

## STRUCTURED MATRIX NUMERICAL SOLUTION OF THE NONLINEAR SCHRÖDINGER EQUATION BY THE INVERSE SCATTERING TRANSFORM

ANTONIO ARICÒ, CORNELIS VAN DER MEE, SEBASTIANO SEATZU

ABSTRACT. The initial-value problem for the focusing nonlinear Schrödinger (NLS) equation is solved numerically by following the various steps of the inverse scattering transform. Starting from the initial value of the solution, a Volterra integral equation is solved followed by three FFT to arrive at the reflection coefficient and initial Marchenko kernel. By convolution these initial data are propagated in time. Using structured-matrix techniques the time evolved Marchenko integral equation is solved to arrive at the solution to the NLS equation.

### 1. INTRODUCTION

In the focusing case, the cubic nonlinear Schrödinger (NLS) equation

$$iq_t = q_{xx} + 2|q|^2q, \quad q = q(x, t), \quad (1.1)$$

where the subscripts  $x \in \mathbb{R}$  and  $t > 0$  denote partial derivatives, has many applications [42, 31, 2, 6, 27, 1, 5]. As usual, we assume the initial potential  $q(x, 0)$  is known. This equation arises in signal propagation in optical fibers [8, 22, 23, 32], wave propagation in nonlinear media [42, 38, 15], and evolution of surface waves on sufficiently deep water [41, 40, 25].

Among the earlier methods to solve the NLS equation numerically are the split-step and Fourier methods used by Lake et al. [25] and by Hardin and Tappert [21]. Taha and Ablowitz [33, 34] made a comparative analysis of numerical methods to solve the NLS equation such as various finite-difference schemes (e.g. the Ablowitz-Ladik scheme [3, 4]), split-step Fourier methods [21, 25], and pseudospectral methods [18, 17], and decided in favor of the split-step Fourier method with pseudospectral methods as a good second. The dominant numerical method became the split-step Fourier method (e.g., [37, 8, 39]), even though in the 1990's orthogonal spline collocation methods were successfully applied to the NLS equation [30, 29, 28].

---

2000 *Mathematics Subject Classification.* 35Q55, 65M32, 45D05.

*Key words and phrases.* Nonlinear Schrödinger equation; inverse scattering transform; structured matrices; numerical computation.

©2009 Texas State University - San Marcos.

Submitted December 23, 2008. Published January 13, 2009.

Supported by the Italian Ministry of Education, Universities and Research (MIUR) under PRIN grant no. 2006017542-003, and by INdAM-GNCS.

In this paper we propose a method to solve the NLS equation (1.1), based on a new formulation of the inverse scattering transform (IST) method. As we shall prove, this revised formulation will allow us to compute the scattering data without resorting to the Zakharov-Shabat system. The IST method was first developed to solve the Korteweg-de Vries (KdV) equation by using the direct and inverse scattering theory of the Schrödinger equation [19, 20] and subsequently was applied to the NLS equation [42] and other nonlinear evolution equations [1, 2, 5, 6, 26, 27]. Contrary to the numerical methods mentioned above, our method follows the itinerary of the IST and hence guarantees that the NLS solutions obtained are indeed the ones found by using the IST method.

For later use we give some definitions. By  $\mathbb{C}^+$  and  $\mathbb{C}^-$  we denote the open upper and lower complex half-planes and by  $\overline{\mathbb{C}^+}$  and  $\overline{\mathbb{C}^-}$  their closures. Next, let  $H^s(\mathbb{R})$  denote the Sobolev space of those measurable functions  $u$  on  $\mathbb{R}$  whose Fourier transforms  $\hat{u}$  satisfy

$$\|u\|_{H^s(\mathbb{R})} := \left[ \int_{-\infty}^{\infty} d\xi |\hat{u}(\xi)|^2 (1 + \xi^2)^s \right]^{1/2} < +\infty.$$

Then, apart from a factor  $(2\pi)^{-1/2}$ , the Fourier transform  $\mathcal{F}$  is a unitary operator from  $L^{2,s}(\mathbb{R}) := L^2(\mathbb{R}; (1 + \xi^2)^s d\xi)$  onto  $H^s(\mathbb{R})$ .

## 2. INVERSE SCATTERING TRANSFORM REVISITED

The inverse scattering transform method to solve the NLS equation (1.1) in the so-called focusing case is based on the spectral analysis of the Zakharov-Shabat system [42]

$$-\mathbf{i}J \frac{\partial \psi}{\partial x}(\lambda, x) - V(x)\psi(\lambda, x) = \lambda\psi(\lambda, x), \quad x \in \mathbb{R}, \quad (2.1)$$

where  $\lambda$  is a complex spectral parameter,

$$J = \text{diag}(1, -1) = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \quad V(x) = \begin{bmatrix} 0 & \mathbf{i}q(x, 0) \\ \mathbf{i}q(x, 0) & 0 \end{bmatrix} = -V(x)^*,$$

and the complex potential  $q(\cdot, 0) \in L^1(\mathbb{R})$  is the initial state of the potential  $q(x, t)$ . Here overline denotes complex conjugation and the asterisk the matrix adjoint (conjugate transpose), while the matrix potential  $V(x)$  is skew-selfadjoint. Introducing, as usual in this context, the right and left Jost matrices  $\Psi(\lambda, x)$  and  $\Phi(\lambda, x)$  as those complex  $2 \times 2$  matrix solutions of (2.1) satisfying, for  $\lambda \in \mathbb{R}$ , the asymptotic conditions

$$\Psi(\lambda, x) = \text{diag}(e^{\mathbf{i}\lambda x}, e^{-\mathbf{i}\lambda x}) + o(1), \quad x \rightarrow +\infty, \quad (2.2a)$$

$$\Phi(\lambda, x) = \text{diag}(e^{\mathbf{i}\lambda x}, e^{-\mathbf{i}\lambda x}) + o(1), \quad x \rightarrow -\infty, \quad (2.2b)$$

we have, for  $\lambda \in \mathbb{R}$ , the proportionality relations

$$\Psi(\lambda, x) = \Phi(\lambda, x)A_l(\lambda), \quad \Phi(\lambda, x) = \Psi(\lambda, x)A_r(\lambda), \quad (2.3)$$

where the so-called transition matrices  $A_l(\lambda)$  and  $A_r(\lambda)$  are unitary  $2 \times 2$  matrices with unit determinant which are the inverses of each other. Thus there exist

complex numbers  $a(\lambda)$  and  $b(\lambda)$  such that<sup>1</sup>

$$A_l(\lambda) = \begin{bmatrix} \frac{a(\lambda)}{-b(\lambda)} & \frac{b(\lambda)}{a(\lambda)} \end{bmatrix}, \quad A_r(\lambda) = \begin{bmatrix} \frac{\overline{a(\lambda)}}{b(\lambda)} & -b(\lambda) \\ b(\lambda) & a(\lambda) \end{bmatrix}, \quad |a(\lambda)|^2 + |b(\lambda)|^2 = 1.$$

It is easily verified [10] that, for each  $\lambda \in \mathbb{R}$ ,  $\Psi(\lambda, x)$  and  $\Phi(\lambda, x)$  are unitary matrices with unit determinant.

The direct and inverse scattering theory of the Zakharov-Shabat system (2.1) can be found in many sources (e.g., [42, 31, 2, 16, 1, 27, 5]). The direct scattering problem consists of evaluating from an initial potential  $q(x, 0)$  in  $L^1(\mathbb{R})$  the reflection coefficient  $R(\lambda) := -b(\lambda)/a(\lambda)$  and the nontrivial so-called bound state solutions of the Zakharov-Shabat system whose two components belong to  $L^2(\mathbb{R})$ . The bound state spectral parameters turn out to be the zeros of the analytic continuation of  $a(\lambda)$  to  $\mathbb{C}^+$  and their complex conjugates [10, 5]. On the other hand, the inverse scattering problem consists of determining the potential  $q(x, t)$ , with  $q(\cdot, t) \in L^1(\mathbb{R})$  for each  $t > 0$ , from the reflection coefficient  $R(\lambda)$ , the bound state spectral parameters, and finitely many so-called norming constants. These data are used to write down the coupled system of two Marchenko integral equations whose unique solution specifies the potential  $q(x, t)$  and its energy density  $|q(x, t)|^2$ .

Traditionally the inverse scattering transform (IST) to solve the initial-value problem for the NLS equation (1.1) is described in terms of the following three steps:

- (1) Solve the direct scattering problem for (2.1) with initial potential  $q(x, 0)$ . Its solution determines the functions  $a(\lambda)$  and  $b(\lambda)$  resulting in the reflection coefficient  $R(\lambda)$ , the distinct bound state spectral parameters  $\lambda_1, \dots, \lambda_N \in \mathbb{C}^+$ , the norming constants  $\Gamma_{js}$  ( $j = 1, \dots, N$ ,  $s = 0, 1, \dots, n_j - 1$ ,  $n_j$  being the order of  $\lambda_j$  as a zero of  $a(\lambda)$ ), and the initial kernel  $\Omega(\alpha; 0)$  of the Marchenko integral equation.
- (2) Propagate the scattering data in time (cf. [9, 11]) to arrive at

$$R(\lambda; t) = e^{4i\lambda^2 t} R(\lambda), \quad \lambda_j(t) = \lambda_j,$$

$$\begin{bmatrix} \Gamma_{j0}(t) \\ \Gamma_{j1}(t) \\ \vdots \\ \Gamma_{j, n_j-1}(t) \end{bmatrix} = e^{-4iA_j^2 t} \begin{bmatrix} \Gamma_{j0} \\ \Gamma_{j1} \\ \vdots \\ \Gamma_{j, n_j-1} \end{bmatrix},$$

where the  $k, l$ -element of the matrix  $A_j$  is given by  $i\lambda_j \delta_{k,l} + \delta_{k, l+1}$  ( $k, l = 1, \dots, n_j$ ), with  $\delta_{k,l}$  denoting the Kronecker delta. In particular,  $\Gamma_{j0}(t) = e^{4i\lambda_j^2 t} \Gamma_{j0}$  if  $n_j = 1$ . The propagation of the Marchenko kernel in time is then computed as a consequence.

- (3) Solve the inverse scattering problem for the time evolved scattering data to arrive at the solution  $q(x, t)$ . This means solving the coupled system of Marchenko integral equations, associated to the scattering data above.

---

<sup>1</sup>In the sequel we shall make use of the fact that any unitary  $2 \times 2$  matrix with unit determinant has the form  $\begin{bmatrix} a & b \\ -\bar{b} & \bar{a} \end{bmatrix}$ , where  $|a|^2 + |b|^2 = 1$ .

The Marchenko integral equations consist of the following linear system:

$$B_1(x, \alpha; t) = \int_0^\infty d\beta \overline{\Omega(2x + \alpha + \beta; t)} B_2(x, \beta; t), \quad (2.4a)$$

$$B_2(x, \alpha; t) = - \int_0^\infty d\beta \Omega(2x + \alpha + \beta; t) B_1(x, \beta; t) - \Omega(2x + \alpha; t), \quad (2.4b)$$

valid for  $\alpha \geq 0$ ,  $t \geq 0$  and  $x \in \mathbb{R}$ . The Marchenko kernel  $\Omega$  is given by

$$\Omega(\alpha; t) = \hat{R}(\alpha; t) + \sum_{j=1}^N \sum_{s=0}^{n_j-1} \Gamma_{js}(t) \frac{\alpha^s}{s!} e^{i\lambda_j \alpha} \quad (2.5)$$

for  $\alpha \in \mathbb{R}$  and  $t \geq 0$ , where the caret denotes the Fourier transform and  $\hat{R}$  is given in terms of the reflection coefficient  $R(\lambda)$  by the Fourier transform

$$\hat{R}(\alpha; t) = \frac{1}{2\pi} \int_{-\infty}^\infty d\lambda e^{i\lambda \alpha} R(\lambda) e^{4i\lambda^2 t}. \quad (2.6)$$

As we shall see, the functions  $B_1$  and  $B_2$ , which are the unknown functions in (2.4), are strictly connected to the Zakharov-Shabat system. The potential  $q(x, t)$  and the associated energy then follow from

$$q(x, t) = 2B_2(x, 0^+; t), \quad (2.7)$$

$$\int_x^\infty dy |q(y, t)|^2 = -2B_1(x, 0^+; t). \quad (2.8)$$

In this article we do not follow exactly the path laid down by the inverse scattering transform to solve the initial value problem for the NLS equation (1.1). In fact, our method allows us to obtain the reflection coefficient  $R(\lambda)$  without solving the Zakharov-Shabat system.

### 3. DETAILED DESCRIPTION OF THE METHOD

Our method for solving the initial value problem for the NLS equation consists of the following four steps, where the first of three steps above has been subdivided in two:

- (1) Compute  $B_1(x, \alpha; 0)$  and  $B_2(x, \alpha; 0)$  from the initial data  $q(x, 0)$  by solving the Volterra integral system (2.4).
- (2) The scattering functions  $\hat{b}(\lambda)$  and  $\hat{a}(\lambda)$  are first computed using (3.14) below in terms of  $B_1(x, \alpha; 0)$  and  $B_2(x, \alpha; 0)$ . Their Fourier transforms  $b(\lambda)$  and  $a(\lambda)$  are then used to evaluate the reflection coefficient  $R(\lambda) = -b(\lambda)/a(\lambda)$ , and determine its initial Fourier transform  $\hat{R}(\alpha; 0)$  from (2.6). All these steps can be implemented using various FFT. By going through the same steps for scattering data involving two different truncations of the initial potential  $q(x, 0)$ , we arrive at the norming constants  $\Gamma_{js}$ . In this way we solve the direct scattering problem, that is we compute the relevant scattering data, without solving the Zakharov-Shabat system.
- (3) The time evolution of  $\hat{R}(\alpha; t)$  is then obtained by solving the initial-value problem for the linear partial differential equation

$$\frac{\partial \hat{R}}{\partial t} + 4i \frac{\partial^2 \hat{R}}{\partial \alpha^2} = 0 \quad (3.1)$$

where the initial value  $\hat{R}(\alpha; 0)$  can be immediately inferred by (2.6). Adding the norming constant terms as in (2.5), we get the time evolution of the Marchenko kernel  $\Omega(\alpha; t)$ .

- (4) Using  $\Omega(\alpha; t)$  the Marchenko system (2.4) is then solved, while the solution  $q(x, t)$  is evaluated from (2.7) and the associated energy  $|q(x, t)|^2$  from (2.8).

Let us organize our method for solving the initial value problem for the NLS equation in the following six modules.

**3.1. From initial potential  $q(x, 0)$  to  $B_1(x, \alpha)$  and  $B_2(x, \alpha)$ .** From (2.1) and (2.2) we easily derive the Volterra integral equations

$$\Psi(\lambda, x) = e^{i\lambda Jx} - \mathbf{i}J \int_x^\infty dy e^{-i\lambda(y-x)J} V(y) \Psi(\lambda, y), \tag{3.2a}$$

$$\Phi(\lambda, x) = e^{i\lambda Jx} + \mathbf{i}J \int_{-\infty}^x dy e^{-i\lambda(y-x)J} V(y) \Phi(\lambda, y), \tag{3.2b}$$

where the entries  $\mathbf{i}q(x, 0)$  and  $\overline{\mathbf{i}q(x, 0)}$  of  $V(x)$  belong to  $L^1(\mathbb{R})$ . Decomposing either of (3.2) into separate scalar equations, it is easy to see that the first column of  $\Psi(\lambda, x)e^{-i\lambda Jx}$  and the second column of  $\Phi(\lambda, x)e^{-i\lambda Jx}$  are continuous in  $\lambda \in \overline{\mathbb{C}^+}$ , are analytic in  $\lambda \in \mathbb{C}^+$ , and tend to a constant column vector as  $|\lambda| \rightarrow \infty$  in  $\overline{\mathbb{C}^+}$ . Similarly, the second column of  $\Psi(\lambda, x)e^{-i\lambda Jx}$  and the first column of  $\Phi(\lambda, x)e^{-i\lambda Jx}$  are continuous in  $\lambda \in \overline{\mathbb{C}^-}$ , are analytic in  $\lambda \in \mathbb{C}^-$ , and tend to a constant column vector as  $|\lambda| \rightarrow \infty$  in  $\overline{\mathbb{C}^-}$ . For details we refer to [5, 35, 14]. Now write [35, 36, 14]

$$\Psi(\lambda, x) = e^{i\lambda Jx} + \int_x^\infty dy K(x, y)e^{i\lambda Jy}, \tag{3.3a}$$

$$\Phi(\lambda, x) = e^{i\lambda Jx} + \int_{-\infty}^x dy G(x, y)e^{i\lambda Jy}, \tag{3.3b}$$

where for each  $x \in \mathbb{R}$  the following inequality holds:

$$\int_x^\infty dy |K(x, y)| + \int_{-\infty}^x dy |G(x, y)| < +\infty.$$

We now introduce the matrix functions  $B(x, \alpha)$  and  $C(x, \alpha)$  by

$$B(x, \alpha) = K(x, x + \alpha), \quad C(x, \alpha) = G(x, x - \alpha),$$

where  $\alpha \in \mathbb{R}^+$ . Then, as functions of  $\alpha \in \mathbb{R}^+$ , the entries of  $B(x, \alpha)$  and  $C(x, \alpha)$  belong to  $L^1(\mathbb{R}^+)$ . Moreover,

$$\Psi(\lambda, x)e^{-i\lambda Jx} = \text{diag}(1, -1) + \int_0^\infty d\alpha B(x, \alpha)e^{i\lambda J\alpha}, \tag{3.4a}$$

$$\Phi(\lambda, x)e^{-i\lambda Jx} = \text{diag}(1, -1) + \int_0^\infty d\alpha C(x, \alpha)e^{-i\lambda J\alpha}. \tag{3.4b}$$

Using the partitioning (see also [10, 35, 14])

$$Z = \begin{bmatrix} Z_1 & Z_2 \\ Z_3 & Z_4 \end{bmatrix},$$

we obtain, from the unitarity of  $\Psi(\lambda, x)$  and  $\Phi(\lambda, x)$ , that

$$B_1(x, \alpha) = \overline{B_4(x, \alpha)}, \quad B_2(x, \alpha) = -\overline{B_3(x, \alpha)}, \tag{3.5a}$$

$$C_1(x, \alpha) = \overline{C_4(x, \alpha)}, \quad C_2(x, \alpha) = -\overline{C_3(x, \alpha)}. \tag{3.5b}$$

The following result has been proved in detail in [14, 36], while in [10] the proof is given for potentials  $V(x)$  satisfying  $V(x)^* = V(x)$ . Observe that Theorem 3.1 and the second of (3.5a) imply (2.7) and (2.8) for  $t = 0$ .

**Theorem 3.1.** *We have the following identities:*

$$B_1(x, \alpha) = \int_x^\infty dy q(y, 0) B_3(y, \alpha), \quad (3.6a)$$

$$B_3(x, \alpha) = -\frac{1}{2} \frac{1}{q(x + \alpha/2, 0)} - \int_x^{x + \frac{\alpha}{2}} dy \overline{q(y, 0)} B_1(y, \alpha - 2(y - x)). \quad (3.6b)$$

Moreover, (3.6) has a unique solution satisfying

$$\sup_{x \in \mathbb{R}} \int_0^\infty dy (|B_1(x, \alpha)| + |B_3(x, \alpha)|) < +\infty. \quad (3.7)$$

Equations (3.6) suggest a method for computing  $B_1(x, \alpha)$  and  $B_2(x, \alpha)$  from the potential  $q(x, 0)$  when also using the second symmetry relation (3.5a). Alternatively, the linear system

$$C_1(x, \alpha) = - \int_{-\infty}^x dy q(y, 0) C_3(y, \alpha), \quad (3.8a)$$

$$C_3(x, \alpha) = \frac{1}{2} \frac{1}{q(x - \alpha/2, 0)} + \int_{x - \alpha/2}^x dy \overline{u(y)} C_1(y, \alpha + 2(y - x)), \quad (3.8b)$$

is uniquely solvable under the condition that

$$\sup_{x \in \mathbb{R}} \int_0^\infty dy (|C_1(x, \alpha)| + |C_3(x, \alpha)|) < +\infty.$$

Using the second of the symmetry relations (3.5b) we can compute  $C_1(x, \alpha)$  and  $C_2(x, \alpha)$  from  $q(x, 0)$  by solving (3.8).

**3.2. From  $B_1(x, \alpha)$  and  $B_2(x, \alpha)$  to the Marchenko kernel.** Writing the reflection coefficient in the form

$$R(\lambda) = \int_{-\infty}^\infty d\alpha e^{-i\lambda\alpha} \hat{R}(\alpha), \quad (3.9)$$

the Marchenko integral equations have the form (2.4), where, putting  $\Omega(\alpha) = \Omega(\alpha; 0)$  and  $\hat{R}(\alpha) = \hat{R}(\alpha, 0)$ , we have

$$\Omega(\alpha) = \hat{R}(\alpha) + \sum_{j=1}^N \sum_{s=0}^{n_j-1} \Gamma_{js} \frac{\alpha^s}{s!} e^{i\lambda_j \alpha}. \quad (3.10)$$

Here  $\lambda_1, \dots, \lambda_N$  are the distinct bound state spectral parameters in  $\mathbb{C}^+$  and  $\Gamma_{js}$  are the corresponding norming constants, where  $\Gamma_{j, n_j-1} \neq 0$  [9, 14]. Recalling that  $a(\lambda)$  extends to a function that is continuous in  $\lambda \in \overline{\mathbb{C}^+}$ , is analytic in  $\lambda \in \mathbb{C}^+$ , and tends to 1 as  $|\lambda| \rightarrow \infty$  in  $\overline{\mathbb{C}^+}$ , we **assume**<sup>2</sup> that  $a(\lambda) \neq 0$  for  $\lambda \in \mathbb{R}$  and define the transmission coefficient  $T(\lambda)$  by

$$T(\lambda) = \frac{1}{a(\lambda)}.$$

Then it easily follows that the bound state spectral parameter values  $\lambda_j \in \mathbb{C}^+$  are the (finitely many) poles of  $T(\lambda)$ .

<sup>2</sup>A technical assumption of this type appears in [2, 5, 14].

The following theorem shows that for sufficiently large  $x \in \mathbb{R}$  the Marchenko kernel  $\Omega(\gamma) = \Omega(\gamma; 0)$  can be found from  $B_1(x, \alpha)$  and  $B_2(x, \alpha)$  by solving (2.4b) for  $\Omega$  [14, App. B.1].

**Theorem 3.2.** *Suppose that, for some  $x \in \mathbb{R}$ , the function*

$$\Psi_1(\lambda, x) = e^{i\lambda x} \left[ 1 + \int_0^\infty d\alpha e^{i\lambda\alpha} B_1(x, \alpha) \right] = e^{i\lambda x} + \int_x^\infty dy e^{i\lambda y} K_1(x, y)$$

*does not vanish for  $\lambda \in \overline{\mathbb{C}^+}$ . Then the convolution integral equation*

$$\Omega(x; \alpha) + \int_\alpha^\infty d\gamma B_1(x, \gamma - \alpha) \Omega(x; \gamma) = -B_2(x, \alpha), \quad \alpha \in \mathbb{R}^+, \quad (3.11)$$

*has a unique solution satisfying*

$$\int_0^\infty d\alpha |\Omega(x; \alpha)| < +\infty.$$

*Moreover, there exists  $x_0 \in \mathbb{R}$  such that (3.11) is uniquely solvable for  $x > x_0$ .*

*Proof.* If  $\Psi_1(\lambda, x) \neq 0$  for each  $\lambda \in \overline{\mathbb{C}^+}$ , there exists  $Z(x, \alpha)$  with  $Z(x, \cdot) \in L^1(\mathbb{R}^+)$  such that

$$\frac{e^{i\lambda x}}{\Psi_1(\lambda, x)} = 1 + \int_0^\infty d\alpha e^{i\lambda\alpha} Z(x, \alpha), \quad \lambda \in \overline{\mathbb{C}^+}.$$

Using that

$$Z(x, \alpha) + B_1(x, \alpha) + \int_0^\alpha d\gamma B_1(x, \gamma) Z(x, \alpha - \gamma) = 0, \quad \alpha \in \mathbb{R}^+,$$

it is easily verified that

$$\Omega(x; \alpha) = -B_2(x, \alpha) - \int_\alpha^\infty d\gamma Z(x, \gamma - \alpha) B_2(x, \gamma)$$

is the unique solution of (3.11). Equations (3.6a) and (3.7) in combination with  $q(\cdot, 0) \in L^1(\mathbb{R})$  imply that

$$\lim_{x \rightarrow +\infty} \int_0^\infty d\alpha |B_1(x, \alpha)| = 0.$$

Choosing  $x_0 \in \mathbb{R}$  such that  $\int_0^\infty d\alpha |B_1(x, \alpha)| < 1$  for  $x > x_0$ , we get

$$|\Psi_1(\lambda, x) - e^{i\lambda x}| < 1, \quad x > x_0 \text{ and } \lambda \in \overline{\mathbb{C}^+},$$

which implies the unique solvability of (3.11) for  $x > x_0$ .  $\square$

Equations (2.2b) and (2.3) imply

$$\lim_{x \rightarrow -\infty} \sup_{\lambda \in \overline{\mathbb{C}^+}} |\Psi_1(\lambda, x) - e^{i\lambda x} a(\lambda)| = 0.$$

Thus there exists  $x_1 \in \mathbb{R}$  such that  $\Psi_1(\lambda, x)$  does not vanish for  $x < x_1$  and  $\lambda \in \overline{\mathbb{C}^+}$ , i.e., (3.11) is uniquely solvable for  $x < x_1$  if and only if  $a(\lambda) \neq 0$  for every  $\lambda \in \overline{\mathbb{C}^+}$ , i.e., if and only if there are no bound states. By the argument principle [13] it then easily follows that the combined zero order of  $\Psi_1(\lambda, x)$ , under the hypothesis that  $\Psi_1(\lambda, x) \neq 0$  for  $\lambda \in \mathbb{R}$ , is given by

$$p(x) = \frac{1}{2\pi} \left[ \arg(e^{-i\lambda x} \Psi_1(\lambda, x)) \right]_{\lambda=-\infty}^{+\infty}.$$

We have  $p(x) = 0$  for  $x > x_0$  and  $p(x)$  equal to the combined pole order of the transmission coefficient for  $x$  in some left half-line, with jumps occurring at those values of  $x$  where  $\Psi_1(\lambda, x)$  has a zero  $\lambda \in \mathbb{R}$ .

**Corollary 3.3.** *Suppose  $x \in \mathbb{R}$ . Then the following statements are true:*

- (1) *Equation (3.11) has at least one solution  $\Omega(x; \alpha)$  such that*

$$\int_0^\infty d\alpha |\Omega(x; \alpha)| < +\infty$$

and

$$\int_\alpha^\infty d\gamma \overline{B_2(x, \gamma - \alpha)} \Omega(x; \gamma) = \overline{B_1(x, \alpha)}, \quad \alpha \in \mathbb{R}^+. \quad (3.12)$$

- (2) *Equation (3.11) is a Fredholm integral equation of the second kind if and only if  $\Psi_1(\lambda, x) \neq 0$  for  $\lambda \in \mathbb{R}$ .*  
 (3) *The number of linearly independent solutions of the homogeneous counterpart of (3.11) coincides with  $p(x)$ .*

*Proof.* The first part follows by observing that the solution  $\Omega(x; \alpha) = \Omega(2x + \alpha)$  of (3.11) also satisfies (3.12), because (3.11) and (3.12) together coincide with the coupled Marchenko system (2.4) on switching known and unknown functions. Next, applying the Fourier transform to (3.11) for  $\alpha \in \mathbb{R}^+$ , we obtain

$$e^{i\lambda x} \Psi_1(-\lambda, x) \hat{\Omega}(x; \lambda) = -\hat{B}_2(x, \lambda), \quad \lambda \in \mathbb{R},$$

which implies the second and third parts.  $\square$

**3.3. Separation of the Marchenko kernel.** To implement the time evolution of the initial Marchenko kernel  $\Omega(\alpha)$  without knowing in advance the reflection and bound state contributions, we proceed as follows. Singling out the first row of the limit of  $\Psi(\lambda, x)e^{-i\lambda Jx}$  as  $x \rightarrow -\infty$ , we obtain from (3.2a) with the help of (2.2a) and (2.3)

$$e^{-i\lambda x} \Psi_1(\lambda, x) = 1 + \int_x^\infty dy q(y, 0) \Psi_3(\lambda, y) e^{-i\lambda y},$$

$$e^{-i\lambda x} \Psi_2(\lambda, x) = \int_x^\infty dy e^{-i\lambda y} q(y, 0) \Psi_4(\lambda, y).$$

Taking the limit as  $x \rightarrow -\infty$  and using (3.4a) we get

$$a(\lambda) = 1 + \int_0^\infty d\alpha e^{i\lambda\alpha} \hat{a}(\alpha), \quad (3.13a)$$

$$b(\lambda) = \int_{-\infty}^\infty d\alpha e^{-i\lambda\alpha} \hat{b}(\alpha), \quad (3.13b)$$

where [cf. (3.5a)]

$$\hat{a}(\alpha) = \int_{-\infty}^\infty dy q(y, 0) B_3(y, \alpha) = - \int_{-\infty}^\infty dy q(y, 0) \overline{B_2(y, \alpha)}, \quad (3.14a)$$

$$\begin{aligned} \hat{b}(\alpha) &= \frac{1}{2} \left[ q(\alpha/2, 0) + \int_{-\infty}^\alpha dy q(y/2, 0) B_4(y/2, \alpha - y) \right] \\ &= \frac{1}{2} \left[ q(\alpha/2, 0) + \int_{-\infty}^\alpha dy q(y/2, 0) \overline{B_1(y/2, \alpha - y)} \right]. \end{aligned} \quad (3.14b)$$

Using truncated potentials as specified below, the numerical solution of (3.14) can be greatly simplified.

**3.4. Computation of the Initial Marchenko Kernel.** To compute the initial Marchenko kernel without solving the Zakharov-Shabat system, we introduce a technique based on the use of truncated potentials. For  $\xi \in \mathbb{R}$  we define as a truncated potential the function

$$q_\xi(x, 0) = \begin{cases} q(x, 0), & x > \xi, \\ 0, & x < \xi, \end{cases} \quad (3.15)$$

which is associated to the initial potential  $q(x, 0)$ . Then the corresponding right Jost matrix is given by

$$\Psi_\xi(\lambda, x) = \begin{cases} \Psi(\lambda, x), & x \geq \xi, \\ e^{i\lambda J(x-\xi)} \Psi(\lambda, \xi), & x \leq \xi. \end{cases}$$

Hence

$$a_\xi(\lambda) = e^{-i\lambda\xi} \Psi_1(\lambda, \xi), \quad T_\xi(\lambda) = \frac{1}{a_\xi(\lambda)} = \frac{e^{i\lambda\xi}}{\Psi_1(\lambda, \xi)}, \quad (3.16a)$$

$$b_\xi(\lambda) = e^{-i\lambda\xi} \Psi_2(\lambda, \xi), \quad R_\xi(\lambda) = -\frac{b_\xi(\lambda)}{a_\xi(\lambda)} = -\frac{\Psi_2(\lambda, \xi)}{\Psi_1(\lambda, \xi)}. \quad (3.16b)$$

Consequently,  $p(\xi)$  coincides with the combined pole order of the transmission coefficient  $T_\xi(\lambda)$  corresponding to the truncated potential  $q_\xi$ .

Let us now explain an easy algorithm for computing separately the contributions to the initial Marchenko kernel of the reflection coefficient and of the bound states. First we compute  $B_1(x, \alpha)$  and  $B_2(x, \alpha)$  from the potential  $q(x, 0)$ . Then  $\hat{a}(\alpha)$  and  $\hat{b}(\alpha)$  are computed with the help of (3.14). These Fourier transforms are used to get  $b(\lambda)$  and  $a(\lambda)$ , to evaluate the initial reflection coefficient  $R(\lambda) = -b(\lambda)/a(\lambda)$ , and finally to compute its Fourier transform  $\hat{R}(\alpha)$ .

We note that an appropriate use of the truncated potential may greatly simplify the computation of  $\hat{a}(\alpha)$  and  $\hat{b}(\alpha)$ . Indeed, denoting by  $\hat{a}_\xi$  and  $\hat{b}_\xi$  the functions  $\hat{a}$  and  $\hat{b}$  associated with the truncated potential, we have

$$\hat{a}_\xi(\alpha) = \begin{cases} B_1(\xi, \alpha), & \alpha \geq 0, \\ 0, & \alpha < 0, \end{cases} \quad \hat{b}_\xi(\alpha) = \begin{cases} -B_3^*(\xi, \alpha - 2\xi), & \alpha \geq 2\xi, \\ 0, & \alpha < 2\xi. \end{cases} \quad (3.17)$$

If  $\|q\|_1 \leq (\pi/2)$ , there are no bound states [24] and hence  $\Omega(\alpha) = \hat{R}(\alpha)$ . On the other hand, if  $\|q\|_1 > (\pi/2)$ , we choose  $\zeta \in \mathbb{R}$  such that  $\|q_\zeta\|_1 < (\pi/2)$  and compute the corresponding  $\hat{R}_\zeta(\alpha)$ . Further, we compute the Marchenko kernel  $\Omega_\zeta(\alpha)$  by solving (2.4) at  $t = 0$ . Then the bound state part of the Marchenko kernel coincides with  $\Omega_\zeta(\alpha) - \hat{R}_\zeta(\alpha)$  and it can be identified by a least squares technique.

**3.5. Time evolution of the Marchenko kernel.** The Fourier transformed reflection coefficient  $\hat{R}(\alpha; t)$  and the Marchenko kernel  $\Omega(\alpha; t)$  both satisfy the partial differential equation (3.1). The initial value problem for this PDE has a unique solution in each Sobolev space  $H^s(\mathbb{R})$  and its solution is represented by a strongly continuous group of unitary operators  $U(t)$  acting on the initial data. This is easily

verified by moving (3.1) to  $L^{2,s}(\mathbb{R})$  by using  $(2\pi)^{-1/2}\mathcal{F}$  as a unitary equivalence, as indicated by the diagram

$$\begin{array}{ccc} L^{2,s}(\mathbb{R}) & \xrightarrow{e^{4i\lambda^2 t}} & L^{2,s}(\mathbb{R}) \\ (2\pi)^{-1/2}\mathcal{F} \downarrow & & \downarrow (2\pi)^{-1/2}\mathcal{F} \\ H^s(\mathbb{R}) & \xrightarrow{U(t)} & H^s(\mathbb{R}) \end{array}$$

In [9] the time evolution of the Marchenko kernel has been given in the multisoliton case, where the reflection coefficient  $R(\lambda) \equiv 0$ . In this case there exist a complex  $p \times p$  matrix  $A$  having all of its eigenvalues in the right half-plane, a complex column vector  $B$  and a complex row vector  $C$  such that

$$\Omega(\alpha; 0) = Ce^{-\alpha A}B.$$

It then follows that the time evolved Marchenko kernel is given by

$$\Omega(\alpha; t) = Ce^{-\alpha A}e^{-4itA^2}B.$$

The free Schrödinger group closely related to  $U(t)$  has been studied in detail in [12, Ch. 2], where Lemma 3.4 is proved in a different way.

**Lemma 3.4.** *Let  $\hat{R}(\cdot; 0)$  be an element of  $L^1(\mathbb{R}) \cap L^2(\mathbb{R})$ . Then the unique solution  $\hat{R}(\cdot; t)$  of the partial differential equation*

$$\frac{\partial \hat{R}}{\partial t} + 4i \frac{\partial^2 \hat{R}}{\partial \alpha^2} = 0 \tag{3.18}$$

in  $L^2(\mathbb{R})$  is given by the expression

$$\hat{R}(\alpha; t) = [U(t)\hat{R}(\cdot; 0)](\alpha) = \frac{1+i}{4\sqrt{2\pi|t|}} \int_{-\infty}^{\infty} d\beta e^{-\frac{1}{16t}i(\alpha-\beta)^2} \hat{R}(\beta; 0). \tag{3.19}$$

If  $\hat{R}(\cdot; 0) \in L^2(\mathbb{R})$ , the solution of (3.18) in  $L^2(\mathbb{R})$  is given by

$$\hat{R}(\alpha; t) = [U(t)\hat{R}(\cdot; 0)](\alpha) = \lim_{N \rightarrow +\infty} \frac{1+i}{4\sqrt{2\pi|t|}} \int_{-N}^N d\beta e^{-\frac{1}{16t}i(\alpha-\beta)^2} \hat{R}(\beta; 0). \tag{3.20}$$

*Proof.* Suppose  $\hat{R}(\cdot; 0) \in L^2(\mathbb{R})$ . Then using Plancherel's theorem twice we get

$$\begin{aligned} \hat{R}(\alpha; t) &= \lim_{N \rightarrow +\infty} \frac{1}{2\pi} \int_{-N}^N d\lambda e^{-i\lambda\alpha} \hat{R}(\lambda; t) = \lim_{N \rightarrow +\infty} \frac{1}{2\pi} \int_{-N}^N d\lambda e^{-i\lambda\alpha} e^{4i\lambda^2 t} \hat{R}(\lambda; 0) \\ &= \lim_{N \rightarrow +\infty} \frac{1}{2\pi} \int_{-N}^N d\lambda e^{-i\lambda\alpha} e^{4i\lambda^2 t} \int_{-\infty}^{\infty} d\beta e^{i\lambda\beta} \hat{R}(\beta; 0). \end{aligned}$$

Supposing that  $\hat{R}(\cdot; 0) \in L^1(\mathbb{R}) \cap L^2(\mathbb{R})$ , we apply Fubini's Theorem to obtain

$$\begin{aligned} \hat{R}(\alpha; t) &= \lim_{N \rightarrow +\infty} \int_{-\infty}^{\infty} d\beta \left( \frac{1}{2\pi} \int_{-N}^N d\lambda e^{-i\lambda(\alpha-\beta)} e^{4i\lambda^2 t} \right) \hat{R}(\beta; 0) \\ &= \lim_{N \rightarrow +\infty} \int_{-\infty}^{\infty} d\beta \left( \frac{1}{2\pi} \int_{-N}^N d\lambda e^{4it[\lambda - \frac{1}{8t}(\alpha-\beta)]^2} \right) e^{-\frac{1}{16t}i(\alpha-\beta)^2} \hat{R}(\beta; 0). \end{aligned}$$

Making the change of variable  $\eta = 2\sqrt{|t|}[\lambda - \frac{1}{8t}(\alpha - \beta)]$ , we now get

$$\hat{R}(\alpha; t) = \lim_{N \rightarrow +\infty} \int_{-\infty}^{\infty} d\beta \left( \frac{1}{4\pi\sqrt{|t|}} \int_{2\sqrt{|t|}[-N - \frac{1}{8t}(\alpha-\beta)]}^{2\sqrt{|t|}[N - \frac{1}{8t}(\alpha-\beta)]} d\eta e^{i\eta^2} \right). \tag{3.21}$$

Using the Fresnel integrals [7, 7.3.1-7.3.2]

$$C(z) = \int_0^z dt \cos\left(\frac{\pi}{2}t^2\right), \quad S(z) = \int_0^z dt \sin\left(\frac{\pi}{2}t^2\right),$$

which satisfy  $C(+\infty) = S(+\infty) = \frac{1}{2}$  (cf. [7, 7.3.0]), we easily calculate

$$\begin{aligned} & \lim_{N \rightarrow +\infty} \frac{1}{4\pi\sqrt{|t|}} \int_{2\sqrt{|t|}[-N-\frac{1}{8t}(\alpha-\beta)]}^{2\sqrt{|t|}[N-\frac{1}{8t}(\alpha-\beta)]} d\eta e^{i\eta^2} = \frac{1}{2\pi\sqrt{|t|}} \int_0^\infty d\eta e^{i\eta^2} \\ & = \frac{1}{2\pi\sqrt{|t|}} \left[ \int_0^\infty d\eta \cos(\eta^2) + \mathbf{i} \int_0^\infty d\eta \sin(\eta^2) \right] = \frac{1 + \mathbf{i}}{4\sqrt{2\pi|t|}}. \end{aligned}$$

Using the Theorem of Dominated Convergence, (3.21) can be written as

$$\begin{aligned} \hat{R}(\alpha; t) &= \int_{-\infty}^\infty d\beta \lim_{N \rightarrow +\infty} \left( \frac{1}{4\pi\sqrt{|t|}} \int_{2\sqrt{|t|}[-N-\frac{1}{8t}(\alpha-\beta)]}^{2\sqrt{|t|}[N-\frac{1}{8t}(\alpha-\beta)]} d\eta e^{i\eta^2} \right) \\ &\quad \times e^{-\frac{1}{16t}\mathbf{i}(\alpha-\beta)^2} \hat{R}(\beta; 0) \\ &= \frac{1 + \mathbf{i}}{4\sqrt{2\pi|t|}} \int_{-\infty}^\infty d\beta e^{-\frac{1}{16t}\mathbf{i}(\alpha-\beta)^2} \hat{R}(\beta; 0), \end{aligned}$$

which implies (3.19). Equation (3.20) now easily follows.  $\square$

We now derive the following result.

**Theorem 3.5.** *Suppose  $\hat{R} \in L^1(\mathbb{R}) \cap L^2(\mathbb{R})$ . Then the Marchenko kernel is given by*

$$\Omega(\alpha; t) = \hat{R}(\alpha; t) + C e^{-\alpha A} e^{-4itA^2} B, \quad (3.22)$$

where  $A$ ,  $B$  and  $C$  are matrices and

$$\hat{R}(\alpha; t) = \frac{1 + \mathbf{i}}{4\sqrt{2\pi|t|}} \int_{-\infty}^\infty d\beta e^{-\frac{1}{16t}\mathbf{i}(\alpha-\beta)^2} \hat{R}(\beta; 0). \quad (3.23)$$

**3.6. Solving Marchenko equations to get NLS solution.** Now that the time evolved Marchenko kernel  $\Omega(\alpha, t)$  has been evaluated, we solve the system of Marchenko equations (2.4) and then apply (2.7) to arrive at the NLS solution  $q(x, t)$ . To compute the squared modulus  $|q(x, t)|^2$ , we employ (2.8) in the following form:

$$|q(x, t)|^2 = 2 \frac{\partial B_1}{\partial x}(x, 0^+; t). \quad (3.24)$$

#### 4. ALGORITHMS

To solve the NLS equation (1.1) we start with a truncated potential  $q_\xi(x, 0)$  and apply six steps, under the hypothesis that  $q(x, 0)$  has at most one bound state. We note that our method recognizes automatically if the initial potential allows one bound state or none. In other words, assume that  $q_\xi$  has at most one bound state.

The six steps are as follows:

4.1. **Solution of the Volterra system.** We have to solve the system

$$B_{1,\xi}(x, \alpha) - \int_x^{+\infty} q_\xi(y)B_{3,\xi}(y, \alpha)dy = 0, \tag{4.1a}$$

$$\int_x^{x+\frac{\alpha}{2}} \overline{q_\xi(y)}B_{1,\xi}(y, \alpha - 2(y - x))dy + B_{3,\xi}(x, \alpha) = -\frac{1}{2}\overline{q_\xi(x + \alpha/2)}. \tag{4.1b}$$

where  $q_\xi(x, 0)$ ,  $x \in \mathbb{R}$ , is given and  $B_{1,\xi}(x, \alpha)$  and  $B_{3,\xi}(x, \alpha)$ ,  $x \in \mathbb{R}$  and  $\alpha \in \mathbb{R}^+$ , are the functions to compute. The system is solved in a Cartesian grid by recursively applying a local formula obtained by the composite Simpson's rule. The recursion scheme is applied in each row  $\{\alpha_j = 2hj\}$  of the grid starting with  $j = 2$ , and going on from right to left in each row grid  $\{x_i = ih\}$ , as Fig. 1 shows. Note that  $B_{1,\xi}$ ,

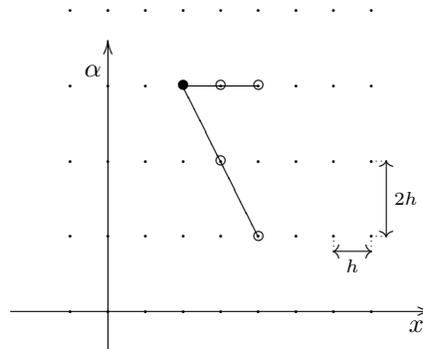


FIGURE 1. Pattern used for solving the Volterra system (4.1)

$B_{3,\xi}$  can be obtained by using the relations

$$B_{1,\xi}(x, \alpha) = \begin{cases} B_1(x, \alpha), & x \geq \xi, \\ B_1(\xi, \alpha), & x < \xi, \end{cases} \tag{4.2a}$$

$$B_{3,\xi}(x, \alpha) = \begin{cases} B_3(x, \alpha), & x \geq \xi, \\ B_3(\xi, 2x + \alpha - 2\xi), & x < \xi, 2x + \alpha \geq 2\xi, \\ 0, & x < \xi, 2x + \alpha < 2\xi. \end{cases} \tag{4.2b}$$

Hence, to solve (4.1) for any fixed  $\xi$ , we can limit ourselves to solving it for  $x \geq \xi$ , after replacing  $B_{1,\xi}$  and  $B_{3,\xi}$  with  $B_1$  and  $B_3$  and  $q_\xi$  with  $q$ .

4.2. **Computation of  $\hat{a}_\xi$  and  $\hat{b}_\xi$ .** As we are considering truncated potentials, we do not need to use the formulas (3.14). Indeed, more simply, we can compute them by using (3.17). Note that, as a consequence of the decay of  $B_1$  and  $B_3$ , which is of the same order as for  $q$ , the above formulas could also be used numerically in the case of a non-truncated potential. Let us emphasize that, in such a way, we are able to compute  $\hat{a}_\xi$  and  $\hat{b}_\xi$  without resorting to the Zakharov-Shabat system.

4.3. **Computation of  $\hat{R}_\xi(\alpha)$ .** The computation of  $\hat{R}_\xi$  can be carried out by means of three FFT's. In fact we need two FFT's to compute  $a_\xi(\lambda)$  and  $b_\xi(\lambda)$  from  $\hat{a}_\xi(\alpha)$  and  $\hat{b}_\xi(\alpha)$ . We need a third FFT to compute  $\hat{R}_\xi(\alpha)$  from  $R_\xi(\lambda) = -b_\xi(\lambda)/a_\xi(\lambda)$ .

**4.4. Computation of the Initial Marchenko kernel.** To compute the Marchenko kernel we still have to evaluate the parameters of a possible bound state. For this purpose, we resort to an artifice: we introduce an additional truncated potential  $q_\zeta$ , with  $\zeta > \xi$  so large as not to admit a bound state, which is true if  $\|q_\zeta\|_1 < \pi/2$ . As a consequence  $\Omega_\zeta(\alpha) = \hat{R}_\zeta(\alpha)$ , while  $\Omega_\xi(\alpha) = \hat{R}_\xi(\alpha) + \Gamma_\xi e^{-\gamma_\xi \alpha}$ , where  $\Gamma_\xi = 0$  if and only if there is no bound state.

We now note that for  $\alpha \geq 2\zeta$  we have  $B_1(\alpha, \cdot) = B_{1,\xi}(\alpha, \cdot) = B_{1,\zeta}(\alpha, \cdot)$  and  $B_2(\alpha, \cdot) = B_{2,\xi}(\alpha, \cdot) = B_{2,\zeta}(\alpha, \cdot)$ , which implies that both  $\Omega_\xi(\alpha)$  and  $\Omega_\zeta(\alpha)$  solve the same integral system, so that  $\Gamma_\xi e^{-\gamma_\xi \alpha} = \hat{R}_\zeta(\alpha) - \hat{R}_\xi(\alpha)$ . As a result we can compute numerically  $\hat{R}_\zeta(\alpha) - \hat{R}_\xi(\alpha)$  for  $\alpha \geq 2\zeta$  and then apply a least squares technique to estimate the parameters  $\Gamma_\xi$  and  $\gamma_\xi$ . Hereafter, for the sake of simplicity, we shall omit the subscript  $\xi$ .

**4.5. Time evolution of the Marchenko kernel.** Let us assume we have one bound state and the order of the corresponding zero  $\gamma$  of  $a(\lambda)$  is 1. In this case  $\Omega(\alpha, t) = \hat{R}(\alpha, t) + \Gamma e^{-\gamma \alpha} e^{-4i\gamma^2 t}$  where  $\hat{R}(\alpha, t)$  is the solution of the initial value differential problem

$$\begin{cases} \frac{\partial \hat{R}}{\partial t} + 4i \frac{\partial^2 \hat{R}}{\partial \alpha^2} = 0, & \alpha \in \mathbb{R}, t > 0 \\ \hat{R}(\alpha, 0) = \hat{R}(\alpha) \end{cases}$$

For an effective approximation of  $\hat{R}(\alpha, t)$  we distinguish two situations:

- we have to compute  $\hat{R}(\alpha, t)$  at a fixed  $t = t_0$ , with  $t_0$  not too small ( $t_0 \geq 1$ , say);
- we have to compute  $\hat{R}(\alpha, t)$  for  $0 < t < t_0$ .

In the former case we compute  $\hat{R}(\alpha, t_0)$  by using (3.19), i.e., we compute a discrete convolution. In the latter case the best strategy consists of discretizing the differential equation with respect to  $\alpha$  and then solving the resulting equation by using the Discrete Fourier Transform (DFT).

The first step generates the biinfinite system

$$\frac{\partial \hat{R}_j}{\partial t} = -\frac{4i}{h^2} (\hat{R}_{j+1} - 2\hat{R}_j + \hat{R}_{j-1}), \quad \hat{R}_j = \hat{R}_j(jh, t), \quad h > 0, j \in \mathbb{Z}. \quad (4.3)$$

Using the DFT; i.e., the transform

$$\tilde{S}(z) = \mathcal{F}\{S_j\} = \sum_{j=-\infty}^{\infty} S_j z^j, \quad z = e^{i\theta},$$

we convert the difference equation (4.3) into the ordinary differential equation

$$\frac{\partial}{\partial t} \mathcal{F}\{\hat{R}(z, t)\} = \frac{8i}{h^2} (1 - \cos(\theta)) \mathcal{F}\{\hat{R}(z, t)\}$$

whose solution is

$$\mathcal{F}\{\hat{R}(z, t)\} = e^{-\frac{4it}{h^2} (z+z^{-1}-2)} \mathcal{F}\{\hat{R}(z, 0)\},$$

where  $\mathcal{F}\{\hat{R}(z, 0)\}$  is known. The computation of  $\mathcal{F}\{\hat{R}(z, t)\}/\mathcal{F}\{\hat{R}(z, 0)\}$  can then be done resorting to a Bessel function and the inverse DFT gives us  $\{\hat{R}(jh, t)\}$ .

**4.6. Evolution in time of the initial potential.** As explained in Section 2 the evolution in time of the initial potential, as the one of the initial energy, is immediately given (formulas (2.7) e (2.8)) by the solution of the Marchenko system (2.4). For fixed values of  $t$  and  $x$ , we discretize the Marchenko systems at the equispaced points  $\{\alpha_i = ih\}$  by using the composite Simpson rule at the knots  $\{\beta_j = jh\}$ . In this way we obtain the linear system

$$\begin{pmatrix} I & -H^*D \\ HD & I \end{pmatrix} \begin{pmatrix} \mathbf{b}_1 \\ \mathbf{b}_2 \end{pmatrix} = \begin{pmatrix} \mathbf{0} \\ -\hat{\mathbf{R}} \end{pmatrix}$$

where  $D = \frac{h}{3} \text{diag}(1, 4, 2 \dots, 2, 4, 1)$ ,  $\mathbf{b}_s = B_s(ih, 0, t)$  for  $s = 1, 2$ ,  $H$  is the Hankel matrix defined by  $H_{ij} = \Omega(2x + \alpha_i + \beta_j)$  and  $\hat{\mathbf{R}} = \hat{R}(2ih, t)$ . This system can be written as follows

$$\begin{cases} (D + DHDH^*D)\mathbf{b}_2 = -D\mathbf{R}, \\ \mathbf{b}_1 = H^*D\mathbf{b}_2, \end{cases}$$

where in the first equation the matrix is symmetric positive definite and the solution is smooth so that it can be easily obtained by the Conjugate Gradient (CG) method.

As remarked before, the potential  $q(x_i, t)$  is given by  $2B_2(x_i, 0, t)$  and its energy  $\int_{x_i}^{+\infty} |q(y, t)|^2 dy$  by  $-2B_1(x_i, 0, t)$ .

## 5. NUMERICAL RESULTS

To assess the effectiveness of our method, we solved the NLS equation assuming as the initial potential the one defined in (3.15), where  $q(x, 0) = -8e^{2x}/(1+4e^{4x})$  is a single lobe potential [24]. More precisely, it is the one soliton potential considered in Appendix 8, where  $a = p = c = 1$ . As  $\|q\|_1 = \pi$ , the truncated potential  $q_\xi$  leads to at most one bound state. Since  $\int_{x_0}^{\infty} |q(x, 0)| dx = \frac{\pi}{2}$  (see Appendix 7 for further details), there is exactly one bound state if and only if  $\xi \leq x_0 = -\ln(\sqrt{2})$ . The possibility of solving the NLS equation, by using this initial potential, justifies the choice. The analytical solution of the corresponding NLS equation, as well as the analytical computation of the initial Marchenko kernel  $\Omega_\xi$  associated to the above family of truncated potentials  $q_\xi$ , are given in Appendix 8.

In our numerical experiments we considered the two truncated potentials:  $q_{-1}(x, 0)$  and  $q_1(x, 0)$ , which lead to one and zero bound states, respectively. As input data, we used the sampling of the initial potential in a grid of  $2^{10} + 1$  equispaced points of the interval  $[-7.5, 9]$ , roughly speaking is the support of  $q$ . We need this choice to make the steps described in Section 4.

Taking  $q_{-1}(x, 0)$ , the algorithm recognizes automatically the existence of one bound state and approximates, at a satisfactory precision, the parameters  $\Gamma$  and  $\gamma$  identifying the bound state. In our experiments we computed the potential in the rectangle  $\mathcal{D} = \{(x, t), \text{ s.t. } x \in [-1.90, 1.65] \text{ and } t \in [1, 1.6]\}$ , where the solution is not negligible (note that in the final step of the algorithm we can choose the subdomain where we want to compute the potential). The infinite norm of the pointwise discretization error; i.e., of the difference between the left and the right hand side of the NLS equation in the grid points of the domain considered is  $\simeq 10^{-3}$  if we take  $q_{-1}$  as the initial potential and  $\simeq 10^{-6}$  in the  $q_1$  case (this is mainly due to the fact that  $x_0$  is much further from 1 than from  $-1$ ).

In Figures 2 and 3, respectively, we depicted the real and imaginary parts, as well as the modulus, of the discretization error in  $\mathcal{D}$  pertaining to the potentials  $q_{-1}$  and  $q_1$ , respectively.

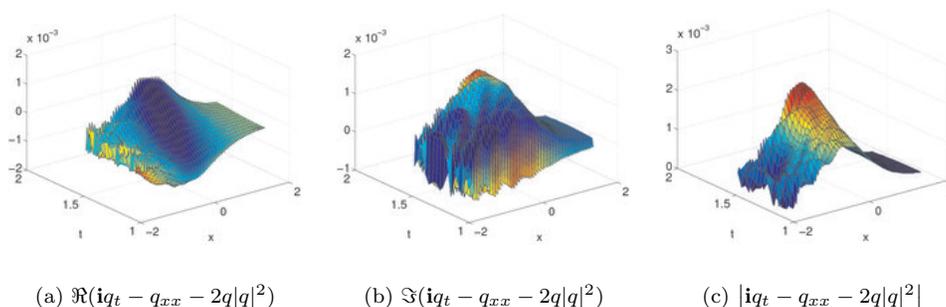


FIGURE 2. Discretization error determined by  $q_{-1}$  (in  $\mathcal{D}$ )

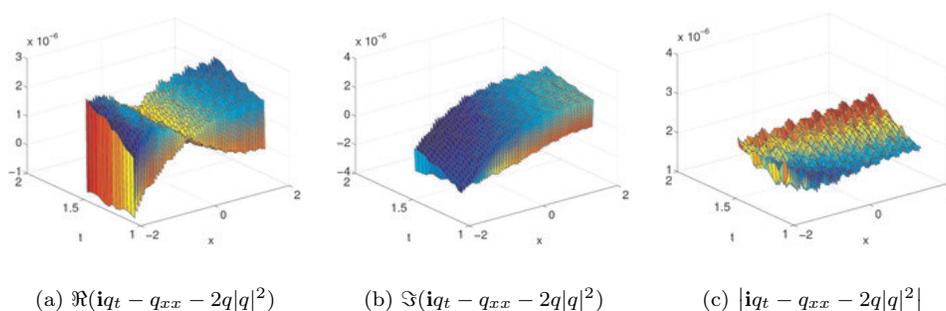


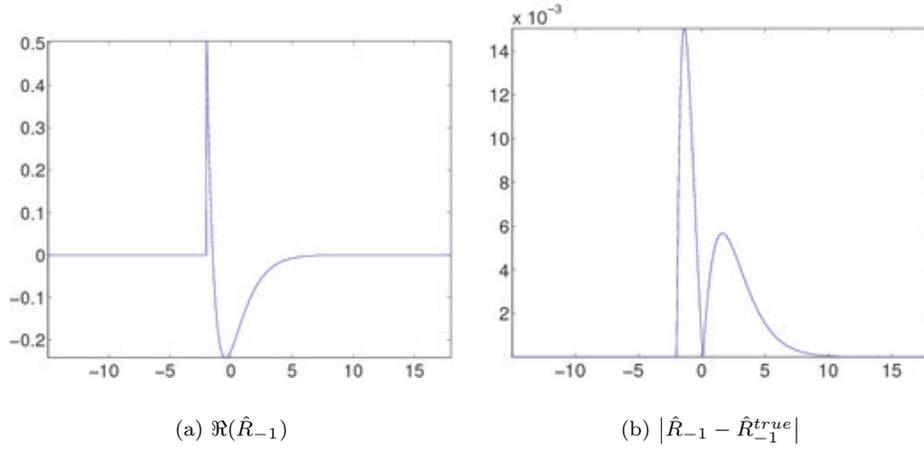
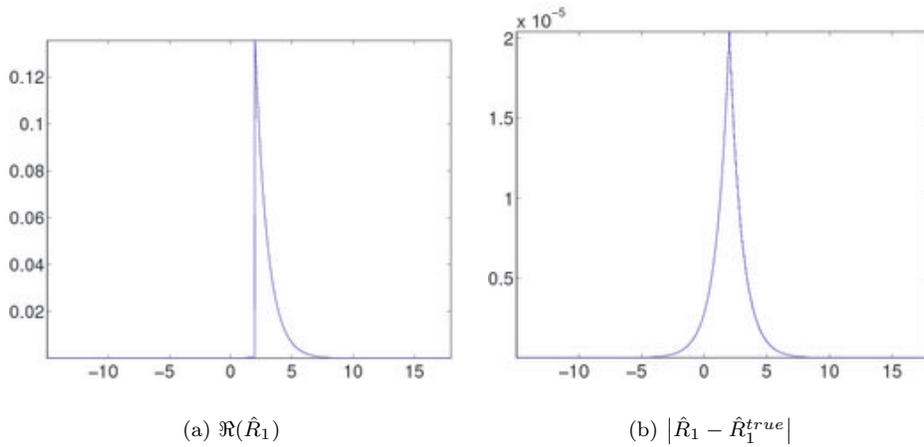
FIGURE 3. Discretization error determined by  $q_1$  (in  $\mathcal{D}$ )

The reflection coefficient  $\hat{R}_\xi$  is real (see Appendix 8). Our numerical computations give, for both  $\xi = 1$  and  $\xi = -1$ , a componentwise imaginary part which is  $\simeq 10^{-17}$ . Hence, in Figures 4 and 5 we give the real part of  $\hat{R}_\xi$  and the discretization error in the interval  $[-15, 18]$ .

Finally in Figures 6 and 7 we visualize the time evolution of  $q_{-1}$  and  $q_1$ , respectively (in  $\mathcal{D}$ ).

## 6. CONCLUSIONS

In this paper we give a new method to solve the NLS equation (1.1). Though it follows the path of the IST, it works without solving the Zakharov-Shabat system. From the numerical point of view it uses the structure of the kernels in the Marchenko integral equations optimally. The effectiveness of our method has been ascertained under the hypothesis that the initial potential has at most one bound state. It is an open problem to develop a method to treat the general case of  $n$  bound states. A second open problem, of great relevance to telecommunications,

FIGURE 4.  $\Re(\hat{R}_{-1}(x, 0))$  and the associated pointwise errorFIGURE 5.  $\Re(\hat{R}_1(x, 0))$  and the associated pointwise error

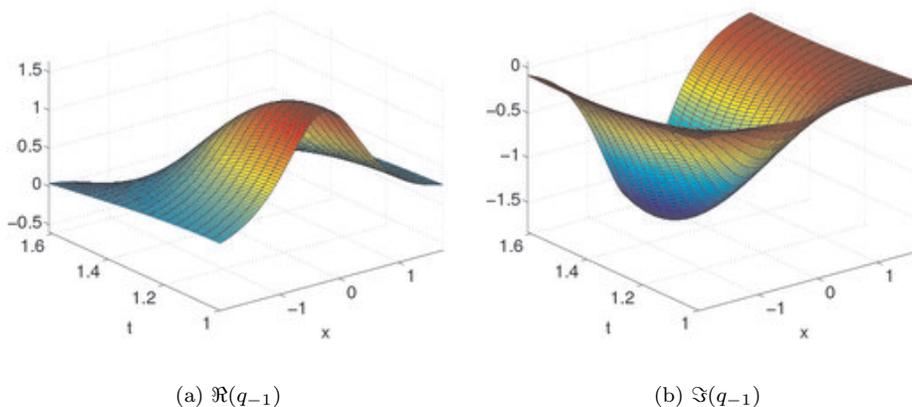
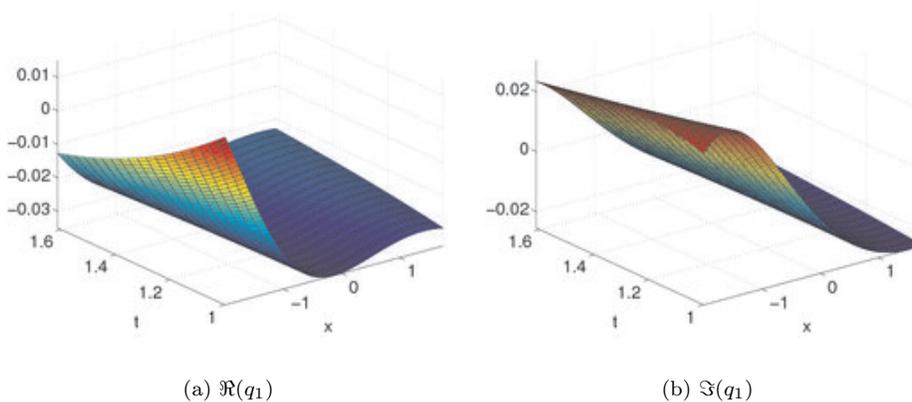
concerns the extension of our method to the solution of NLS equation with a damping factor in the energy term.

## 7. NUMBER OF BOUND STATES

In this appendix we summarize the results in [24] concerning the number of bound states:

- (1) There are no bound states if  $\|q\|_1 \leq (\pi/2)$ .
- (2) There are no bound states if  $q$  is real and

$$\|q\|_1 \leq \max(\|\max(q, 0)\|_1, \|\max(-q, 0)\|_1) \leq \frac{\pi}{2}.$$

FIGURE 6. Real and imaginary parts of  $q_{-1}(x, t)$ FIGURE 7. Real and imaginary parts of  $q_1(x, t)$ 

- (3) If  $q$  is a real potential of constant sign such that

$$(2N - 1)\frac{\pi}{2} < \|q\|_1 \leq (2N + 1)\frac{\pi}{2}, \quad (7.1)$$

then there are at least  $N$  positive imaginary bound state spectral parameters and no bound state spectral parameter in  $\mathbb{C}^+ \setminus (i\mathbb{R}^+)$  of maximal imaginary part among the bound state spectral parameters in  $\mathbb{C}^+$ .

- (4) If  $q$  is a single lobe potential [i.e., if  $q$  is real and has constant sign, and  $|q|$  is nonincreasing on  $\mathbb{R}^+$  and nondecreasing on  $\mathbb{R}^-$ ], then the number of positive imaginary bound state spectral parameters is exactly  $N$  and there are no bound state spectral parameters off the imaginary axis.

Thus if both  $\int_x^\infty dy \max(q(y, 0), 0) < (\pi/2)$  and  $\int_x^\infty dy \max(-q(y, 0), 0) < (\pi/2)$ , then  $p(x) = 0$ . Further, if  $q$  is a single lobe potential satisfying

$$(2N - 1)\frac{\pi}{2} < \int_x^\infty dy |q(y, 0)| \leq (2N + 1)\frac{\pi}{2}$$

for some positive integer  $N$ , then  $p(x) = N$ .

8. TRUNCATED ONE SOLITON POTENTIALS

In this appendix we give the Jost solutions and scattering coefficients of the truncated one-soliton potential.

Consider the initial potential

$$q(x, 0) = \frac{-2ce^{-2ax}}{1 + \frac{|c|^2}{4p^2}e^{-4px}}, \quad x \in \mathbb{R},$$

where  $a = p + iq$  with  $p > 0$  and  $0 \neq c \in \mathbb{C}$ , which stands for one soliton potential. The application of direct and inverse scattering transform leads to the following data:

$$\begin{aligned} \|q\|_1 &= \pi, \quad \Omega(\alpha) = ce^{-a\alpha}, \\ B_1(x, \alpha) &= \frac{-\frac{|c|^2}{2p}e^{-4px}e^{-\bar{a}\alpha}}{1 + (|c|^2/4p^2)e^{-4px}}, \quad B_2(x, \alpha) = \frac{-ce^{-2ax}e^{-a\alpha}}{1 + (|c|^2/4p^2)e^{-4px}}, \\ \Psi_1(\lambda, x) &= e^{i\lambda x} \frac{\lambda - i\gamma(x)}{\lambda + i\bar{a}}, \quad \Psi_2(\lambda, x) = \frac{ice^{-2ax}e^{-i\lambda x}}{(\lambda - ia)[1 + (|c|^2/4p^2)e^{-4px}]}, \end{aligned}$$

where

$$\gamma(x) = p \frac{-1 + \frac{|c|^2}{4p^2}e^{-4px}}{1 + (|c|^2/4p^2)e^{-4px}} + iq.$$

Moreover, as it is easy to check, the NLS solution is given by

$$q(x, t) = \frac{-2ce^{-2p(x-4qt)}e^{-2iq(x-2qt,0)}e^{-4itp^2}}{1 + (|c|^2/4p^2)e^{-4p(x-4qt)}}.$$

Now use subscripts  $\xi$  to denote quantities pertaining to the truncated potential  $q_\xi$ . Then the functions which characterize the reflection coefficient  $R(\lambda)$  are:

$$a_\xi(\lambda) = e^{-i\lambda\xi} \Psi_1(\lambda, \xi) = \frac{\lambda - i\gamma(\xi)}{\lambda + i\bar{a}} = 1 - \int_0^\infty d\alpha [\gamma(\xi) + \bar{a}]e^{i\lambda\alpha}e^{-\bar{a}\alpha},$$

and

$$\begin{aligned} b_\xi(\lambda) &= e^{-i\lambda\xi} \Psi_2(\lambda, \xi) \\ &= \frac{ice^{-2a\xi}e^{-2i\lambda\xi}}{(\lambda - ia)[1 + (|c|^2/4p^2)e^{-4p\xi}]} \\ &= \frac{-c}{1 + (|c|^2/4p^2)e^{-4p\xi}} \int_{2\xi}^\infty d\alpha e^{-i\lambda\alpha}e^{-a\alpha}. \end{aligned}$$

Note that  $i\gamma(\xi) \in \mathbb{C}^+$  if and only if  $\xi < x_0 := [\ln(|c|/2p)]/2p$ , which implies that we have a bound state if and only if  $\xi < x_0$ . Therefore,

$$R_\xi(\lambda) = -\frac{b_\xi(\lambda)}{a_\xi(\lambda)} = \frac{-ice^{-2a\xi}e^{-2i\lambda\xi}}{1 + (|c|^2/4p^2)e^{-4p\xi}} \frac{\lambda + i\bar{a}}{\lambda - ia} \frac{1}{\lambda - i\gamma(\xi)}$$

and

$$T_\xi(\lambda) = \frac{\lambda + \mathbf{i}\bar{a}}{\lambda - \mathbf{i}\gamma(\xi)}.$$

Let us now apply the inversion formula

$$\hat{R}_\xi(\alpha) = \frac{ce^{-2a\xi}}{1 + (|c|^2/4p^2)e^{-4p\xi}} \frac{1}{2\pi\mathbf{i}} \int_{-\infty}^{\infty} d\lambda e^{i\lambda(\alpha-2\xi)} \frac{\lambda + \mathbf{i}\bar{a}}{\lambda - \mathbf{i}a} \frac{1}{\lambda - \mathbf{i}\gamma(\xi)}.$$

For  $\xi > x_0$  we get

$$\Omega_\xi(\alpha) = \hat{R}_\xi(\alpha) = \begin{cases} \frac{2pc}{[a-\gamma(\xi)][1+(|c|^2/4p^2)e^{-4p\xi}]} e^{-a\alpha} = ce^{-a\alpha}, & \alpha > 2\xi, \\ \frac{-ce^{2\xi[\gamma(\xi)-a]}}{1+(|c|^2/4p^2)e^{-4p\xi}} \frac{\gamma(\xi)+\bar{a}}{\gamma(\xi)-a} e^{-\gamma(\xi)\alpha}, & \alpha < 2\xi. \end{cases}$$

On the other hand, for  $\xi < x_0$  we have  $N = 1$ ,  $n_1 = 1$ ,  $\lambda_1 = \mathbf{i}\gamma(\xi)$ , and

$$\Gamma(\xi) = -\frac{c}{1 + (|c|^2/4p^2)e^{-4p\xi}} \frac{\gamma(\xi) + \bar{a}}{\gamma(\xi) - a} e^{2\xi[\gamma(\xi)-a]},$$

whence

$$\hat{R}_\xi(\alpha) = \begin{cases} ce^{-a\alpha} - \Gamma(\xi)e^{-\gamma(\xi)\alpha}, & \alpha > 2\xi, \\ 0, & \alpha < 2\xi. \end{cases}$$

As a result, for  $\xi < x_0$  we have

$$\Omega_\xi(\alpha) = \hat{R}_\xi(\alpha) + \Gamma_{10}e^{-\gamma(\xi)\alpha} = \begin{cases} ce^{-a\alpha}, & \alpha > 2\xi, \\ \Gamma_{10}e^{-\gamma(\xi)\alpha}, & \alpha < 2\xi. \end{cases}$$

Thus in either case ( $\xi < x_0$  and  $\xi > x_0$ ) we have found the same expression for  $\Omega_\xi(\alpha)$ , both resorting to the Zakharov-Shabat system and ignoring it.

Let us compute now

$$\int_\xi^\infty dx |q(x, 0)| = 2|c| \int_\xi^\infty dx \frac{e^{-2px}}{1 + (|c|^2/4p^2)e^{-4px}} \\ z=(|c|/2p)e^{-2px} \quad 2 \int_0^{(|c|/2p)e^{-2p\xi}} \frac{dz}{1 + z^2} = 2 \arctan\left(\frac{|c|}{2p}e^{-2p\xi}\right).$$

Thus  $\int_\xi^\infty dx |q(x, 0)| = (\pi/2)$  if and only if  $\xi = x_0$  which implies that  $q_\xi(x)$  has one bound state if  $\xi \leq x_0$  and no bound state if  $\xi > x_0$ . Also,

$$\int_{-\infty}^\infty dx |q(x, 0)|^2 = \left[\frac{4p}{1 + (|c|^2/4p^2)e^{-4px}}\right]_{x=-\infty}^\infty = 4p.$$

### REFERENCES

- [1] M. J. Ablowitz and P. A. Clarkson, *Solitons, Nonlinear Evolution Equations and Inverse Scattering*, Cambridge Univ. Press, Cambridge, 1991.
- [2] M. J. Ablowitz, D. J. Kaup, A. C. Newell, and H. Segur, *The inverse scattering transform-Fourier analysis for nonlinear problems*, Stud. Appl. Math. **53**, 249–315 (1974).
- [3] M. J. Ablowitz and J. F. Ladik, *A nonlinear difference scheme and inverse scattering*, Studies in Appl. Math. **55**, 213–229 (1976).
- [4] M. J. Ablowitz and J. F. Ladik, *On the solution of a class of nonlinear partial difference equations*, Studies in Appl. Math. **57**, 1–12 (1976/77).
- [5] M. J. Ablowitz, B. Prinari, and A. D. Trubatch, *Discrete and Continuous Nonlinear Schrödinger Systems*, Cambridge Univ. Press, Cambridge, 2004.
- [6] M. J. Ablowitz and H. Segur, *Solitons and the Inverse Scattering Transform*, SIAM, Philadelphia, 1981.

- [7] M. Abramowitz and I. A. Stegun, *Handbook of Mathematical Physics*, Dover Publ., New York, 1964.
- [8] G. P. Agrawal, *Nonlinear Fiber Optics*, 3rd ed., Academic Press, New York, 2001.
- [9] T. Aktosun, F. Demontis, and C. van der Mee, *Exact solutions to the focusing nonlinear Schrödinger equation*, *Inverse Problems* **23**, 2171–2195 (2007).
- [10] T. Aktosun, M. Klaus, and C. van der Mee, *Direct and inverse scattering for selfadjoint Hamiltonian system on the line*, *Integral Equations and Operator Theory* **38**, 129–171 (2000).
- [11] Th. Busse, *Generalized Inverse Scattering Transform for the Nonlinear Schrödinger Equation*, Ph.D. Thesis, University of Texas at Arlington, 2008.
- [12] Th. Cazenave, *Semilinear Schrödinger Equations*, Courant LNM **10**, Amer. Math. Soc., Providence, RI, 2003.
- [13] J. B. Conway, *Functions of One Complex Variable*, Graduate Texts in Mathematics **11**, Springer, Berlin, 1973.
- [14] F. Demontis, *Direct and Inverse Scattering of the Matrix Zakharov-Shabat System*, Ph.D. Thesis, University of Cagliari, Italy, 2007.
- [15] R. K. Dodd, J. C. Eilbeck, J. D. Gibbon, and H. C. Morris, *Solitons and Nonlinear Wave Equations*, Academic Press, London, 1982.
- [16] W. Eckhaus and A. van Harten, *The Inverse Scattering Transformation and the Theory of Solitons*, North-Holland, Amsterdam, 1981.
- [17] B. Fornberg, *A Practical Guide to Pseudospectral Methods*, Cambridge University Press, Cambridge, 1996.
- [18] B. Fornberg and G. B. Whitham, *A Numerical and theoretical study of certain nonlinear wave phenomena*, *Philos. Trans. Roy. Soc. London, Series A*, **289**(1361), 373–404 (1973).
- [19] C. S. Gardner, J. M. Greene, M. D. Kruskal, and R. M. Miura, *Method for solving the Korteweg-de Vries equation*, *Phys. Rev. Lett.* **19**, 1095–1097 (1967).
- [20] C. S. Gardner, J.M. Greene, M. D. Kruskal, and R. M. Miura, *The Korteweg-de Vries equation and generalizations. VI. Methods for exact solution*, *Commun. Pure Appl. Math.* **27**, 97–133 (1974).
- [21] R. H. Hardin and F. D. Tappert, *Applications of the split-step Fourier method to the numerical solution of non-linear and variable-coefficient wave equations*, SIAM-SIGNUM Fall Meeting, Austin, October, 1972, *SIAM Rev. Chronicle* **15**, 423 (1973).
- [22] A. Hasegawa and M. Matsumoto, *Optical Solitons in Fibers*, 3rd ed., Springer, Berlin, 2002.
- [23] A. Hasegawa and F. Tappert, *Transmission of stationary nonlinear optical pulses in dispersive dielectric fibers. I. Anomalous dispersion*, *Appl. Phys. Lett.* **23**, 142–144 (1973).
- [24] M. Klaus and J. K. Shaw, *On the eigenvalues of Zakharov-Shabat systems*, *SIAM J. Math. Anal.* **34**(4), 759–773 (2003).
- [25] B. M. Lake, H.C. Yuen, H. Rungaldier, and W. E. Ferguson, *Nonlinear deep-water waves; theory and experiment. Part 2. Evolution of a continuous wave train*, *J. Fluid Mech.* **83**, 49–74 (1977).
- [26] V. A. Marchenko, *Sturm-Liouville Operators and Applications*, Birkhäuser OT**22**, Basel and Boston, 1986; also: Naukova Dumka, Kiev, 1977 [Russian].
- [27] S. Novikov, S. V. Manakov, L. P. Pitaevskii, and V. E. Zakharov, *Theory of Solitons: The Inverse Scattering Method*, Consultants Bureau, New York, 1984.
- [28] M. P. Robinson, *The solution of nonlinear Schrödinger equations using orthogonal spline collocation*, *Comput. Math. Appl.* **33**, 39–57 (1997); also: *Comput. Math. Appl.* **35**, 151 (1998).
- [29] M. P. Robinson and G. Fairweather, *Orthogonal spline collocation methods for Schrödinger-type equations in one space variable*, *Numer. Math.* **68**, 355–376 (1994).
- [30] M. P. Robinson, G. Fairweather, and B. M. Herbst, *On the numerical solution of the cubic Schrödinger equation in one space variable*, *J. Comput. Phys.* **104**, 277–284 (1993).
- [31] A. C. Scott, F. Y. F. Chu, and D. W. McLaughlin, *The soliton: A new concept in applied science*, *Proc. IEEE* **61**, 1443–1483 (1973).
- [32] J. K. Shaw, *Mathematical Principles of Optical Fiber Communications*, CBMS-NSF Regional Conference Series **76**, SIAM, Philadelphia, 2004.
- [33] Th. R. Taha and M. J. Ablowitz, *Analytical and numerical aspects of certain nonlinear evolution equations. I. Analytical*, *J. Comput. Phys.* **55**, 192–202 (1984).

- [34] Th. R. Taha and M. J. Ablowitz, *Analytical and numerical aspects of certain nonlinear evolution equations. II. Numerical, nonlinear Schrödinger equation*, J. Comput. Phys. **55**, 203–230 (1984).
- [35] C. van der Mee *Direct and inverse scattering for skewselfadjoint Hamiltonian systems*. In: J.A. Ball, J.W. Helton, M. Klaus, and L. Rodman (eds.), *Current Trends in Operator Theory and its Applications*, Birkhäuser OT **149**, Basel and Boston, 2004, pp. 407–439.
- [36] J. Villarroel, M. J. Ablowitz, and B. Prinari, *Solvability of the direct and inverse problems for the nonlinear Schrödinger equation*, Acta App. Math. **87**, 245–280 (2005).
- [37] J. A. C. Weideman and B. M. Herbst, *Split-step methods for the solution of the nonlinear Schrödinger equation*, SIAM J. Numer. Anal. **23**, 485–507 (1986).
- [38] G. B. Whitham, *Linear and Nonlinear Waves*, John Wiley, New York, 1974.
- [39] X. Xu and T. Taha, *Parallel split-step Fourier methods for nonlinear Schrödinger-type equations*, J. Math. Model. Algorithms 2, (2003), **3**, 185–201.
- [40] H. C. Yuen and B. M. Lake, *Nonlinear deepwater waves: Theory and experiment*, Phys. Fluids **18**, 756–760 (1975).
- [41] V. E. Zakharov, *Stability of periodic waves of finite amplitude on the surface of a deep fluid*, J. Appl. Mech. Tech. Phys. **4**, 190–194 (1968).
- [42] V. E. Zakharov and A. B. Shabat, *Exact theory of two-dimensional self-focusing and one dimensional self-modulation of waves in nonlinear media*, Sov. Phys. JETP **34**, 62–69 (1972).

DIP. MATEMATICA E INFORMATICA, UNIVERSITÀ DI CAGLIARI, VIALE MERELLO 92, 09123 CAGLIARI, ITALY

*E-mail address*, Antonio Aricò: [arico@unica.it](mailto:arico@unica.it)

*E-mail address*, Cornelis van der Mee: [cornelis@krein.unica.it](mailto:cornelis@krein.unica.it)

*E-mail address*, Sebastiano Seatzu: [seatzu@unica.it](mailto:seatzu@unica.it)