Numerical Solution of the Direct Scattering Problem for the Nonlinear Schrödinger Equation

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***Abstract*—We illustrate a numerical method to compute the scattering data for the Zhakarov-Shabat system associated to the initial value problem for the nonlinear Schrödinger equation. This numerical method which, to our best knowledge, is the first method proposed to compute all scattering data under general assumptions, is based on the version of the Inverse Scattering Transform method proposed by one of the authors.**

I. Introduction

The problem we are addressing is the initial value problem for the nonlinear Schrödinger equation

$$\begin{cases} iu_t + u_{xx} \pm 2|u|^2 u = 0, & x \in \mathbb{R}, \quad t > 0, \\ u(x,0) = u_0(x), & x \in \mathbb{R}, \end{cases} \tag{1}$$

where i denotes the imaginary unit, $u(x,t)$ is the unknown potential, the subscripts x and t designate partial derivatives with respect to position and time and $u_0 \in L^1(\mathbb{R})$ is the initial potential. The plus sign regards the focusing case and the minus sign the defocusing case.

This equation, a prototype of the important class of nonlinear partial differential equations of integrable type, has important physical applications. In fact, it arises in modeling signal processing in optical bers [1] as well as surface waves on deep waters [2].

In 1972 Zakharov and Shabat [3] showed that (1) can be associated to the rst order linear system

$$\begin{cases} \frac{\partial \psi_1}{\partial x} + i\lambda\psi_1 &= u(x,t)\psi_2, \\ \frac{\partial \psi_2}{\partial x} - i\lambda\psi_2 &= \mp u^*(x,t)\psi_1, \end{cases} \tag{2}$$

where λ is the spectral parameter and the asterisk denotes complex conjugation. With the help of this system, known as the ZS system, the solution $u(x,t)$ of (1) can be obtained from the initial potential $u(x,0)$ by means of the inverse scattering transform (IST) technique. More precisely, it can be obtained by performing the following three steps:

a. Solve the direct scattering problem for the ZS system, i.e., determine the initial scattering data from the initial potential $u(x,0)$;

b. Evolve the initial scattering data in time;

c. Solve the corresponding inverse scattering problem for the ZS system, i.e., determine the potential $u(x,t)$ from the scattering data evolved in time.

Considering that an effective method to solve steps b-c has been proposed in [4], under the hypothesis that the initial scattering data are known, in this paper we illustrate a numerical method to solve the direct problem associated to (1). Although, in large part, it coincides with that proposed in [5], it contains the following important novelty: it allows us to compute the scattering data whenever the initial potential has jump discontinuities.

The paper is organized as follows. In Section II we recall the de nition and the properties necessary for the illustration of the method. In Section III we illustrate the main steps of our numerical method. In Section IV we report the numerical results and in Section V we give the conclusions.

II. Definition and properties

For the sake of clarity, let us recall the de nition and properties most important for this paper. We start recalling that the Jost solutions [6] [7] are those 2×2 matrix solutions to the ZS system (2) which satisfy the asymptotic conditions

$$(\bar{\mathbf{\Psi}}(\lambda,x), \mathbf{\Psi}(\lambda,x)) = e^{-i\lambda \mathbf{J}x}\,[\mathbf{I} + o(1)], \quad x \to \infty \tag{3}$$

$$(\mathbf{\Phi}(\lambda,x), \bar{\mathbf{\Phi}}(\lambda,x)) = e^{-i\lambda \mathbf{J}x}\,[\mathbf{I} + o(1)], \quad x \to -\infty \tag{4}$$

where $\lambda \in \mathbb{R}$, $\mathbf{J} = diag(1,-1)$, $\mathbf{I}$ denotes the identity matrix and the overbar is used to distinguish two different functions.

Since the Jost solutions (3) and (4) satisfy the same linear rst order system, there exist transition matrices

$$A_\ell(\lambda) = \begin{pmatrix} a_{\ell 1}(\lambda) & a_{\ell 2}(\lambda) \\ a_{\ell 3}(\lambda) & a_{\ell 4}(\lambda) \end{pmatrix}, \tag{5}$$

$$A_r(\lambda) = A_\ell(\lambda)^{-1} = \begin{pmatrix} a_{r1}(\lambda) & a_{r2}(\lambda) \\ a_{r3}(\lambda) & a_{r4}(\lambda) \end{pmatrix} \tag{6}$$

such that

$$(\bar{\mathbf{\Psi}}(\lambda,x), \mathbf{\Psi}(\lambda,x)) = (\mathbf{\Phi}(\lambda,x), \bar{\mathbf{\Phi}}(\lambda,x)) A_\ell(\lambda).$$

These matrices are essential to the computation of the so-called scattering matrix

$$\mathbf{S}(\lambda, \mathbf{0}) \equiv \mathbf{S}(\lambda) = \begin{pmatrix} T(\lambda) & L(\lambda) \\ R(\lambda) & T(\lambda) \end{pmatrix} \tag{7}$$

where $T(\lambda)$ represents the (initial) transmission coef cient and $L(\lambda)$ and $R(\lambda)$ stand for the (initial) re ection coef cients from the left and the right, respectively. This matrix for $\lambda \in \mathbb{R}$ satis es the following symmetric properties [6] [7]

$$\mathbf{S}^\dagger(\lambda)\mathbf{S}(\lambda) = \mathbf{S}(\lambda)\mathbf{S}^\dagger(\lambda) = \mathbf{I}, \tag{8}$$

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in the defocusing case and

$$\mathbf{S}^{\dagger}(\lambda)\,\mathbf{J}\,\mathbf{S}(\lambda) = \mathbf{S}(\lambda)\,\mathbf{J}\,\mathbf{S}^{\dagger}(\lambda) = \mathbf{J}, \tag{9}$$

in the focusing case where the dagger symbol denotes the matrix conjugate transpose.

If $T(\lambda)$ has no poles in the complex upper half-plane $\mathbb{C}^+$, there are no discrete spectral data to identify. Otherwise, denoting by $\lambda_1, \ldots, \lambda_n$ the so-called bound states, i.e., the nitely many poles of $T(\lambda)$ in $\mathbb{C}^+$, and by $m_1, \ldots, m_n$ the corresponding multiplicities, we have to identify the parameters $\{n, m_j, \lambda_j\}$ as well as the coef cients $\{(\Gamma_l)_{js}, (\Gamma_r)_{js}\}$ of the initial spectral sums from the left and from the right

$$S_l(\alpha) = \sum_{j=1}^{n} e^{i\lambda_j \alpha} \sum_{s=0}^{m_j-1} (\Gamma_l)_{js} \frac{\alpha^s}{s!}, \qquad \alpha \geq 0, \tag{10}$$

$$S_r(\alpha) = \sum_{j=1}^{n} e^{i\lambda_j \alpha} \sum_{s=0}^{m_j-1} (\Gamma_r)_{js} \frac{\alpha^s}{s!}, \qquad \alpha \leq 0. \tag{11}$$

In (10) and (11) the coef cients $(\Gamma_l)_{js}$ and $(\Gamma_r)_{js}$ are the so-called norming constants from the left and from the right, respectively, and $0! = 1$. In the IST method a crucial role is played by the initial Marchenko kernels from the left $\Omega_l(\alpha)$ and from the right $\Omega_r(\alpha)$ which are connected to the above scattering coef cients and spectral sums as follows:

$$\Omega_l(\alpha) = \rho(\alpha) + S_l(\alpha), \qquad \text{for } \alpha \geq 0, \tag{12}$$

$$\Omega_r(\alpha) = \ell(\alpha) + S_r(\alpha), \qquad \text{for } \alpha \leq 0, \tag{13}$$

where, using Fourier transforms and their inverses,

$$\rho(\alpha) = \mathcal{F}^{-1}\{R(\lambda)\}, \qquad \ell(\alpha) = \frac{1}{2\pi}\mathcal{F}\{L(\lambda)\}. \tag{14}$$

III. Numerical Method

As shown in [5], the scattering data consisting of $S(\lambda, 0)$, the bound states with their multiplicity and the norming constants can be computed by means of the following four consecutive steps:

Step 1: Starting from the initial potential $u(x, 0)$, we compute, for $y \geq x$, the pairs of auxiliary functions $(\overline{K}^{\text{up}}(x, y), \overline{K}^{\text{dn}}(x, y))$ and $(K^{\text{up}}(x, y), K^{\text{dn}}(x, y))$ and, for $y \leq x$, the two pairs of auxiliary functions $(\overline{M}^{\text{up}}(x, y), \overline{M}^{\text{dn}}(x, y))$ and $(M^{\text{up}}(x, y), M^{\text{dn}}(x, y))$. The rst two pairs of functions can be obtained by solving the following systems of two structured Volterra integral equations (see, for instance, [7] and [8]):

$$\overline{K}^{\text{up}}(x, y) + \int_x^{\infty} u_0(z)\overline{K}^{\text{dn}}(z, z + y - x)\, dz = 0, \tag{15a}$$

$$\overline{K}^{\text{dn}}(x, y) - \int_x^{\frac{1}{2}(x+y)} u_0(z)\overline{K}^{\text{up}}(z, x + y - z)\, dz = \tfrac{1}{2} v_0(\tfrac{1}{2}(x + y)), \tag{15b}$$

and for the pair $(K^{\text{up}}, K^{\text{dn}})$ the structured Volterra system

$$K^{\text{up}}(x, y) + \int_x^{\frac{1}{2}(x+y)} u_0(z)K^{\text{dn}}(z, x + y - z)\, dz = -\tfrac{1}{2} u_0(\tfrac{1}{2}(x + y)), \tag{16a}$$

$$K^{\text{dn}}(x, y) - \int_x^{\infty} v_0(z)K^{\text{up}}(z, z + y - x)\, dz = 0. \tag{16b}$$

Notice that $v_0(x) = \pm\overline{u_0(x)}$, according to the $\pm$ sign in (1). Similarly, for $y \leq x$, the pairs $(\overline{M}^{\text{up}}, \overline{M}^{\text{dn}})$ and $(M^{\text{up}}, M^{\text{dn}})$ of auxiliary functions are the solutions of analogous systems of two structured Volterra equations. Considering that the auxiliary functions are, basically, the Fourier transforms of the Jost functions, these equations have been obtained by using the analyticity properties of the Jost functions [6] [7].

Step 2: The entries of the scattering matrix $S(\lambda, 0)$ can be computed by resorting to the following representation [7]:

$$T(\lambda) = \frac{1}{a_{l4}(\lambda)} = \frac{1}{a_{r1}(\lambda)}, \tag{17}$$

$$L(\lambda) = \frac{a_{l2}(\lambda)}{a_{l4}(\lambda)} = -\frac{a_{r2}(\lambda)}{a_{r1}(\lambda)}, \qquad R(\lambda) = -\frac{a_{l3}(\lambda)}{a_{l4}(\lambda)} = \frac{a_{r3}(\lambda)}{a_{r1}(\lambda)}, \tag{18}$$

where the $\{a_{lj}(\lambda)\}_j$ and $\{a_{rj}(\lambda)\}_j$ denote the entries of the transition matrices from the left and the right, respectively. As shown in [5], these entries can be computed as follows:

$$\begin{cases} a_{\ell 1}(\lambda) &= 1 - \displaystyle\int_{\mathbb{R}^+} e^{-i\lambda z}\, \bar{\Phi}^{\text{dn}}(z)dz, \\ a_{\ell 2}(\lambda) &= -\displaystyle\int_{\mathbb{R}} e^{2i\lambda y} u_0(y)dy - \int_{\mathbb{R}} e^{i\lambda z}\Phi^{\text{dn}}(z)dz, \\ a_{\ell 3}(\lambda) &= \displaystyle\int_{\mathbb{R}} e^{-2i\lambda y} v_0(y)dy + \int_{\mathbb{R}} e^{-i\lambda z}\bar{\Phi}^{\text{up}}(z)dz, \\ a_{\ell 4}(\lambda) &= 1 + \displaystyle\int_{\mathbb{R}^+} e^{i\lambda z}\Phi^{\text{up}}(z)dz, \end{cases} \tag{19}$$

where

$$\bar{\Phi}^{\text{dn}}(z) = \int_{\mathbb{R}} u_0(y)\bar{K}^{\text{dn}}(y, y + z)dy, \tag{20}$$

$$\Phi^{\text{dn}}(z) = \int_{-\infty}^{\frac{z}{2}} u_0(y)K^{\text{dn}}(y, z - y)dy, \tag{21}$$

$$\Phi^{\text{up}}(z) = \int_{\mathbb{R}} v_0(y)K^{\text{up}}(y, y + z)dy, \tag{22}$$

$$\bar{\Phi}^{\text{up}}(z) = \int_{-\infty}^{\frac{z}{2}} v_0(y)\bar{K}^{\text{up}}(y, z - y)dy. \tag{23}$$

In other words, once the auxiliary functions $\{\bar{K}^{\text{up}}, \bar{K}^{\text{dn}}\}$ and $\{K^{\text{up}}, K^{\text{dn}}\}$ have been obtained, the entries $\{a_{\ell,j}(\lambda)\}_j$ of the transition matrix for the left can be computed by resorting to proper quadrature formulae. An analogous procedure allows us to compute the entries $\{a_{r,j}(\lambda)\}_j$ of the transition matrix from the right [5]. After that the spectral matrix can be computed by using the procedure before illustrated.

In the literature other methods have been proposed to compute the transition matrices such as the T-matrix method [9] which is theoretically exact whenever the initial potential is piecewise constant. To our best knowledge, our method is the only one that allows one to compute the transition matrices under general hypotheses.

Step 3: De nition (14) suggests to compute $\rho(\alpha)$ and $\ell(\alpha)$ by resorting to the inverse and direct discrete Fourier transform. However, this procedure is effective whenever the initial potential is continuous, that is $u_0 \in C(\mathbb{R})$. If this is not the case, that is if $u_0 \in L^1(\mathbb{R})$ but $u_0 \notin C(\mathbb{R})$, the Fourier transforms $\rho(\alpha)$ and $\ell(\alpha)$ can be approximated by solving the following

structured Fredholm integral equations [5]

$$\rho(\alpha) + \int_0^\infty \Phi^{\text{up}}(z)\,\rho(z+\alpha)dz = -\frac{1}{2}v_0\left(\frac{\alpha}{2}\right) - \bar{\Phi}^{\text{up}}(\alpha), \tag{24}$$

$$\ell(\alpha) + \int_0^\infty \Phi^{\text{up}}(z)\,\ell(\alpha-z)dz = -\frac{1}{2}u_0\left(\frac{\alpha}{2}\right) - \Phi^{\text{dn}}(\alpha) \tag{25}$$

where Φ^{up}, $\bar{\Phi}^{\text{up}}$ and Φ^{dn} are given in (21)-(23).

Step 4: Following [7, (2.50a)-(2.50b)], we can claim [5] that for $y \geq x \geq 0$ the Marchenko kernel Ω_l is connected to the auxiliary functions $\overline{K}^{\text{dn}}$ and K^{dn} as follows:

$$\Omega_l(x+y) + \int_x^\infty K^{\text{dn}}(x,z)\Omega_l(z+y) = -\overline{K}^{\text{dn}}(x,y). \tag{26}$$

Assuming the auxiliary functions are known, (26) can be interpreted as a structured Fredholm integral equation having the initial Marchenko kernels Ω_l as its unknown. For $y \leq x \leq 0$ the Marchenko kernel Ω_r is connected to the auxiliary functions $\overline{M}^{\text{dn}}$ and M^{dn} by an analogous equation. It is important to note that, from the computational point of view, each Marchenko kernel can be treated as a function of only one variable, as we only have to deal with the sum of the two variables. As a result, the computation of Ω_l and Ω_r can be carried out maintaining the accuracy of the auxiliary functions [5].

Step 5: Once the inverse and direct Fourier transforms $\rho(\alpha)$ and $\ell(\alpha)$ of re ection coef cients $R(\lambda)$ and $L(\lambda)$ have been computed we can identify the parameters and coef cients of the spectral sums $S_l(\alpha)$ and $S_r(\alpha)$, noting that

$$S_l(\alpha) = \Omega_l(\alpha) - \rho(\alpha), \qquad S_r(\alpha) = \Omega_r(\alpha) - \ell(\alpha). \tag{27}$$

In fact, setting $M = m_1 + ... + m_n$, the matrix-pencil method proposed in [10] allows one to compute the parameters $\{n, m_j, \lambda_j\}$ and the coef cients $\{(\Gamma_l)_{js}\}$, given $S_\ell(\alpha)$ in $2N$ $(N > M)$ equidistant points $\alpha_j = a + jh$, $j = 0, 1, ..., 2N-1$ of an interval $[a, b]$ under the assumption that a reasonable overestimate $\tilde{M}$ of M is known.

The coef cients $\{(\Gamma_l)_{js}\}$ can then be computed by solving in the least square sense a linear system of order $N \times M$.

IV. Numerical Results

Let us now present some results concerning three examples.

A. Example 1

The rst example is the one-soliton potential

$$u_0(x) = 2i\eta\, e^{i(2\xi x+\phi)}\text{sech}(x_0 - 2\eta x), \tag{28}$$

where $\xi, \phi, x_0 \in \mathbb{R}$ and $0 \neq \eta \in \mathbb{R}$. In the numerical results reported below $x_0 = \phi = 0$, $\xi = 0.1$ and $\eta = 2$, so that the peak point position is $\mu_0 \equiv \frac{x_0}{2\eta} = 0$. As the initial scattering data associated to (28) can be obtained exactly [3], [1], we can compute very accurately the relative approximation error for all scattering data. In particular, assuming L large enough to have

$$|u_0(x)| < 10^{-16}, \quad |x| > L,$$

and assuming the symbol $\sim$ to denote the computed approximation of Marchenko kernels, we have obtained

$$\max_{x\in[0,L]}\left|\frac{\tilde{\Omega}_\ell(x) - \Omega_\ell(x)}{\Omega_\ell(x)}\right| \simeq \max_{x\in[-L,0]}\left|\frac{\tilde{\Omega}_r(x) - \Omega_r(x)}{\Omega_r(x)}\right| \simeq 3.2e-07.$$

Moreover, adopting analogous distinctions between exact and computing data, and assuming $\tilde{M} = 5$ we have obtained

$$n = 1, \quad m_1 = 1, \quad |\rho(\alpha)| \leq 10^{-16}, \quad \frac{|\tilde{\lambda} - \lambda|}{|\lambda|} = 4.11e-09$$

$$\frac{|\tilde{\Gamma}_\ell - \Gamma_\ell|}{|\Gamma_\ell|} = 3.24e-07, \qquad \frac{|\tilde{\Gamma}_r - \Gamma_r|}{|\Gamma_r|} = 3.24e-07.$$

B. Example 2

As a second example we consider the initial potential

$$u_0(x) = q_0 e^{i\mu x} e^{-x^2/\sigma},$$

where $q_0 > 0$, $\sigma > 0$, and $\mu \in \mathbb{R}$ which has been considered in [11] in the defocusing case.

We consider both the focusing case and the defocusing case with more values of q_0, μ, and σ.

In the focusing case with $q_0 = 2.5$, $\mu = 1$, and $\sigma = 2$, as shown in [5], we have two simple bound states $\{\lambda_1, \lambda_2\}$ whose real part is $-\frac{1}{2}$. Assuming $[-8, 8]$ as the support of the initial potential, our method recognizes these two simple bound states having real part equal to $-\frac{1}{2}$. In fact, in our case we obtain $\lambda_1 = -0.50 + 1.97i$ and $\lambda_2 = -0.50 + 0.79i$.

In the defocusing case, our method recognizes that there are no bound states. Taking $q_0 = 1.9$, $\mu = 1$ and $\sigma = 2$, for example, we obtain

$$\max_{\alpha\in[0,16]}|\Omega_\ell(\alpha) - \rho(\alpha)| \simeq \max_{\alpha\in[-16,0]}|\Omega_r(\alpha) - \ell(\alpha)| \simeq 10^{-10},$$

which means that $S_\ell(\alpha) = S_r(\alpha) = 0$. Moreover, we have checked the numerical validity of the algebraic symmetry properties (8). The results are at all satisfactory as Figure 1 shows where the behavior of the error function

$$E(\lambda) = \left\|\frac{1}{2}(\mathbf{S}^\dagger(\lambda)\mathbf{S}(\lambda) + \mathbf{S}(\lambda)\mathbf{S}^\dagger(\lambda)) - \mathbf{I}\right\|,$$

in the Gaussian defocusing case is depicted in the interval $\lambda \in [-16, 16]$, being $|u_0(x)| < 10^{-16}$ for $|x| > 8$.

C. Example 3

Let us now consider the initial truncated potential

$$u_{0,\tau}(x) = \begin{cases} 0, & x < \tau, \\ u_0(x), & x > \tau, \end{cases} \tag{29}$$

where u_0 is the initial potential de ned in (28) with $x_0 = \phi = 0$, $\xi = 0.1$, $\eta = 2$, and $\mu_0 = 0$. It is easy to prove that $u_{0,\tau}(x)$ has a bound state if $\tau < 0$ and we have no bound states if $\tau > 0$. By choosing $\tau = -1$ and $\tau = 1$, we obtain two truncated potentials whose behaviors are depicted in Figures 2 and 3, respectively. Let us also remark that, because the initial potential has a jump of discontinuity, the inverse and

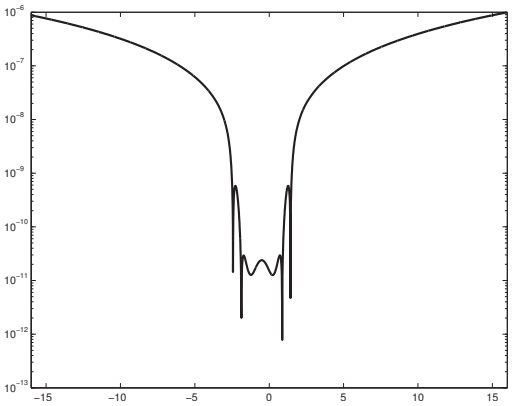

Fig. 1. E in semi logarithmic scale

direct Fourier transform of the re ection coef cients have been computed by solving equations (24)-(25) rather than (14) and (18).

In the case $\tau = -1$, our method recognizes that we have a single bound state at $\lambda = 1.99 + 0.1i$ with norming constants $\Gamma_\ell = 4.00i$ and $\Gamma_r = -4.00i$, and it also numerically veri es the symmetry property (9).

In the case $\tau = 1$, the method recognizes that the re ection coef cients are different from zero and also that there are no bound states.

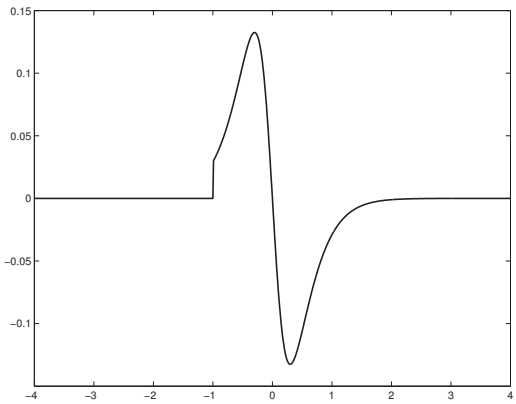

Fig. 2. Truncated one-soliton potential ($\tau = -1$)

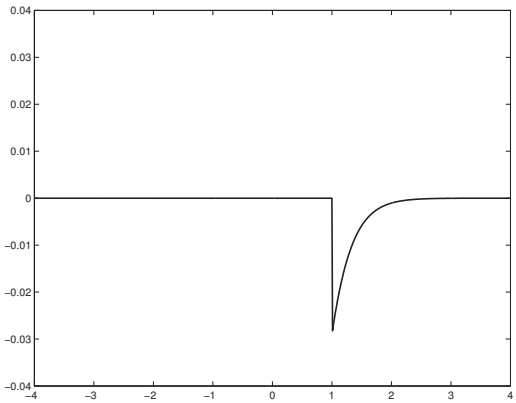

Fig. 3. Truncated one-soliton potential ($\tau = 1$)

V. Conclusions

Our method allows us to effectively compute the scattering data for the NLS equation with continuous initial potential as well as when it has jump discontinuities.

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