \quad j = 1, \ldots, N_1. \quad (2.47)$$

In finite volume the rapidities of physical particles are also quantized. Their quantized values can be determined from $y_0(\theta)$:

$$\frac{1}{i} \log y_0(\theta_k + i\frac{\pi}{2}) = 2\pi I_k, \quad k = 1, \ldots, N. \quad (2.48)$$

All the above quantum numbers $I_{\alpha_j}$'s are half integers. A state is then identified by a choice of the quantum numbers $(I_{h_j}, I_{c_j}, \ldots)$. We note that the NLIE itself can impose constraints on the allowed values of the magnonic quantum numbers. Moreover there are relations among the numbers of different species of source objects. They are called counting equations and in this model there are two of them:

$$N_2 + 2N_S^V - 2N_S = M_C + 2J + 2M_W, \quad (2.49)$$

$$N_1 - 2N_S^R = J + M_1 - M_R, \quad (2.50)$$

where $M_1$ denotes the number of close and wide objects lying farther than $\frac{\pi}{2}$ from the real axis, $M_R$ stands for the number of real Bethe roots of the asymptotic Bethe Ansatz equations of the model, and $N_S^R$ means the number of the real special objects. Real special objects can be either real Bethe roots or real type I holes. They are called specials because at the positions of real specials the counting function of real Bethe roots is no more monotonically increasing: i.e. $\frac{d}{dx}Z_1(x) < 0$. We note that the counting equation (2.50) is valid when all the type I holes are real, while (2.49) is valid also for complex holes as far as their imaginary parts lie within the interval $[-\gamma, \gamma]$.

In the TBA analysis of the sine-Gordon theory [10] it turned out that the energy expression for an $N$-particle state consists of two terms: the sum of the kinetic energies of $N$ non-interacting particles plus an integral expression similar to (1.2) containing the $Y$-function corresponding to the massive node of the $Y$-system. Assuming this formula to be valid also for the $O(3)$ NLS model the energy can be

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6Real roots are those zeroes of $1 + b_0(\theta)$ along the real axis which are not type I holes. They correspond to real solutions of the asymptotic Bethe equations.
expressed in terms of the solutions of the NLIE:

\[ E = \sum_{k=1}^{N} \cosh \theta_k - \int_{-\infty}^{\infty} \frac{d\theta}{2\pi} \cosh \theta \ln Y_0(\theta). \]  

(2.51)

3 NLIE in the IR limit and solution of the asymptotic Bethe equations for 2-particle states

In this subsection we analyse the structure of the asymptotic solution of the NLIE equations based on the explicit T-system solution (2.3). We consider zero momentum 2-particle states, with states corresponding to \( J = 0, 1, 2 \) in the isospin space.
The analytic properties of the problem are determined by the magnonic Bethe roots and the zeroes of the transfer matrices $\tilde{T}_1(\theta)$ and $T_2(\theta)$ inside the physical strip. From (2.3) we see that the above data depend on $J$ and the two physical rapidities $\theta_{1,2}$ and for zero-momentum (symmetric) states with fixed $J$ the state can be characterized by the magnitude of $\theta_1$.

The result of the calculation is as follows.

$J = 2$ state:
For all real values of the rapidities $\theta_1$ and $\theta_2$:

- $Q_0(\theta) = 1$,
- $\tilde{T}_1(\theta)$ has two real zeroes,
- $T_2(\theta)$ has four real zeroes.

$J = 1$ state:
For any symmetric state $\theta_1 = -\theta_2$: $Q_0(\theta) = \theta$, and the distribution of zeroes of the transfer matrices depend on the magnitude of $\theta_1$.

$0 < \theta_1 < \frac{\sqrt{3}}{2} \pi \simeq 2.72070$
- $\tilde{T}_1(\theta)$ has no zeroes,
- $T_2(\theta)$ has two real zeroes.

$\frac{\sqrt{3}}{2} \pi < \theta_1 < \pi \simeq 3.14159$
- $\tilde{T}_1(\theta)$ has two complex zeroes,
- $T_2(\theta)$ has two real zeroes.

$\pi < \theta_1 < \sqrt{\frac{3}{2} + \frac{1}{2} \sqrt{\frac{43}{3}}} \pi \simeq 5.78682$
- $\tilde{T}_1(\theta)$ has two real zeroes,
- $T_2(\theta)$ has two real zeroes.

\footnote{The strip $|\text{Im}\theta| \leq \frac{\pi}{2}$ in the complex plane.}
\[
\sqrt{\frac{3}{2} + \frac{1}{2}\sqrt{\frac{4\pi}{3}}} < \theta_1 < \frac{\sqrt{15}}{2}\pi \simeq 6.08367
\]

- \(\hat{T}_1(\theta)\) has two real zeroes,
- \(T_2(\theta)\) has two real and two complex zeroes.

\(\sqrt{\frac{15}{2}\pi} < \theta_1\)

- \(\hat{T}_1(\theta)\) has two real zeroes,
- \(T_2(\theta)\) has four real zeroes and there is a special object in the corresponding NLIE as well.

\[J = 0\text{ state:}\]

For this state the \(Q_0\) function in the IR limit reads as:

\[
Q_0(\theta) = (\theta - u_0 + i\zeta)(\theta - u_0 - i\zeta), \quad u_0 = \frac{\theta_1 + \theta_2}{2},
\]

where \(\zeta = \frac{1}{2}\sqrt{\frac{4\pi^2}{3} + \frac{(\theta_1 - \theta_2)^2}{3}}\). Depending on the magnitude of the rapidities for this state there are seven regions corresponding to the various possibilities for the distribution of the relevant zeroes of the transfer matrices \(\hat{T}_1\) and \(T_2\). In our numerical investigations for \(J = 0\) we considered only the simplest symmetric states with \(0 < \theta_1 < \sqrt{\frac{17 - \sqrt{241}}{6}}\pi \simeq 1.55809\). In this case neither \(\hat{T}_1\) nor \(T_2\) has zeroes in the physical strip.

4 Numerical results

We have considered the NLIE description of the cases \(N = 0\) (vacuum) and \(N = 1\) (mass gap) previously [11, 18]. Some numerical results for these cases are given in the \(\epsilon_0, \epsilon_1\) columns of Table [1].

We now discuss the \(N = 2\) (2-particle) cases extensively. This is the next non-trivial case, with possible isospin values \(J = 0, 1, 2\). Concretely, we consider only zero momentum states with physical rapidities \(\theta_{1,2} = \pm H\) with the smallest possible momentum values. In addition, we also consider some special \(N = 3, J = 1\) 3-particle states with physical rapidities \(\theta_{1,3} = \pm H, \theta_2 = 0\), which leads to an
NLIE very similar to the one corresponding to the RI1b region for 2-particle states discussed below.

In all cases we started from the large $\ell$ BY solution and found the numerical solution of the NLIE equation by iteration. We used the following parameters:

- $h = 0.04$ (step size for the Simpson formula in rapidity space)
- $h' = 0.004$ (step size for the Fourier integrals)
- $\Lambda = 240$ (cutoff in rapidity space)
- $\epsilon = 10^{-12}$ (absolute accuracy for solving the quantization conditions)

With these parameters, it was necessary to perform a few hundred iterations (corresponding to less than 1 hour CPU on a laptop). In this way a (relative) accuracy of about $2 \cdot 10^{-8}$ is achieved for both the energy values and the position of the roots, except very close to the boundary points between regions where qualitative changes occur (discussed below).

For $N = 2$, $J = 2$ there is just one region: starting from large $\ell$, we can gradually come down to the UV region $\ell \sim 10^{-6}$ without any qualitative change in the algorithm. The qualitative description is correctly given by the BY-equations: there are two pairs of real roots for $T_2$ (arranged symmetrically around the origin) and one pair of real roots for $\tilde{T}_1$ (also symmetrical). Some numerical results are given in Table 1 ($\epsilon_{22}$ column).

The case $N = 2$, $J = 1$ is more complex. From the large $\ell$ BY equations we see that in this case only $T_2$ has a single pair of real roots. Let us denote this region RI1a. From the BY equations we get the estimate $\ell \gtrsim 0.74$, below which $\tilde{T}_1$ has (a complex conjugate pair of) imaginary roots inside the physical strip. Indeed, we can monitor the imaginary $\tilde{T}_1$ roots as they move towards the physical strip by solving the RI1a NLIE equations for decreasing $\ell$ values and we estimate that the boundary of RI1a is at $\ell \cong 0.65$, below which (region RI1c) we have to solve the NLIE with one complex conjugate pair of imaginary roots for $\tilde{T}_1$ and one pair of real roots for $T_2$. The limits of this region are

$$0.37 \lesssim \ell \lesssim 0.65$$  \hspace{1cm} (4.1)

(as opposed to the $0.49 \lesssim \ell \lesssim 0.74$ estimate from the BY solution).

At $\ell = 0.37$ the imaginary $\tilde{T}_1$ roots meet at the origin and as $\ell$ decreases further they move away symmetrically from the origin along the real axis. We denote this
region by RI1b. According to the BY solution, RI1b ends at $\ell \approx 0.036$ but the BY equations are no longer relevant for such small $\ell$ values and in fact we find that RI1b extends all the way to the UV limit $\ell \to 0$. The three regions of the $N = 2$, $J = 1$ problem are summarized in Table 2. Some numerical results are given in Table 1 (\(\varepsilon_{21}\) column).

| region | range       | \(\bar{T}_1\) roots | \(T_2\) roots |
|--------|-------------|-----------------------|---------------|
| RI1a   | $\ell > 0.65$ | -                     | 1 real pair   |
| RI1c   | $0.37 < \ell < 0.65$ | 1 imaginary pair    | 1 real pair   |
| RI1b   | $\ell < 0.37$ | 1 real pair           | 1 real pair   |

Table 2: The regions in the $N = 2$, $J = 1$ case.

For $N = 2$, $J = 0$ we have not considered all regions. The large $\ell$ RI0a region is characterized by no roots for either \(\bar{T}_1\) or \(T_2\). It corresponds to $\ell \gtrsim 2$, below which an imaginary pair of \(T_2\) roots enters the physical strip. The $N = 2$, $J = 0$ problem corresponds to a number of different regions, but this is not discussed here in detail.
Rotator spectrum

At small physical volumes, $\ell \to 0$, the only relevant degrees of freedom are those corresponding to the zero modes of the $\sigma$ fields and the low lying energy levels are the eigenvalues of the effective Hamiltonian $^{[21]}$

$$\mathcal{H}_{\text{eff}} = \frac{1}{2\Theta_{\text{eff}}} \hat{L}^2,$$

(4.2)

where $\hat{L}^2$ is the quadratic Casimir operator with eigenvalues $J(J+1)$ and $\Theta_{\text{eff}}$ is the effective moment of inertia (which depends on the volume $\ell$). More precisely, the lowest energy levels in the isospin $J$ sector are given as

$$\tilde{\epsilon}_J(\ell) = \ell \tilde{E}_J(\ell) \cong g(\ell) J(J+1),$$

(4.3)

where $g(\ell)$ is some effective running coupling. This effective rotator spectrum is valid in perturbation theory (PT) up to 2-loop level $^{[22, 23]}$. The lowest energy levels correspond to the totally symmetric tensor states, which in our notation are the $J = N$ states (diagonal scattering or $U(1)$ sector).

The $J = 1$ case corresponds to the mass gap. In this case the PT result is known up to 3-loop order $^{[24]}$:

$$\tilde{\epsilon}_1(\ell) = 2\pi \alpha (1 + \alpha^2 + 1.19 \alpha^3) + O(\alpha^5),$$

(4.4)

where $\alpha$ is a convenient running coupling defined by

$$\frac{1}{\alpha} + \ln \alpha = \ln \frac{32\pi}{\ell} + \Gamma'(1) - 1.$$  

(4.5)

Here the constants on the right hand side of this equation are chosen such that the 1-loop term in $^{[14]}$ vanishes. For general isospin no direct calculation exists beyond 1-loop order $^{[22]}$, but using the validity of the rotator spectrum up to 2-loop order $^{[23]}$ we have

$$\tilde{\epsilon}_J(\ell) = J(J+1)\pi \alpha (1 + \alpha^2) + O(\alpha^4).$$

(4.6)

Using the numerical results in Table $^{[1]}$ we established that

$$\tilde{\epsilon}_2(\ell) = 6\pi \alpha (1 + \alpha^2) + O(\alpha^5),$$

(4.7)

$^8$Note that $\tilde{E}_J(\ell) = E_J(\ell) - E_0(\ell)$, i.e. the energy eigenvalues are measured from the lowest energy state (vacuum).
Figure 3: The UV spectrum of the O(3) model as function of the running coupling $\alpha$, corresponding to the range $0.000001 < \ell < 0.1$. The two low energy data sets contain the $J = 1$ and $J = 2$ rotator energy levels and the corresponding solid lines are the PT predictions (4.4) and (4.7), respectively. Far above the rotator spectrum energies of the $N = 2$, $J = 1$ excited states are shown. Here the solid line is the constant $4\pi$.

i.e. the 3-loop term in (4.7) vanishes or is very small.

The excited states above the rotator spectrum start at

$$\tilde{\epsilon}^*(\ell) \cong 4\pi,$$

(4.8)

corresponding to two massless particles of momentum $\pm \frac{2\pi}{\ell}$.

The UV spectrum of the $\sigma$ model, obtained by numerically solving the NLIE equations down to $\ell = 10^{-6}$ agrees very well with the above rotator picture. This is shown in Figure 3.

The Bajnok-Janik formula

Recently [4] a generalization of Lüscher’s well-known result [3] about the finite size corrections of particle masses has been suggested. According to this conjecture, in 2-dimensional relativistic integrable models one first defines the auxiliary function

$$\mathcal{F}(\theta) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dy \ e^{-\ell \cosh y} \Lambda(y + iq\theta),$$

(4.9)

$\tilde{\epsilon}^*(\ell)$ for the modifications necessary for the nonrelativistic model relevant in the AdS/CFT problem see [4].
where $\theta = (\theta_1, \theta_2, \ldots, \theta_N)$ are the physical rapidities of an $N$-particle state and $\Lambda(\theta|\theta)$ is the eigenvalue of the transfer matrix corresponding to the state in question.

Then the leading (for large $\ell$) finite size correction to the particle rapidities are given by the solution of the modified Bethe-Yang equations

$$e^{i\ell \sinh \theta_j} \Lambda(\theta_j|\theta) \left( 1 + i \frac{\partial F}{\partial \theta_j} \right) = -1, \quad j = 1, 2, \ldots, N. \quad (4.10)$$

Finally the energy formula, which includes the leading FS corrections is given by

$$E = \sum_{j=1}^{N} \cosh \theta_j - \frac{1}{2\pi} \int_{-\infty}^{\infty} dy \cosh y e^{-\ell \cosh y} \Lambda(y + iq|\theta). \quad (4.11)$$

Here the particle rapidities $\theta_j$ are solutions of the modified BY equations (4.10).

Since the above conjecture has been questioned for states with non-diagonal scattering in the case of the O(4) model [2], we decided to numerically investigate the validity of it in our model. The results are shown in Tables 3-6. In all cases we studied (2-particle states with isospin 0,1,2 and a 3-particle state with isospin 1) (4.10) and (4.11) seem to correctly give the leading FS corrections for the particle rapidities and the energy of the state, respectively.

| $\ell$ | $H^{(0)}$ | $H^{(1)}$ | $H$ | $E^{(0)}$ | $E^{(1)}$ | $E$ |
|-------|-----------|-----------|-----|----------|----------|-----|
| 1     | 1.322083  | 1.316882  | 1.317113 | 4.017806 | 3.965831 | 3.969807 |
| 2     | 0.912509  | 0.911777  | 0.911788 | 2.892078 | 2.881859 | 2.882081 |
| 3     | 0.705671  | 0.705531  | 0.705532 | 2.518982 | 2.516186 | 2.516206 |
| 4     | 0.576883  | 0.576852  | 0.576852 | 2.342126 | 2.341269 | 2.341271 |

Table 3: Test of the Bajnok-Janik conjecture for zero momentum $N = 2, J = 2$ states. $H^{(0)}$ is the rapidity from the BY equation, $H^{(1)}$ from the modified BY equation (4.10) and $H$ is the exact rapidity. The energy values $E^{(0)}, E^{(1)}$ and $E$ are defined analogously.

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Table 4: Test of the Bajnok-Janik conjecture for zero momentum $N = 2, J = 1$ states. $H^{(0)}$ is the rapidity from the BY equation, $H^{(1)}$ from the modified BY equation (4.10) and $H$ is the exact rapidity. The energy values $E^{(0)}, E^{(1)}$ and $E$ are defined analogously.

| $\ell$ | $H^{(0)}$ | $H^{(1)}$ | $H$ | $E^{(0)}$ | $E^{(1)}$ | $E$   |
|-------|-----------|-----------|-----|-----------|-----------|------|
| 1     | 2.424832  | 2.426304  | 2.426517 | 11.388820 | 11.579614 | 11.606615 |
| 2     | 1.756669  | 1.757402  | 1.757428 | 5.965728  | 6.006502  | 6.008211  |
| 3     | 1.392858  | 1.393083  | 1.393086 | 4.274704  | 4.285133  | 4.285278  |
| 4     | 1.155252  | 1.155316  | 1.155317 | 3.489801  | 3.492757  | 3.492771  |

Table 5: Test of the Bajnok-Janik conjecture for zero momentum $N = 2, J = 0$ states. $H^{(0)}$ is the rapidity from the BY equation, $H^{(1)}$ from the modified BY equation (4.10) and $H$ is the exact rapidity. The energy values $E^{(0)}, E^{(1)}$ and $E$ are defined analogously.

| $\ell$ | $H^{(0)}$ | $H^{(1)}$ | $H$ | $E^{(0)}$ | $E^{(1)}$ | $E$   |
|-------|-----------|-----------|-----|-----------|-----------|------|
| 2     | 1.444416  | 1.448838  | 1.448743 | 4.475261  | 4.464046  | 4.465255 |
| 3     | 1.055912  | 1.057006  | 1.056993 | 3.222472  | 3.212762  | 3.212965 |
| 4     | 0.818360  | 0.818622  | 0.818621 | 2.707934  | 2.703854  | 2.703885 |
| 5     | 0.661971  | 0.662035  | 0.662035 | 2.454443  | 2.452936  | 2.452940 |

A Construction of the T-system and TQ-system

In this appendix we construct T-system elements satisfying (2.7), (2.8) for $k \geq 1$, (2.9) and (2.10) for $k \geq 2$ and the modified relations (2.21) and (2.22), assuming that a solution of the O(3) Y-system is found satisfying (1.3) and the Y-functions have roots corresponding to the sets (2.16).

We start by constructing the functions $\hat{T}_2$ and $\hat{T}_3$ satisfying

$$\hat{T}_k(\theta + iq) \hat{T}_k(\theta - iq) = Y_k(\theta)$$

for $k = 2, k = 3$ with the additional assumption that they are bounded for large $\theta$ and their roots are the elements of the sets $t_2, t_3$. The solution of this problem is the fundamental problem in the theory of the TBA integral equations and is given explicitly by ($k = 2, 3$)

$$\hat{T}_k(\theta) = \prod_{\alpha} \tanh \left( \frac{\theta - t^{(\alpha)}_k}{2} \right) \exp \left\{ \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{du}{\cosh(\theta - u)} \ln Y_k(u) \right\}.$$
Table 6: Test of the Bajnok-Janik conjecture for zero momentum $N = 3, J = 1$ states. $H^{(0)}$ is the rapidity from the BY equation, $H^{(1)}$ from the modified BY equation (4.10) and $H$ is the exact rapidity. The energy values $E^{(0)}, E^{(1)}$ and $E$ are defined analogously.

| $\ell$ | $H^{(0)}$ | $H^{(1)}$ | $H$ | $E^{(0)}$ | $E^{(1)}$ | $E$ |
|--------|-----------|-----------|-----|-----------|-----------|-----|
| 1      | 2.441754  | 2.443044  | 2.443196 | 12.580190 | 12.762041 | 12.786246 |
| 2      | 1.786837  | 1.787192  | 1.787205 | 7.138026  | 7.176748  | 7.178369  |
| 3      | 1.425225  | 1.425320  | 1.425321 | 5.399247  | 5.409763  | 5.409915  |
| 4      | 1.185639  | 1.185665  | 1.185665 | 4.578328  | 4.581482  | 4.581498  |

where $t_k^{(\alpha)}$ are the elements of $t_k$. We now define $\hat{T}_4$ by

$$\hat{T}_4(\theta) = \frac{y_3(\theta)}{T_2(\theta)}. \tag{A.3}$$

Using the Y-system equations and (2.16) it is easy to show that the roots of $\hat{T}_4$ are the set $t_4$ and it satisfies $[A.1]$ with $k = 4$. Similarly we construct $\hat{T}_5, \hat{T}_6, \ldots$ recursively. We also define

$$\hat{T}_1(\theta) = \frac{y_2(\theta)}{T_3(\theta)} \tag{A.4}$$

and see that its roots are in $t_1$ and it satisfies

$$\hat{T}_1(\theta + iq) \hat{T}_1(\theta - iq) = Y_1(\theta) Y_0(\theta). \tag{A.5}$$

So far we have constructed $\hat{T}_1, \hat{T}_2, \ldots$ satisfying

$$\hat{T}_k(\theta + iq) \hat{T}_k(\theta - iq) = Y_k(\theta) [1 + \delta_{k1} y_0(\theta)] \tag{A.6}$$

for $k \geq 1$,

$$\hat{T}_{k-1}(\theta) \hat{T}_{k+1}(\theta) = y_k(\theta) \tag{A.7}$$

for $k \geq 2$ and the T-system equations

$$\hat{T}_k(\theta + iq) \hat{T}_k(\theta - iq) = 1 + \hat{T}_{k+1}(\theta) \hat{T}_{k-1}(\theta) \tag{A.8}$$

for $k \geq 2$. The T-system functions can be completed by $\hat{T}_0$ by requiring (A.8) to hold for $k = 1$ also. Note that $\hat{T}_0$ does not have any roots in the physical strip.
The last step is to perform a gauge transformation with \( g(\theta) = \varphi_0(\theta + iq) \). This gives

\[
\phi(\theta) = \varphi_0(\theta) \varphi_0(\theta + 2iq)
\]

and

\[
T_k(\theta) = \varphi_0(\theta + i(k + 1)q) \varphi_0(\theta - i(k + 1)q) \tilde{T}_k(\theta).
\]

Note that \( T_k \) has the same set of roots in the physical strip \( (t_k) \) as \( \tilde{T}_k \) and it is a smooth deformation of the corresponding T-function in the large \( \ell \) Bethe Ansatz solution.

Having constructed the T-system elements we now turn to the TQ-relations \(^{22,23}\). It is possible to show that they are equivalent to the single second order difference equation \(^{25}\)

\[
\phi(\theta) Q(\theta - 2iq) + \phi(\theta - 2iq) Q(\theta + 2iq) = A(\theta) Q(\theta),
\]

where

\[
A(\theta) = \frac{\phi(\theta) T_0(\theta - 3iq) + \phi(\theta - 2iq) T_2(\theta - iq)}{T_1(\theta - 2iq)}.
\]

In the large \( \ell \) limit this can be further simplified:

\[
A(\theta) = T_1(\theta).
\]

Throughout this paper our main assumption was that the exact solution is a smooth deformation of the one obtained from the Bethe Ansatz at large \( \ell \). Here we make this statement more precise. Since the exact TBA equations differ from the ones valid in the large \( \ell \) limit only by terms related to \( Y_0 \), which is exponentially small in the physical strip, we obviously have

\[
Y_k(\theta) \sim Y_k^{BA}(\theta), \quad |\text{Im} \, \theta| < \frac{\pi}{2}, \quad k = 1, 2, \ldots,
\]

where \( \sim \) here means up to exponentially small corrections (in \( \ell \)) and we introduced the superscript \(^{BA}\) for objects of the Bethe Ansatz solution. Next, from the set of Y-system equations \(^{1,3}\) we see that the deformation is actually exponentially small in the larger domain

\[
Y_k(\theta) \sim Y_k^{BA}(\theta), \quad |\text{Im} \, \theta| < \frac{k\pi}{2}, \quad k = 1, 2, \ldots
\]
Inspecting the relation between the T-system and Y-system functions we can see that

\[ T_k(\theta) \sim T_{k}^{\text{BA}}(\theta), \quad |\text{Im } \theta| < \frac{(k + 1)\pi}{2}, \quad k = 1, 2, \ldots \]  

(A.16)

Finally from the TQ-relations (2.23) we see that it is natural to assume that

\[ Q(\theta) \sim Q_{0}^{\text{BA}}(\theta) = Q_0(\theta), \quad |\text{Im } \theta| > 0. \]  

(A.17)

Thus \( Q(\theta) \) is close to the polynomial \( Q_0(\theta) \) in the upper half plane (and its complex conjugate \( \bar{Q}(\theta) \) in the lower half plane).

In the large \( \ell \) limit it can be shown [26] that the two linearly independent solutions of (A.11) are \( Q_0(\theta) \) (which is a polynomial of degree \( M \)) and \( R_0(\theta) \), an other polynomial of degree \( 2N + 1 - M > M \). We will assume a similar polynomial behaviour of \( Q(\theta) \) in the upper half plane for large \( \theta \) thus we can characterize the smoothly deformed solution \( Q(\theta) \) uniquely by the requirement that (in the upper half plane)

\[ Q(\theta) \sim \theta^M, \]  

(A.18)

asymptotically for large \( \theta \).

**B NLIE in Fourier space**

In this Appendix we derive the NLIE in the special case where the functions \( T_1 \) and \( T_2 \) have only real roots in the physical strip and also the roots of \( Q(\theta) \) satisfy

\[ |\text{Im } u_j| < \gamma + \frac{\pi}{2}, \quad Q(u_j) = 0, \quad j = 1, 2, \ldots M. \]  

(B.1)

The set of real \( T_1 \) roots will be denoted by \( \{r_j\} \). This is the union of the set of physical rapidities with the set of type I holes. This important special case covers all 2-particle states discussed in this paper (at least for large enough volume) and many other multi-particle states of interest. The derivation in the most general case is more complicated, but goes essentially along the same lines.

We start with some definitions. To any bounded meromorphic function \( \psi(z) \) we associate the Fourier transform of its logarithmic derivative along a line parallel to the real axis:

\[ \psi(z) \implies \tilde{\psi}(k, \alpha) = \int_{-\infty}^{\infty} \frac{\psi' (x + i\alpha)}{\psi(x + i\alpha)} dx e^{ikx}. \]  

(B.2)
For the complex conjugate we have:

\[ \tilde{\psi}(z) \implies \tilde{\psi}(k, \alpha) = \tilde{\psi}^*(-k, -\alpha). \]  

(B.3)

The function \( \psi(z) \) has roots at \( R_\mu \) and poles at \( P_\nu \). We have

\[ e^{-k\alpha} \tilde{\psi}(k, \alpha) - e^{-k\beta} \tilde{\psi}(k, \beta) = 2\pi i \left\{ \sum_{\alpha < \text{Im} R_\mu < \beta} e^{ikR_\mu} - \sum_{\alpha < \text{Im} P_\nu < \beta} e^{ikP_\nu} \right\}. \]  

(B.4)

In the limit \( \beta \to +\infty \) we have

\[ e^{-k\alpha} \tilde{\psi}(k, \alpha) = 2\pi i \left\{ \sum_{\text{Im} R_\mu > \alpha} e^{ikR_\mu} - \sum_{\text{Im} P_\nu > \alpha} e^{ikP_\nu} \right\}. \]  

(B.5)

We start from (2.25,2.26) and (2.28,2.29), which we recall here for \( k = 1 \):

\[ b_1(\theta) = \frac{Q(\theta + 3iq) T_1(\theta - iq)}{Q(\theta - 3iq) \phi(\theta + iq)}, \]  

(B.6)

\[ B_1(\theta) = \frac{Q(\theta + iq) T_2(\theta)}{Q(\theta - 3iq) \phi(\theta + iq)}. \]  

(B.7)

\[ b_1(\theta) \tilde{b}_1(\theta) = \ell_1(\theta) = [1 + y_1(\theta)] \left[ 1 + e^{-\ell \cosh \theta} y_1(\theta) \right], \]  

(B.8)

\[ B_1(\theta + iq) \tilde{B}_1(\theta - iq) = \ell_2(\theta) = 1 + y_2(\theta). \]  

(B.9)

We now define

\[ \tau_1(k) = 2\pi i \sum_j e^{ikr_j}, \quad \tau_2(k) = 2\pi i \sum_j e^{ikh_j}. \]  

(B.10)

Some further definitions:

\[ \tau(k) = e^{-qk} \tilde{T}_1(k, q) - \tilde{T}_2(k, q), \]  

(B.11)

\[ \tilde{\ell}_1(k) = \tilde{\ell}_1(k, 0), \quad \tilde{\ell}_2(k) = \tilde{\ell}_2(k, 0), \quad \tilde{b}(k) = \tilde{b}_1(k, \gamma), \quad \tilde{B}(k) = \tilde{B}_1(k, \gamma). \]  

(B.12)

From the ratio of (B.3) and (B.7) we have

\[ \tilde{b}(k) = \tilde{B}(k) + \tilde{T}_1(k, \gamma - q) + \tilde{Q}(k, \gamma + 3q) - \tilde{T}_2(k, \gamma) - \tilde{Q}(k, \gamma + q). \]  

(B.13)
Since $Q(\theta)$ is analytic in the upper half plane and has no roots in $[\gamma + q, \infty]$ we conclude using (B.5) that
\[ \check{Q}(k, \gamma + q) = \check{Q}(k; \gamma + 3q) = 0, \quad k > 0. \] (B.14)

Furthermore using (B.4) we see that
\[ \tilde{T}_1(k, \gamma - q) = e^{k(\gamma - 2q)}\tilde{T}_1(k, q) + e^{(\gamma - q)k}\tau_1(k), \quad \tilde{T}_2(k, \gamma) = e^{k(\gamma - q)}\tilde{T}_2(k, q) \] (B.15)
and thus we can write
\[ \check{b}(k) = \check{B}(k) + e^{(\gamma - q)k}[\tau(k) + \tau_1(k)], \quad k > 0. \] (B.16)

We now use the facts that $T_1(\theta)$ has no roots in $[-q, -q + \gamma]$, $Q(\theta)$ has no roots in $[3q, 3q + \gamma]$, $\phi(\theta)$ has no roots in $[q, q + \gamma]$, $\check{Q}(\theta)$ has no roots in $[-3q, -3q + \gamma]$, and conclude from (B.6) using (B.4) that
\[ \check{b}_1(k, 0) = e^{-k\gamma}\check{b}(k) \] (B.17)
and using (B.8) that
\[ \check{b}_1(k, 0) + \check{b}_1(-k, 0) = \check{\ell}_1(k) = e^{-k\gamma}\check{b}(k) + e^{k\gamma}\check{b}^*(-k). \] (B.18)
This can be used to write a relation also for negative $k$:
\[ \check{b}(k) = e^{k\gamma}\check{\ell}_1(k) - e^{2k\gamma}\check{B}^*(-k) - e^{k(\gamma + q)}[\tau^*(-k) - \tau_1(k)], \quad k < 0. \] (B.19)

Similarly using that $T_2(\theta)$ has no roots in $[\gamma, q]$, $Q(\theta)$ has no roots in $[\gamma + q, 2q]$, $\phi(\theta)$ has no roots in $[\gamma + q, 2q]$, $\check{Q}(\theta)$ has no roots in $[\gamma - 3q, -2q]$, we conclude from (B.7) using (B.4) that
\[ \check{B}_1(k, q) = e^{k(q - \gamma)}\check{B}(k) \] (B.20)
and also using (B.9) we have
\[ \tilde{\ell}_2(k) = e^{k(q-\gamma)} \tilde{B}(k) + e^{k(\gamma-q)} \tilde{B}^*(-k). \]  
(B.21)

We now go back to the original relations (2.10) and (2.22) and write
\[ \tilde{\ell}_1(k) = \tilde{T}_1(k, q) + \tilde{T}_1(k, -q) - \tilde{\phi}(k, q) - \tilde{\bar{\phi}}(k, -q) \]  
(B.22)
and
\[ \tilde{\ell}_2(k) = \tilde{T}_2(k, q) + \tilde{T}_2(k, -q) - \tilde{\phi}(k, 2q) - \tilde{\bar{\phi}}(k, -2q). \]  
(B.23)

Since \( \tilde{\phi}(\theta) \) has no roots in \([-2q, -q]\) and \( \phi(\theta) \) has no roots in \([q, \infty]\) we see that
\[ e^{2qk} \tilde{\phi}(k, -2q) = e^{qk} \tilde{\bar{\phi}}(k, -q) \]  
(B.24)
and
\[ \tilde{\phi}(k, 2q) = \tilde{\bar{\phi}}(k, q) = 0, \quad k > 0. \]  
(B.25)

Further we note that
\[ e^{kq} \tilde{T}_1(k, -q) - e^{-qk} \tilde{T}_1(k, q) = \tau_i(k), \quad i = 1, 2. \]  
(B.26)

Combining (B.22) and (B.23) we thus have
\[ e^{-qk} \tilde{\ell}_1(k) - \tilde{\ell}_2(k) = \tau(k) \left( 1 + e^{-2qk} \right) + e^{-2qk} \tau_1(k) - e^{-qk} \tau_2(k), \quad k > 0, \]  
(B.27)
and, after some algebra and using (B.21)
\[ \tau(k) = g(k) \left\{ \tilde{\ell}_1(k) - e^{(2q-\gamma)} \tilde{B}(k) - e^{k\gamma} \tilde{B}^*(-k) + \tau_2(k) - e^{-qk} \tau_1(k) \right\}, \quad k > 0, \]  
(B.28)
where
\[ g(k) = \frac{1}{2 \cosh qk}. \]  
(B.29)

From this we get for negative \( k \), after complex conjugation:
\[ \tau^*(-k) = \tau_1(k) + g(k) \left\{ \tilde{\ell}_1(k) - e^{-k\gamma} \tilde{B}(k) - e^{k(\gamma-2q)} \tilde{B}^*(-k) - \tau_2(k) - e^{-qk} \tau_1(k) \right\}, \quad k < 0. \]  
(B.30)
Finally we use (B.28) in (B.16) and similarly (B.30) in (B.19) and get for positive \( k \):

\[
\tilde{b}(k) = g(k) \left\{ e^{-qk} \tilde{B}(k) - e^{k(2\gamma - q)} \tilde{B}^*(-k) \\
+ e^{k(\gamma - q)} \tilde{\ell}_1(k) + e^{k(\gamma - q)} \tau_2(k) + e^{k\gamma} \tau_1(k) \right\}, \quad k > 0
\]  

(B.31)

and for negative \( k \):

\[
\tilde{b}(k) = g(k) \left\{ e^{qk} \tilde{B}(k) - e^{k(2\gamma + q)} \tilde{B}^*(-k) \\
+ e^{k(\gamma - q)} \tilde{\ell}_1(k) + e^{k(\gamma + q)} \tau_2(k) + e^{k\gamma} \tau_1(k) \right\}, \quad k < 0.
\]  

(B.32)

Combining the last two equations we now write the NLIE in Fourier space as

\[
\tilde{b}(k) = g(k) \left\{ e^{-q|k|} \tilde{B}(k) - e^{2k\gamma - q|k|} \tilde{B}^*(-k) \\
+ e^{k(\gamma - q)} \tilde{\ell}_1(k) + e^{k\gamma - q|k|} \tau_2(k) + e^{k\gamma} \tau_1(k) \right\}.
\]  

(B.33)

This is the Fourier space version of the first equation of the NLIE (2.30) in our special case.

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