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Nonlinear integral equations for finite volume excited-state energies of the $O(3)$ and $O(4)$ nonlinear σ-models

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Abstract

We propose nonlinear integral equations for the finite volume one-particle energies in the $O(3)$ and $O(4)$ nonlinear σ-models. The equations are written in terms of a finite number of components and are therefore easier to solve numerically than the infinite component excited-state TBA equations proposed earlier. Results of numerical calculations based on the nonlinear integral equations and the excited-state TBA equations agree within numerical precision.

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1. Introduction

A better theoretical understanding of finite size (FS) effects is one of the most important problems in quantum field theory (QFT). The study of FS effects is a useful method of analysing the structure of QFT models and it is an indispensable tool in the numerical simulation of lattice field theories.

Finite size effects can be studied through the volume dependence of the mass gap of the theory, the usefulness of which is demonstrated [1] by the introduction of the Lüscher–Weisz–Wolff (LWW) running coupling that enables interpolation between the large volume (non-perturbative) and the small volume (perturbative) regions in both two-dimensional sigma models and QCD.

The study of the Lüscher–Weisz–Wolff running coupling is useful in the two-dimensional $O(N)$ nonlinear sigma (NLS) models, because according to recently performed high-precision Monte Carlo measurements of the LWW running coupling [2] the cut-off effects look linear in these models, in contrast to perturbative considerations. The knowledge of the exact value of the LWW coupling enables one to make better fits for the cut-off effects, and thus to determine more accurately the functional form of the lattice artefacts.

Our aim in this paper is to propose nonlinear integral equations (NLIEs) for the one-particle states of the $O(3)$ and $O(4)$ NLS models that allow for a fast and accurate numerical calculation of the LWW coupling. Although this calculation has recently been done in [3] using the excited-state thermodynamic Bethe ansatz (TBA) technique [4–9], the difficulties corresponding to the infinite number of components in the TBA equations make the numerical calculations slow and at the same time restrict their accuracy too. Therefore, it is desirable to work with the more convenient NLIE technique.

Another point of the construction of these excited-state NLIEs is to demonstrate that, similarly to the case of the sine-Gordon model [10, 11], the NLIE technique can be extended to describe the finite size excited states also in the family of NLS models.

The infinite sets of TBA equations for the ground states of the $O(3)$ and $O(4)$ NLS models were given in [12, 13] and [14, 15], respectively. The derivation of the equations was based on the fact that NLS models can be represented as (limits of) certain perturbed conformal field theories [12–15].

The TBA description of the excited states is less systematic in the continuum models than it is for the ground-state problem. Although a lot of different methods have been worked out to obtain excited-state TBA equations in different models [4–9], a general construction has not been discovered yet. The generalization of the TBA equations of the $O(3)$ and $O(4)$ NLS models to one-particle excited states was proposed recently [3]. The sigma-model TBA equations consist of infinitely many components, which makes their numerical analysis difficult.

The NLIEs for the ground state of the $O(3)$ NLS model were proposed in [16], based on the statement according to which the $O(3)$ NLS model can be expressed as a certain limit of appropriately perturbed Z_N parafermion conformal field theories [12].

The ground-state NLIEs for the $O(4)$ NLS model were derived in [17], using the integrable lattice regularization of the model [20–22].

Our main purpose in this paper is to propose excited-state NLIEs for the one-particle states of the $O(3)$ and $O(4)$ NLS models. This is achieved in sections 4 and 5 using the assumption that the excited-state NLIEs differ from the ground state ones only in additional source terms, and if it is necessary in additional quantization conditions.

The paper is organized as follows. In section 2, we recall the TBA integral equations, Y-systems and NLIEs corresponding to the ground-state problem. In section 3, we briefly summarize the one-particle TBA equations of the models. In sections 4 and 5, we propose excited-state NLIEs for the $O(4)$ and $O(3)$ NLS models, respectively. Numerical solutions of the NLIEs and their comparison to perturbation theory and to TBA results are discussed in section 6. Finally, our conclusions are summarized in section 7.

2. The ground-state problem of the $O(4)$ and $O(3)$ NLS models (TBA and NLIE)

In this section, we give a short review of the ground-state TBA equations, Y-systems and nonlinear integral equations (NLIEs) for the $O(4)$ and $O(3)$ NLS models.

The ground-state energy of a two-dimensional integrable model enclosed in a finite box with periodic boundary conditions can be determined by the solutions of the TBA integral equations [18]. The TBA equations of the $O(4)$ and $O(3)$ NLS models can be encoded in infinite Dynkin diagrams (see figures 1(a) and (b)).

The unknown functions y_a are associated with nodes of the Dynkin diagram and the TBA equations are of the form [12–15]

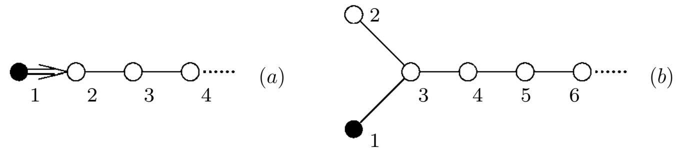

Figure 1. Dynkin diagrams associated with the Y-systems of the (*a*) $O(4)$ and (*b*) $O(3)$ σ-models.

$$y_a(x) = \exp\left\{\delta_{a1}\mathcal{D}(x) + \sum_{b=1}^{\infty} I_{ab}(K * \log Y_b)(x)\right\}, \qquad a = 1, 2, \ldots \tag{1}$$

where

$$Y_a(x) = 1 + y_a(x), \qquad K(x) = \frac{1}{4\cosh\frac{\pi}{2}x}, \qquad \mathcal{D}(x) = -ml\cosh\left(\frac{\pi}{2}x\right), \tag{2}$$

the $*$ denotes the convolution, i.e. $(f * g)(x) = \int_{-\infty}^{\infty} \mathrm{d}y\, f(x-y)g(y)$, m is the mass gap in infinite volume, l is the box size and I_{ab} is the incidence matrix of the Dynkin diagram. The TBA equations of the $O(4)$ NLS model correspond to the diagram shown in figure 1(*a*) [14, 15], where the oriented double line at the beginning of the diagram means

$$I_{12} = 2, \qquad I_{21} = 1. \tag{3}$$

The TBA equations of the $O(3)$ NLS model are encoded into a D_∞ diagram shown in figure 1(*b*). The ground-state energy can be calculated from the solutions of the TBA equations [12–15]

$$E_0(l) = -\frac{m}{4}\int_{-\infty}^{\infty} \mathrm{d}x \cosh\left(\frac{\pi x}{2}\right)\log Y_1(x). \tag{4}$$

The solutions of the TBA equations also satisfy the so-called Y-system equations [19]

$$y_a(x+\mathrm{i})y_a(x-\mathrm{i}) = \prod_b Y_b(x)^{I_{ab}}. \tag{5}$$

There is another alternative to calculate the ground-state energy of the $O(4)$ NLS model, namely the nonlinear integral equation technique. The nonlinear integral equations for the ground state of the $O(4)$ NLS were derived in [17] using the light-cone lattice approach of the model of [20]. The nonlinear integral equations in this case are of the form

$$\begin{aligned}
&\log y_1(x) = \mathcal{D}(x) + 2(K^{+\gamma} * \log U)(x) + 2(K^{-\gamma} * \log \bar{U})(x),\\
&\log a(x) = (F * \log U)(x) - (F^{+2(1-\gamma)} * \log \bar{U})(x) + (K^{-\gamma} * \log Y_1)(x),\\
&\log \bar{a}(x) = (F * \log \bar{U})(x) - (F^{-2(1-\gamma)} * \log U)(x) + (K^{+\gamma} * \log Y_1)(x),\\
&U(x) = 1 + a(x), \qquad \bar{U}(x) = 1 + \bar{a}(x), \qquad Y_1(x) = 1 + y_1(x),
\end{aligned} \tag{6}$$

where $0 < \gamma < 1/2$ is an arbitrary fixed parameter,

$$F(x) = \int_{-\infty}^{\infty} \frac{\mathrm{d}q}{2\pi}\frac{\mathrm{e}^{-|q|-\mathrm{i}qx}}{2\cosh(q)}, \tag{7}$$

and we have used the notation

$$f^{\pm\eta}(x) = f(x \pm \mathrm{i}\eta). \tag{8}$$

In this case, the form of the ground-state energy is the same as it is in the TBA case (4). Equations (6) contain only three real unknown functions because $y_1(x)$ and $Y_1(x)$ are real and $\bar{a}(x)$ is the complex conjugate of $a(x)$, therefore they serve as an efficient basis for numerical

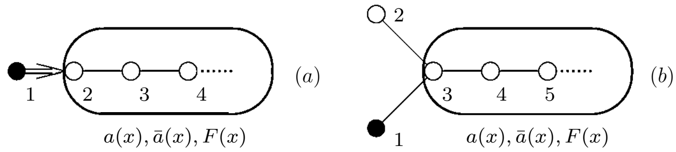

Figure 2. Graphical representation for the NLIEs of the (*a*) $O(4)$ and (*b*) $O(3)$ σ-models.

calculations. The graphical notation of these equations is depicted in figure 2(*a*). The big 'bubble' denotes the complex auxiliary functions which sum up the contributions of those TBA nodes, which are inside it. In our notation, the names of the complex unknown functions and the kernel function are indicated.

In [17], equations (6) were derived on a Bethe ansatz solvable lattice and certainly the TBA equations of the model can also be derived from the Bethe ansatz solution of the model. Thus, it turns out that the function $y_1(x)$ of equations (6) is exactly the same as the function $y_1(x)$ of the TBA equations (1). Furthermore, the connection between the complex $a(x)$ and $\bar{a}(x)$ variables and the TBA variables can be expressed by the following formula:

$$U(x + \mathrm{i}\gamma)\bar{U}(x - \mathrm{i}\gamma) = Y_2(x), \tag{9}$$

which is a very important formula from the NLIE technique point of view, because this relation allows one to reduce the infinite component TBA system to a finite component NLIE.

NLIEs are also available for the ground state of the $O(3)$ NLS model. In [16], NLIEs were proposed for a class of perturbed parafermion conformal field theories, which reduce to the $O(3)$ NLS model in a certain limit [12]. Taking the appropriate limit, the NLIEs take the form

$$\begin{aligned}
\log y_1(x) &= \mathcal{D}(x) + \log y_2(x),\\
\log y_2(x) &= (K^{+\gamma} * \log U)(x) + (K^{-\gamma} * \log \bar{U})(x),\\
\log a(x) &= (F * \log U)(x) - (F^{+2(1-\gamma)} * \log \bar{U})(x)\\
&\quad + (K^{-\gamma} * \log Y_1)(x) + (K^{-\gamma} * \log Y_2)(x), \qquad (10)\\
\log \bar{a}(x) &= (F * \log \bar{U})(x) - (F^{-2(1-\gamma)} * \log U)(x)\\
&\quad + (K^{+\gamma} * \log Y_1)(x) + (K^{+\gamma} * \log Y_2)(x),\\
U(x) &= 1 + a(x), \qquad \bar{U}(x) = 1 + \bar{a}(x), \qquad Y_a(x) = 1 + y_a(x), \qquad a = 1, 2
\end{aligned}$$

where $0 < \gamma < 1/2$ is an arbitrary fixed parameter, the kernel and source functions are the same as in (2), (7) and the ground-state energy is given by formula (4) as in the TBA case. The graphical representation of these equations is given in figure 2(*b*).

Although these equations are only conjectured ones, one can recognize that the functions $y_1(x)$ and $y_2(x)$ are the same as those of the corresponding TBA equations (1), $a(x)$ and $\bar{a}(x)$ are the complex conjugates of each other and the connection between the TBA and NLIE variables can be expressed (similarly to the $O(4)$ case) by the formula

$$U(x + \mathrm{i}\gamma)\bar{U}(x - \mathrm{i}\gamma) = Y_3(x), \tag{11}$$

which somehow ensures the reduction of the infinite component Y-system.

3. TBA equations for the one-particle states of the $O(4)$ and $O(3)$ NLS models

In this section, we briefly review the first excited-state TBA equations of the $O(4)$ and $O(3)$ NLS models proposed in [3].

In [3], the main assumption was (based on previous experience with the sine-Gordon case) that the Y-system (5) describes not only the ground state of the model, but remains valid also for the first excited state. Then Lüscher's mass gap formula [23], valid for asymptotically large volumes, was used to determine the infinite volume solution of the excited-state Y-system, which is sufficient to derive the one-particle excited-state TBA equations. It is important from the NLIE technique point of view that the infinite volume solutions of the Y-system can be expressed by an infinite volume t-system, which is of the form

$$t_p(x+\mathrm{i})t_p(x-\mathrm{i}) = B(x-\mathrm{i}p)B(x+\mathrm{i}p) + t_{p-1}(x)t_{p+1}(x), \qquad p = 1, 2, \ldots \tag{12}$$

where

$$t_0(x) = 0, \tag{13}$$

$$B(x) = x, \qquad \text{in the } O(4) \text{ case} \tag{14}$$

and

$$B(x) = x^2 + 1, \qquad \text{in the } O(3) \text{ case.} \tag{15}$$

The solution of (12) can be represented in the following form:

$$t_p(x) = \sum_{l=1}^{p} \lambda_l^{(p)}(x), \qquad \lambda_l^{(p)}(x) = B[x + \mathrm{i}(2l - p - 1)]. \tag{16}$$

Using the infinite volume t-system (12), the infinite volume solutions of the Y-system can be given as

$$\begin{aligned} y_p^{\infty}(x) &= \frac{t_{p-1}(x)t_{p+1}(x)}{B(x-\mathrm{i}p)B(x+\mathrm{i}p)}, \\ Y_p^{\infty}(x) &= \frac{t_p(x-\mathrm{i})t_p(x+\mathrm{i})}{B}(x-p)B(x+\mathrm{i}p), \qquad p = 1, 2, \ldots \end{aligned} \tag{17}$$

The infinite volume Y-systems of the $O(3)$ and $O(4)$ NLS models [3] are of the form

$$y_p^{\infty}(x+\mathrm{i})y_p^{\infty}(x-\mathrm{i}) = Y_{p-1}^{\infty}(x)Y_{p+1}^{\infty}(x) \qquad p = 2, 3, \ldots \tag{18}$$

where $y_1^{\infty}(x) = 0$, because the Y-system element corresponding to the massive node of the Dynkin diagram tends to zero in the infinite volume limit. The usefulness of these infinite volume solutions is that they give the qualitative position of the zeros of the $y_a(x)$ functions of the Y-system, which is sufficient [3, 24] for the derivation of excited-state TBA integral equations. Thus, the one-particle TBA equations of the $O(4)$ NLS model are of the form [3]

$$y_a(x) = \tau^2(x) \exp\left\{\delta_{a1}\mathcal{D}(x) + \sum_{b=1}^{\infty} I_{ab}(K * \log Y_b)(x)\right\}, \qquad a = 1, 2, \ldots \tag{19}$$

where

$$\tau(x) = \tanh\left(\frac{\pi x}{4}\right), \tag{20}$$

and I_{ab} is the incidence matrix of figure 1(a). The energy of this state takes the form

$$E_1(l) = m - \frac{m}{4}\int_{-\infty}^{\infty} \mathrm{d}x \cosh\left(\frac{\pi x}{2}\right) \log Y_1(x). \tag{21}$$

Similarly the one-particle TBA equations of the $O(3)$ NLS model can be read off from [3] and take the form

$$
\begin{aligned}
&y_1(x) = \mathrm{e}^{\mathcal{D}(x)} y_2(x),\\
&y_2(x) = \tau(x-h_3)\tau(x+h_3)\exp\{(K * \log Y_3)(x)\}\\
&y_a(x) = \tau(x-h_{a-1})\tau(x+h_{a-1})\tau(x-h_{a+1})\tau(x+h_{a+1})\exp\left(\left\{\sum_{b=1}^{\infty} I_{ab}(K * \log Y_b)(x)\right\}\right)\\
&\qquad\qquad a = 3, 4, \ldots
\end{aligned}
\tag{22}
$$

and in addition to these integral equations one has to impose quantization conditions for the h_a zeros of the $y_a(x)$ functions to ensure that $y_a(\pm h_a \pm \mathrm{i}) = -1$, which is a consequence of the (5) Y-system relations. These quantization equations can be obtained by the analytic continuation of (22) and are of the form

$$
\begin{aligned}
&\gamma(h_s - h_{s-1}) + \gamma(h_s + h_{s-1}) + \gamma(h_s - h_{s+1}) + \gamma(h_s + h_{s+1})\\
&\qquad - \frac{1}{\mathrm{i}}\sum_{b=1}^{\infty} I_{sb}(K^{-1} * \log Y_b)(x) = \pi,
\end{aligned}
\tag{23}
$$

for $s = 3, 4, \ldots$, where $h_2 = 0$, $\gamma(x) = 2\arctan\tau(x)$ and

$$
(K^{-1} * \log Y_b)(x) = \mathrm{i}\mathcal{P}\int_{-\infty}^{\infty} \frac{\mathrm{d}y}{4}\frac{\log Y_b(y)}{\sinh\frac{\pi}{2}(x-y)}
\tag{24}
$$

is a principal value integration.

Our main goal in this paper is to propose NLIEs equivalent to these infinite component excited-state TBA equations.

4. Nonlinear integral equations for the first excited state of the $O(4)$ NLS model

In this section, we propose nonlinear integral equations for the first excited state of the $O(4)$ NLS model. The proposal is based on the assumption that the excited-state NLIEs differ from the ground state ones only in additional source terms, plus if it is necessary in quantization conditions. In addition, we assume that the functional form of these additional source terms does not depend directly on the volume. They can depend on the volume only through some complex objects, on which we impose quantization conditions. Such objects may be the zeros of the Y-system elements, or some roots of the Bethe ansatz equations as happens in the sine-Gordon case [11]. These assumptions are valid for the NLIEs in the sine-Gordon model, where the form of the excited-state NLIEs of [11] differ from the ground-state NLIE of [10] only in additional source terms and in quantization conditions.

In this model, one can even give a physical interpretation of the various terms of the equation. The integral term represents the contribution of the infinite number of real Bethe ansatz roots. The presence of these roots can be regarded as filling the Dirac sea and thus the presence of this term in the NLIE of the sine-Gordon model is somehow related to the vacuum structure of the theory. For an excited state of the model one has to consider a slightly modified configuration of the Bethe ansatz roots. It turns out that in the sine-Gordon model, these modifications can be taken into account by adding source terms to the NLIE of the ground-state problem [11]. Similarly, the excited-state TBA equations of the sine-Gordon model differ from the ground state ones only by some source terms [24]. Finally, additional support for our assumptions comes from a direct calculation in the higher spin vertex model, which reduce to the $O(4)$ NLS model in the infinite spin limit. These calculations show that excited-state NLIEs differ from the ground state ones again only by some source terms, which depend on the volume only through some complex objects, on which quantization conditions have to be imposed. (As an additional example see [28] for the $S = 1$ special case.) However, we cannot directly derive the one-particle NLIEs of the $O(4)$ NLS model from the (limit of the) higher spin vertex model, since the solvable lattice model is describing only a subsector of the Hilbert space of the model [20, 21] and unfortunately the one-particle states are not in this subsector.

Accepting these assumptions our task is to find the necessary source terms of the excited-state NLIEs. This is achieved similarly to the case of the derivation of the excited-state TBA equations of the model, where the infinite volume solutions of the equations allowed one to deduce the TBA integral equations [24]. The unknown functions of the excited-state problem will be denoted in the same way as in equations (6). Assuming that relation (9) holds also for the first excited states, we can use this relation in the equation for the massive mode in (1). This leads to the following ansatz for the first excited-state NLIE problem:

$$\begin{aligned}
&\log y_1(x) = \mathcal{D}(x) + \log \tau^2(x) + 2(K^{+\gamma} * \log U)(x) + 2(K^{-\gamma} * \log \bar{U})(x),\\
&\log a(x) = \mathcal{F}_a(x) + (F * \log U)(x) - (F^{+2(1-\gamma)} * \log \bar{U})(x) + (K^{-\gamma} * \log Y_1)(x),\\
&\log \bar{a}(x) = \mathcal{F}_{\bar{a}}(x) + (F * \log \bar{U})(x) - (F^{-2(1-\gamma)} * \log U)(x) + (K^{+\gamma} * \log Y_1)(x),\\
&U(x) = 1 + a(x), \qquad \bar{U}(x) = 1 + \bar{a}(x), \qquad Y_1(x) = 1 + y_1(x),
\end{aligned} \tag{25}$$

where $0 < \gamma < 1/2$ is an arbitrary fixed parameter, the energy formula identical to (21) and our task is to determine the presently unknown $\mathcal{F}_a(x)$ and $\mathcal{F}_{\bar{a}}(x)$ source functions. Using the assumption that these functions do not depend on the volume directly, one can determine them from the infinite volume solution of the proposed equations, which can be determined from the solution of the infinite volume t-system (12) and Y-system (18). Using the construction of [17, 25], the infinite volume solutions of the ansatz (25) take the form

$$a_\infty(x) = \frac{\lambda_1^{(2)}(x + \mathrm{i} - \mathrm{i}\gamma)}{\lambda_2^{(2)}(x + \mathrm{i} - \mathrm{i}\gamma)} = \frac{t_1(x - \mathrm{i}\gamma)}{B[x + \mathrm{i}(2 - \gamma)]} = \frac{x - \mathrm{i}\gamma}{x + \mathrm{i}(2 - \gamma)}, \tag{26}$$

$$\bar{a}_\infty(x) = \frac{\lambda_2^{(2)}(x - \mathrm{i} + \mathrm{i}\gamma)}{\lambda_1^{(2)}(x - \mathrm{i} + \mathrm{i}\gamma)} = \frac{t_1(x + \mathrm{i}\gamma)}{B[x - \mathrm{i}(2 - \gamma)]} = \frac{x + \mathrm{i}\gamma}{x - \mathrm{i}(2 - \gamma)}, \tag{27}$$

$$U_\infty(x) = 1 + a_\infty(x) = 2\frac{x + \mathrm{i}(1 - \gamma)}{x + \mathrm{i}(2 - \gamma)}, \tag{28}$$

$$\bar{U}_\infty(x) = 1 + \bar{a}_\infty(x) = 2\frac{x - \mathrm{i}(1 - \gamma)}{x - \mathrm{i}(2 - \gamma)}, \tag{29}$$

and $y_1^\infty(x) = 0$. One can check that $a(x)$ is the complex conjugate of $\bar{a}(x)$ and that these solutions satisfy the relation $U_\infty(x + \mathrm{i}\gamma)\bar{U}_\infty(x - \mathrm{i}\gamma) = Y_2^\infty(x)$, which is the infinite volume limit of (9). Once one knows the infinite volume solutions of the ansatz (25), one can substitute these formulae into them and can compute explicitly the unknown source functions. The most convenient way to do this is to take the derivative of equations (25) and work in Fourier space, and in the end return to the coordinate space and integrate once. After these simple calculations one gets

$$\mathcal{F}_a(x) = \chi(x + \mathrm{i}(1 - \gamma)) + \chi_K(x + \mathrm{i}(1 - \gamma)), \tag{30}$$

$$\mathcal{F}_{\bar{a}}(x) = -\chi(x - \mathrm{i}(1 - \gamma)) - \chi_K(x - \mathrm{i}(1 - \gamma)), \tag{31}$$

where

$$\chi(x) = 2\pi \mathrm{i} \int_0^x \mathrm{d}y\, F(y) = \mathrm{i} \int_{-\infty}^{\infty} \frac{\mathrm{dq}}{q} \sin(qx) \frac{\mathrm{e}^{-|q|}}{2\cosh(q)}, \tag{32}$$

$$\chi_K(x) = 2\pi \mathrm{i} \int_0^x \mathrm{d}y\, K(y) = \mathrm{i} \arctan \sinh\left(\frac{\pi x}{2}\right). \tag{33}$$

Note that these functions are nothing but the odd primitives of the kernel functions of the integral terms of the ground-state equations (6), which is similar to what happens for the NLIE of the sine-Gordon model in the case of the one hole excitation [11].

We solved these NLIEs numerically for a number of cases and the results we found always agreed with those obtained from the numerical solution of the TBA equations (19) (see section 6). This means that the two methods are equivalent. On the other hand, the TBA equations were tested previously by using Lüscher's formula, Monte Carlo measurements [2] and 3-loop perturbation theory [26]. Thus, we are confident that equations (25) with source terms (30), (31) correctly describe the one-particle excited states of the $O(4)$ NLS model. They are superior to the TBA equations since they contain only three real unknown functions leading to faster convergence in numerical calculations.

5. Excited-state nonlinear integral equations for the $O(3)$ NLS model

In this section, following the method described in the previous section, we propose NLIEs for the first excited state of the $O(3)$ NLS model. According to our assumptions the ansatz for the NLIEs is of the form

$$\begin{aligned}
\log y_1(x) &= \mathcal{D}(x) + \log y_2(x), \\
\log y_2(x) &= \log \tau(x - h_3) + \log \tau(x + h_3) + (K^{+\gamma} * \log U)(x) + (K^{-\gamma} * \log \bar{U})(x), \\
\log a(x) &= \mathcal{F}_a(x) + (F * \log U)(x) - (F^{+2(1-\gamma)} * \log \bar{U})(x) \\
&\quad + (K^{-\gamma} * \log Y_1)(x) + (K^{-\gamma} * \log Y_2)(x), \\
\log \bar{a}(x) &= \mathcal{F}_{\bar{a}}(x) + (F * \log \bar{U})(x) - (F^{-2(1-\gamma)} * \log U)(x) \\
&\quad + (K^{+\gamma} * \log Y_1)(x) + (K^{+\gamma} * \log Y_2)(x), \\
U(x) &= 1 + a(x), \qquad \bar{U}(x) = 1 + \bar{a}(x), \qquad Y_a(x) = 1 + y_a(x), \qquad a = 1, 2
\end{aligned} \tag{34}$$

where $0 < \gamma < 1/2$ is an arbitrary fixed parameter, $y_1(x)$ and $y_2(x)$ are the same variables as those in the excited-state TBA equations (22) and h_3 is the zero of the $y_3(x)$ Y-system element of the excited-state problem (i.e. $y_3(\pm h_3 \pm \mathrm{i}) = -1$), therefore an additional quantization equation must be imposed on this zero. This quantization condition can also be derived from the infinite volume solution of our equations and will be discussed at the end of this section. The energy expression in turn is the same as the TBA one (21).

According to our method, first we have to determine the infinite volume solution of our ansatz (34). This can be achieved using the solutions of the infinite volume t-system (12)–(16), and applying the construction of [17, 25]. After some straightforward calculations one gets

$$a_\infty(x) = \frac{\lambda_1^{(3)}(x + \mathrm{i} - \mathrm{i}\gamma) + \lambda_2^{(3)}(x + \mathrm{i} - \mathrm{i}\gamma)}{\lambda_3^{(3)}(x + \mathrm{i} - \mathrm{i}\gamma)} = 2 \frac{(x - \mathrm{i}\gamma)^2}{(x + \mathrm{i}(4 - \gamma))(x + \mathrm{i}(2 - \gamma))}, \tag{35}$$

$$\bar{a}_\infty(x) = \frac{\lambda_2^{(3)}(x - \mathrm{i} + \mathrm{i}\gamma) + \lambda_3^{(3)}(x - \mathrm{i} + \mathrm{i}\gamma)}{\lambda_1^{(3)}(x - \mathrm{i} + \mathrm{i}\gamma)} = 2 \frac{(x + \mathrm{i}\gamma)^2}{(x - \mathrm{i}(4 - \gamma))(x - \mathrm{i}(2 - \gamma))}, \tag{36}$$

$$U_\infty(x) = 1 + a_\infty(x) = 3\frac{(x+h_0+\mathrm{i}(1-\gamma))(x-h_0+\mathrm{i}(1-\gamma))}{(x+\mathrm{i}(4-\gamma))(x+\mathrm{i}(2-\gamma))}, \tag{37}$$

$$\bar{U}_\infty(x) = 1 + \bar{a}_\infty(x) = 3\frac{(x+h_0-\mathrm{i}(1-\gamma))(x-h_0-\mathrm{i}(1-\gamma))}{(x-\mathrm{i}(4-\gamma))(x-\mathrm{i}(2-\gamma))}, \tag{38}$$

$$y_2^\infty(x) = \frac{t_1(x)t_3(x)}{B(x+2\mathrm{i})B(x-2\mathrm{i})} = 3\frac{(x+h_0)(x-h_0)}{(x+3\mathrm{i})(x-3\mathrm{i})}, \tag{39}$$

$$Y_2^\infty(x) = 1 + y_2^\infty(x) = \frac{t_2(x+\mathrm{i})t_2(x-\mathrm{i})}{B(x+2\mathrm{i})B(x-2\mathrm{i})} = 3\frac{(x+\mathrm{i})(x-\mathrm{i})}{(x+3\mathrm{i})(x-3\mathrm{i})}, \tag{40}$$

where $h_0 = \lim_{l\to\infty} h_3 = \sqrt{5/3}$, the infinite volume limit of the zero h_3, and certainly $y_1(x) = 0$ in the infinite volume limit. The infinite volume solutions (35)–(40) also satisfy the important relation $U_\infty(x+\mathrm{i}\gamma)U_\infty(x-\mathrm{i}\gamma) = Y_3^\infty(x)$, which allows one to cut the infinite TBA equations.

Having the infinite volume solutions of our ansatz, using the method detailed in the previous section one can calculate the unknown source terms (at least their infinite volume limit). After simple calculations one gets

$$\mathcal{F}_a(x) = \chi(x+h_0+\mathrm{i}(1-\gamma)) + \chi(x-h_0+\mathrm{i}(1-\gamma)) + 2\chi_K(x+\mathrm{i}(1-\gamma)), \tag{41}$$

$$\mathcal{F}_{\bar{a}}(x) = -\chi(x+h_0-\mathrm{i}(1-\gamma)) - \chi(x-h_0-\mathrm{i}(1-\gamma)) - 2\chi_K(x-\mathrm{i}(1-\gamma)). \tag{42}$$

According to our assumption these source terms may depend on the volume through the objects, which can be found in their arguments, namely through the volume dependence of h_0. Therefore, we replace h_0 by its finite volume value h_3 in (41), (42), and according to our conjecture that will be the form of the source functions for finite volume,

$$\mathcal{F}_a(x) = \chi(x+h_3+\mathrm{i}(1-\gamma)) + \chi(x-h_3+\mathrm{i}(1-\gamma)) + 2\chi_K(x+\mathrm{i}(1-\gamma)), \tag{43}$$

$$\mathcal{F}_{\bar{a}}(x) = -\chi(x+h_3-\mathrm{i}(1-\gamma)) - \chi(x-h_3-\mathrm{i}(1-\gamma)) - 2\chi_K(x-\mathrm{i}(1-\gamma)). \tag{44}$$

Equations (34) must be supplemented by the quantization condition of the zero h_3, similarly to the TBA case. The quantization condition can be found from the infinite volume solutions (35)–(40). One can see from these solutions that $U_\infty(\pm h_0 - \mathrm{i}(1-\gamma)) = 0$. Assuming that this relation remains valid also for finite volume, one can infer that $U(\pm h_3 - \mathrm{i}(1-\gamma)) = 0$, from which follows that

$$a(h_3 - \mathrm{i}(1-\gamma)) = -1. \tag{45}$$

Taking the logarithm of this, and using equations (34) with (43), (44), one gets the quantization condition for h_3

$$\mathcal{A}(h_3) = \pi, \tag{46}$$

where

$$\mathcal{A}(x) = \frac{1}{\mathrm{i}}\chi(x-h_3) + \frac{1}{\mathrm{i}}\chi(x+h_3) + \frac{2}{\mathrm{i}}\chi_K(x) + \frac{1}{\mathrm{i}}(K^{-1} * \log Y_1)(x)$$
$$+ \frac{1}{\mathrm{i}}(K^{-1} * \log Y_2)(x) + \frac{1}{\mathrm{i}}(F^{-(1-\gamma)} * \log U)(x) - \frac{1}{\mathrm{i}}(F^{+(1-\gamma)} * \log \bar{U})(x). \tag{47}$$

To summarize equations (34) with the source functions (43), (44), and supplemented by the quantization, conditions (46), (47) make up the one-particle NLIEs of the $O(3)$ NLS model. In these equations, one can also see that the source functions are nothing but the odd primitives of the kernel functions, as in the $O(4)$ case. Nevertheless in this case the situation is a bit more

Table 1. NLIE and TBA results for the ground-state energy in the $O(4)$ NLS model.

ml	E_0 (NLIE)	E_0 (TBA)
2	−0.162 028 9681(1)	−0.162 028 97(1)
1	−0.643 774 5719(1)	−0.643 7746(1)
10^{-1}	−11.273 364 587(1)	−11.273 364(1)
10^{-2}	−127.226 343 73(1)	−127.2263(1)
10^{-3}	−1343.409 0793(1)	−1343.409(1)
10^{-4}	−13 865.238 816(1)	
10^{-5}	−141 563.8217(1)	
10^{-6}	−1436 683.423(1)	

complicated, because they contain some zeros in their argument, namely the function $\chi(x)$ contains the zero h_3, which corresponds to the zero of the $y_3(x)$ (in the $y_3(\pm h_3 \pm \mathrm{i}) = -1$ sense), and the function $\chi_K(x)$ contains the zero $h_2 = 0$, which corresponds to the zero of the $y_2(x)$ (in the $y_2(\pm h_2 \pm \mathrm{i}) = -1$ sense), but for this object we do not need to impose a quantization equation for symmetry reasons.

Following from the construction of these equations, one can analytically verify by solving these equations iteratively for large l that they give back correctly the same leading order correction to the infinite volume mass gap as is predicted by Lüscher's formula [23]. For not very large volumes we tested these NLIEs through numerical calculations, and we found that these equations give the same numerical results as the earlier proposed excited-state TBA equations (22)–(24) (see section 6). Because the corresponding TBA system was tested by the results of 3-loop order perturbation theory [26] and lattice Monte Carlo measurements [2], thus our new excited-state NLIEs are also consistent with these methods, and correctly describe the first excited-state energy of the $O(3)$ NLS model.

6. Numerical results

In this section, we perform numerical checks on our conjectured one-particle NLIEs. We solved numerically both the TBA equations and the NLIEs for the ground state and for the one-particle states at some values of the volume, and we compared the numerical results of the two different methods. Moreover, we solved our conjectured NLIEs in the deep ultraviolet region so as to be able to compare our numerical results to the predictions of the asymptotically free perturbation theory.

The numerical method used for solving the TBA equations is described in [3]. The numerical solution of the corresponding NLIEs is rather similar. Namely, we solve the NLIEs numerically by iteration. The starting point for the iteration is the $l \to \infty$ solution of the equations and the procedure converges rapidly. The one-particle state problem for the $O(3)$ NLS model is more involved since here one step of the iteration includes the calculation of the integrals occurring in (34) together with the calculation of the zero (h_3) from the quantization condition (46), (47). Again, the starting point of the iteration procedure is given by the $l \to \infty$ solution, both for the unknown functions and for the position of the zero h_3.

We used Simpson's formula, and a cut-off Λ for the numerical evaluation of the integrals running from $-\infty$ to $+\infty$, in such a way that in the region of $|x| > \Lambda$ the unknown functions are approximated by their infinite volume limit. The magnitude of the cut-off Λ at the values of the volume under consideration has to be 100 in the $O(4)$ case and 150 in the $O(3)$ case, so that 9-digit numerical precision could be reached. Our numerical results are summarized in tables 1–4.

Table 2. NLIE and TBA results for the ground-state energy in the $O(3)$ NLS model.

ml	E_0 (NLIE)	E_0 (TBA)
2	−0.122 846 6915(1)	−0.122 8466(1)
1	−0.486 249 5672(1)	−0.486 2496(1)
10^{-1}	−8.006 985 662(1)	−8.006 985(1)
10^{-2}	−87.635 700 19(1)	−87.6357(1)
10^{-3}	−913.954 7387(1)	−913.954(1)
10^{-4}	−9374.188 294(1)	

Table 3. NLIE and TBA results for the one-particle state energy in the $O(4)$ NLS model.

ml	E_1 (NLIE)	E_1 (TBA)
2	0.992 334 0593(1)	0.992 334 06(1)
1	0.938 397 0591(1)	0.938 397 06(1)
10^{-1}	−3.004 108 884(1)	−3.004 1089(1)
10^{-2}	−69.838 027 86(1)	−69.838 028(1)
10^{-3}	−901.281 5867(1)	−901.281 59(1)
10^{-4}	−10 260.214 298(1)	
10^{-5}	−111 091.0324(1)	
10^{-6}	−1172 575.496(1)	

Table 4. NLIE and TBA results for the one-particle state energy in the $O(3)$ NLS model.

ml	E_1 (NLIE)	E_1 (TBA)
2	1.021 697 21(1)	1.021 6972(1)
1	1.084 208 673(1)	1.084 208(1)
10^{-1}	0.777 210 84(1)	0.777 18(1)
10^{-2}	−23.640 7101(1)	−23.643(1)
10^{-3}	−406.195 912(1)	−406.23(1)
10^{-4}	−5150.216 19(1)	

One can see from these numerical data that the numerical results served by our NLIEs agree with those of the TBA equations within the numerical precision.

Now we are able to compare our numerical results to those of the asymptotically free perturbation theory. Having the numerical values of the ground-state energies and the one-particle state energies, we can compute the dimensionless finite volume mass gap numerically (LWW coupling)

$$z(ml) = l[E_1(l) - E_0(l)], \tag{48}$$

for which perturbative results are also available up to 3-loop order [26]. The perturbative formulae necessary to compute the 3-loop perturbative mass gap can be found in [3]. The comparison of our numerical results to the predictions of the perturbation theory can be found in tables 5 and 6. We listed both the 2-loop and 3-loop perturbative results so that one can infer the accuracy of the 3-loop perturbation theory at the scales under investigation. From this comparison, at very small ml values one can experience a very nice 4-digit agreement in the $O(3)$ case, and an almost 6-digit agreement in the $O(4)$ case, which is non-trivial, since the conjecture of our NLIEs was based on the large volume asymptotics of the unknown functions. This perfect agreement makes us confident that our conjectured one-particle NLIEs describe the exact finite volume one-particle energies in the $O(3)$ and $O(4)$ NLS models.

Table 5. NLIE and PT results for the finite volume mass gap $z(ml)$ in the $O(4)$ NLS model.

ml	$z(l)$ (NLIE)	3-loop PT	2-loop PT
10^{-1}	0.826 925 570(1)	0.826 130	0.825 2260
10^{-2}	0.573 883 159(1)	0.573 7662	0.573 5488
10^{-3}	0.442 127 493(1)	0.442 0969	0.442 0193
10^{-4}	0.360 502 452(1)	0.360 4916	0.360 4571
10^{-5}	0.304 727 89(1)	0.304 7233	0.304 7056
10^{-6}	0.264 107 93(1)	0.264 1057	0.264 0957

Table 6. NLIE and PT results for the finite volume mass gap $z(ml)$ in the $O(3)$ NLS model.

ml	$z(l)$ (NLIE)	3-loop PT	2-loop PT
10^{-1}	0.878 419 650(1)	0.876 058	0.873 458
10^{-2}	0.639 949 901(1)	0.639 645	0.638 874
10^{-3}	0.507 758 827(1)	0.507 669	0.507 358
10^{-4}	0.422 397 210(1)	0.422 363	0.422 212

7. Summary and conclusions

In this paper, we proposed NLIEs for the one-particle states in the $O(3)$ and $O(4)$ NLS models. The forms of these excited-state NLIEs are based on the assumption that they differ from the ground state ones only by some source terms, which may depend on the volume through some objects in their argument, on which extra quantization conditions must be imposed. This assumption is mainly motivated by the form of the NLIEs in the sine-Gordon model and by direct calculations in the higher spin vertex model (which go to the $O(4)$ NLS model in the infinite spin limit). Accepting these assumptions and starting from the explicit infinite volume solution of the first excited-state Y-system of the models we were able to find the infinite volume limit of the conjectured equations. This is sufficient to determine the source terms and the quantization conditions. It is interesting to note that in all cases the source terms are the odd primitives of the kernels occurring in the integral terms of the equations, just as in the case of the NLIE in the sine-Gordon model. We have solved these equations numerically and found that results agree with those obtained previously from numerical solution of the excited-state TBA equations and in the deep ultraviolet regime the numerical results also agree with the predictions of the 3-loop perturbation theory. This agreement is convincing evidence for the correctness of our integral equations. The advantage of using these NLIEs (instead of the infinite set of TBA equations) is that here the number of unknown functions is finite (and small).

An interesting generalization of our results would be to propose excited-state NLIEs for the $\phi_{(\mathrm{id,id,adj})}$ perturbation of the $SU(2)_L \times SU(2)_K/SU(2)_{L+K}$ models, which were investigated at rational level K in [16].

It would also be interesting to extend the NLIE technique for all the excited states of the $O(3)$ and $O(4)$ NLS models and for such more complicated TBA systems which can be encoded into the products of two Dynkin diagrams [27].

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