Utilization of the ExactMPF package for solving a discrete analogue of the nonlinear Schrödinger equation by the inverse scattering transform method

Adukov, V. M.; Mishuris, G.

Published in:
Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences
DOI:
10.1098/rspa.2022.0144
Publication date:
2023

Citation for published version (APA):
https://doi.org/10.1098/rspa.2022.0144
Utilization of the ExactMPF package for solving a discrete analogue of the nonlinear Schrödinger equation by the inverse scattering transform method

V. M. Adukov¹ and G. Mishuris²

¹Institute of Natural Sciences and Mathematics, South Ural State University, Chelyabinsk 454080, Russia
²Institute of Mathematics, Physics and Computer Science, Aberystwyth University, Aberystwyth SY23 3BZ, UK

We are revisiting the problem of solving a discrete nonlinear Schrödinger equation by the inverse scattering transform method, by use of the recently developed ExactMPF package within MAPLE Software. ExactMPF allows for an exact Wiener–Hopf factorization of matrix polynomials regardless of the partial indices of the matrix. The package can be widely used in various problems, where Wiener–Hopf factorization as one of the effective mathematical tools is required, as its code has already been disclosed. The analysis presented in this paper contains not only numerical examples of its use, but is also supported by appropriate and accurate \textit{a priori} estimations. The procedure itself guarantees that the ExactMPF package produces all computations arithmetically \textit{exactly}, and a detailed numerical analysis of various aspects of the computational algorithm and approximation strategies is provided in the case of a finite initial impulse.

1. Introduction

The inverse scattering transform (IST) method has been an effective tool in the exact solution of many of the...
nonlinear evolutionary equations of mathematical physics [1–6]. Being now a classic technique, IST remains an important numerical tool to analyse different aspects of the equations [7–18]. The main steps of the IST technique are given below, considering this specific example. However, to highlight a link between the results of this paper and the IST approach, we would like to underline that solving a matrix Riemann boundary value problem (or the Wiener–Hopf factorization problem of matrix functions) is one of the crucial steps of the IST numerical procedure [19–27].

The aim of this paper is to demonstrate how the ExactMPF package developed in [28] can be applied within the IST approach. While we follow the line of reasoning given in the work by Khabibullin & Shagalov [4], new results related to a specific approximation of the matrix functions on the unit circle, with consequences for the Wiener–Hopf factorization, are added. However, the basic advantage of our approach is that error-free calculations are used, avoiding the accumulation of computational errors. We underline the peculiarities of this approach and formulate advice for possible users in the main body of the paper and include all the data of the computations in the electronic supplementary material.

We consider the nonlinear Schrödinger equation:

\[ iq_t + q_{xx} = 2\sigma|q|^2q, \quad \sigma = \pm 1, \] (1.1)

with rapidly decreasing boundary conditions. This means that \(q(t, x)\) is an infinitely differentiable function that decays faster than any exponential as \(|x| \to 0\). The Cauchy problem for the equation (1.1) is formulated by use of the initial condition \(q(0, x) = q_0(x)\).

The general approach to the numerical integration of NLSEs is to discretize the equation [2, Ch.2], [29,30]. We study the discrete analogue of (1.1) that is represented by the following differential-difference equation:

\[ iu_{n,t} = (2u_n - u_{n+1} - u_{n-1}) + \sigma u_n \overline{u_n}(u_{n+1} + u_{n-1}), \] (1.2)

where \(u_n = u_n(\tau) = hq(x_n, \tau)\), \(u_{n,t}\) is a partial derivative in time, \(\tau = t/h^2\) and \(\overline{u_n}\) is the complex conjugate of \(u_n\). Here, \(h\) is a specific discretization length \((x_n = nh), n \in \mathbb{Z}\). The lattice equation (1.2) has been derived by Ablowitz and Ladik [1] in 1975 and since then, has been widely known as the AL (Ablowitz–Ladik) equation. The main purpose of our article is to demonstrate the capability of the newly developed mathematical package ExactMPF to deliver error-free factorization of matrix polynomials in applications. It turns out that solving the Ablowitz–Ladik equation (1.2) by the IST method is one such problem. A variant of ICT method proposed by Khabibullin & Shagalov in [4] is based on a sequential solution of a set of factorization problems for the Laurent matrix polynomials or for matrix functions that are well approximated by the polynomials. For this reason, the ExactMPF package is suited for this task.

Following the procedure in [4], to integrate the equation (1.2), an inverse problem from scattering theory for a 2 \times 2 system of difference equations is used:

\[ y_{n+1} = f_n(z)y_n, \quad f_n(z) = \left( \begin{array}{c} z \nu_n^{(0)} \sigma \overline{u_n^{(0)}} \\ zu_n^{(0)} \end{array} \right). \] (1.3)

Here, \(z\) is a spectral parameter, and \(u_n^{(0)} = u_n(0) = hq(x_n, 0)\) are the initial Cauchy data for the NLSE. We require that the potential \(u_n^{(0)}\) satisfies the conditions:

(i) problem (1.3) does not have a discrete spectrum;
(ii) the potential \(u_n^{(0)}\) is finite and its support is concentrated at the points \(n = -N_0, -N_0 + 1, \ldots, K_0\), where \(N_0 + 1, K_0\) are natural numbers;
(iii) \(\prod_{n=-N_0}^{K_0} (1 - \sigma|u_n^{(0)}|^2) > 0\).

Let us explain these conditions. Condition (i) means that we consider the soliton-free case. This is the most suitable case for testing the package ExactMPF, since it requires considerations of the factorization problem in the classical setting (see [4,6]). The second assumption, (ii), is convenient for numerical implementation, and is usually used as a replacement for any localized potential.
Figure 1. A general algorithm for solving nonlinear discrete NLSE by using the IST method is used in this paper. It follows the scheme (1.2) from Khabibullin & Shagalov [4] but slightly deviates at stage 3. The blue text in our scheme indicates this fact (we discuss this issue in more detail in the main body). The text in other colours (red and purple) highlights the key points of this paper. Specifically, red actions (stages 4–5 and 7–8) correspond to the application of the ExactMPF package. This, however, requires a correction of the matrices $L(n, z, \tau)$ (steps 6–7) to be able to perform the exact factorization.

The third constraint, (iii) guarantees that the matrix function $L(n, z)$ used below admits a canonical factorization. This fact is discussed in the next section.

With some modifications shown in figure 1, we mostly follow the scheme (1.2) for solving a discrete nonlinear evolutionary equation (1.2) by the IST method described in [4]. The major modification is the utilization of the matrix function $L(z)$ instead of $r(z)$, which is explained below. The red text emphasizes the new crucial fact, namely, that the respective factorizations are performed exactly via use of the ExactMPF package at stages 4–5 and 7–8. To make this possible, we have to slightly correct the matrices $L(n, z, \tau)$ (steps 6–7). The following results are new and the theoretical background is given in theorems 3.7–3.13.

2. The IST method for the discrete NLSE: the case of $\tau = 0$

We would like to mention here that the AL equation can be easy numerically solved on a compact interval and in finite time ($0 < t < t_m$) by Runge–Kutta or other numerical methods developed for ODEs. As a result of the computation, one obtains a solution given in all chosen discrete points (in time and space) lying within the entire described domain. It is delivered with a prescribed tolerance and represents the solution of the Cauchy problem up to the moment $t_m$ when the signal reaches the ends of the interval. On the other hand, the method used in this work (and in [4]) represents the solution of the Cauchy problem for (1.2) in the infinite interval (that is for any $n \in \mathbb{Z}$) and at any chosen time $t = t_0$. A finite interval $[-N, K]$ should be chosen by the user to extract the values of the solution. Here $N, K$ are sufficiently large natural numbers such that the support $[-N_0, K_0]$ of the finite initial potential $u_0(0)$ is a subset of $[-N, K]$. We discuss this issue in more detail after theorem 3.1 below.

Now we will consider the solution of (1.2) on the infinite interval, i.e. for $n \in \mathbb{Z}$. First, the direct scattering problem is solved for (1.3) (compare stages 1–2 from figure 1): the scattering matrix $S(z)$ is found via the asymptotics of the solution of (1.3) (for details, see [4]). It ensues that, for a finite initial potential, the scattering matrix $S(z)$ is represented by the formula

$$S(z) = Z^{-K_0-1} f_{K_0}(z) f_{K_0-1}(z) \cdots f_{-N_0}(z) Z^{-N_0}, \quad Z = \begin{pmatrix} z & 0 \\ 0 & 1 \end{pmatrix}, \quad (2.1)$$

and takes the form

$$S(z) = \begin{pmatrix} S_{11}(z) & \sigma S_{12}(z) \\ S_{21}(z) & S_{22}(z) \end{pmatrix}.$$

Note that in formula (2.1) we can take any interval $[-N_0, K_0]$ containing the support of the initial potential. The scattering matrix $S(z)$ will remain unchanged.
It is clear from (2.1) that the elements of the scattering matrix $S(z)$ are the Laurent polynomials (i.e., polynomials with respect to variables $z^{-1}$ and $z$, where $S_{11}(z)$ and $S_{22}(z)$ are polynomials with respect to $z^{-1}$ and $z$, respectively. Moreover, for any $z \neq 0$

$$S_{11}(z) = \overline{S_{22}(z^{-1})}, \quad S_{12}(z) = \overline{S_{21}(z^{-1})} \quad \text{and} \quad S_{22}(0) = S_{11}(\infty) = 1. \quad (2.2)$$

In particular, $S_{11}(z) = \overline{S_{22}(z)}$, $S_{12}(z) = \overline{S_{21}(z)}$ on the unit circle. Note also that from the definition of $S(z)$, it follows that the determinant $D = \det S(z) = S_{11}(z)S_{22}(z) - \sigma S_{12}(z)S_{21}(z)$ is the constant $U_\sigma > 0$ (see [4]), while, on the unit circle, $D = |S_{11}(z)|^2 - \sigma |S_{12}(z)|^2$. It is also shown therein that any zeros of the diagonal elements $S_{11}(z)$ and $S_{22}(z)$ lying in their analyticity domains are the eigenvalues of equation (1.3). Hence, assumption (i) is equivalent to the statement that $S_{11}(z) \neq 0$ for $|z| > 1$ and $S_{22}(z) \neq 0$ for $|z| < 1$. Following [4], we also assume that $S_{22}(z) \neq 0$ for $|z| = 1$, which guarantees that the spectrum of (1.3) does not contain points from the closed unit disc.

The next step in the algorithm is to solve the inverse scattering problem, i.e. to restore the potential $u_n(0)$ by the scattering matrix $S(z)$. Shabat [31] proved that this problem is equivalent to a matrix Riemann boundary value problem. Specifically, using the triangular factorizations of $S(z)$ (see formula (33) from [6, Ch. III, § 3]), we introduce the following matrix function

$$r(z) = \frac{1}{S_{22}(z)} \begin{pmatrix} 1 & -\sigma S_{12}(z) \\ S_{21}(z) & D \end{pmatrix}, \quad (2.3)$$

where $r(z)$ is included in a family of matrix functions

$$r(n, z) = Z^n r(z) Z^{-n} = \frac{1}{S_{22}(z)} \begin{pmatrix} 1 & -\sigma S_{12}(z)z^n \\ S_{21}(z)z^{-n} & D \end{pmatrix}, \quad n \in \mathbb{Z}, \quad (2.4)$$

and the matrix $Z = Z(z)$ has been defined in (2.1). The key point of the IST technique is to employ matrix Riemann boundary problems with the matrix coefficients $r(n, z)$, and this, in turn, requires the Wiener–Hopf factorization of matrix functions $r(n, z)$.

For our purposes, it is more convenient to use Laurent matrix polynomials (see stage 3 in figure 1)

$$L(n, z) = Z^n L(z) Z^{-n} = S_{22}(z) r(n, z) = \begin{pmatrix} 1 & -\sigma S_{12}(z)z^n \\ S_{21}(z)z^{-n} & D \end{pmatrix}, \quad n \in \mathbb{Z}, \quad (2.5)$$

where

$$L(z) = S_{22}(z) r(z) = \begin{pmatrix} 1 & -\sigma S_{12}(z) \\ S_{21}(z) & D \end{pmatrix}, \quad (2.6)$$

instead of the family of rational matrix functions $r(n, z)$. Note that the Laurent matrix polynomial $L(z)$ coincides with the matrix $G_2(z)$ from Zakharov et al. [6].

It is easily seen that $\det L(n, z) = S_{11}(z)S_{22}(z)$. Since $S_{22}(z) (S_{11}(z))$ is a polynomial in $z$ (in $z^{-1}$) and $S_{11}(z) \neq 0$ for $|z| \geq 1$, $S_{22}(z) \neq 0$ for $|z| \leq 1$, this representation is, in fact, a canonical Wiener–Hopf factorization of the scalar Laurent polynomial $\det L(n, z)$. It is not difficult to verify that $L(n, z)$ is a positive definite matrix function for $\sigma = -1$, and that it has a positive definite real part for $\sigma = 1$. These statements will be true only if the second constraint ($D = U_\sigma > 0$) from (iii) is fulfilled. Then (see, for example, [32]) the matrix functions $L(n, z)$ admit left canonical factorizations $L(n, z) = l_+(n, z)l_-(n, z)$.

**Remark 2.1.** If the initial (finite) potential $u_n(0) \in \mathbb{Q}(i)$, $n = -N_0, \ldots, K_0$, then the entries of $L(n, z)$, $n = -N_1, \ldots, K_1$ are polynomials over the field $\mathbb{Q}(i)$. Moreover, since $\det L(n, z)$ admits the exact Wiener–Hopf factorization, $\det L(n, z) = S_{11}(z)S_{22}(z)$, Theorem 2.2 from [28] states that the Laurent matrix polynomials $L(n, z)$ all admit the exact left canonical factorizations that can be found with the help of the ExactMPF package.

Since $S_{22}(z)$ is a polynomial in $z$ and $S_{22}(z) \neq 0$ in $|z| \leq 1$, the rational matrix functions $r(n, z)$ also admit left canonical factorizations $r(n, z) = r_+(n, z)r_-(n, z), |z| = 1$. In the approach presented
in [4], the matrix function \( F(n)(z) = r_+^{-1}(n+1,z)Zr_+(n,z) = r_-(n+1,z)Zr_1^{-1}(n,z) \) plays a crucial part. It is obvious that
\[
F(n) = l_+^{-1}(n+1,z)Zl_+(n,z) = l_-(n+1,z)Zl_1^{-1}(n,z).
\]
Since the factors \( l_-(n+1,z) \) are non-singular and bounded in the exterior of the unit disk (\( |z| \geq 1 \)), the maximal growth of the right-hand side of the latter identity is defined by the matrix \( Z \), we conclude that \( F(n)(z) \) is a matrix polynomial in \( z \) of degree 1 within the entire complex plane.

We will now show how to choose a specific factorization of \( L(n,z) \) by normalizing a suitable factor in such a way that \( F(n)(z) \) has the same form as \( f_n(z) \), as shown in (1.3).

For an arbitrary factorization \( L(n,z) = l_+(n,z)l_-(n,z) \), we denote \( l_+(n,0) = A_n = (\alpha_{ij})_{i,j=1,2} \), \( l_-(n,\infty) = B_n = (\beta_{ij})_{i,j=1,2} \), and \( C_n = A_nB_n = (c_{ij})_{i,j=1,2} \). Obviously, the non-singular matrix \( C_n \) is an invariant of the matrix function \( L(n,z) \), i.e. \( C_n \) does not depend on a normalization of the factorization. In the following, the invariants \( C_n \) play a key role in the analysis, and revealing their structure is also a crucial step. To do this, we will need the following:

Lemma 2.2. If \( L(n,z) = l_+(n,z)l_-(n,z) \) is a factorization of \( L(n,z) \), then
\[
L(n,z) = \widetilde{\text{\( l_+(n,z) \)}}\text{\( \tilde{l}_-(n,z) \)} = \frac{1}{\sigma} J_\sigma \bar{f}_n(\frac{n-1}{z}) J_\sigma \cdot J_\sigma \bar{f}_n(\frac{n-1}{z}) J_\sigma
\]
is also a factorization of \( L(n,z) \). Here
\[
J_\sigma = \begin{pmatrix} 0 & 1 \\ \sigma & 0 \end{pmatrix}
\]
and \( G^\dagger \) is the adjoint matrix of \( G \).

Proof. Since the matrix function \( L(n,z) \) has the following involution property: \( L(n,z) = \sigma J_\sigma L(n,z^{-1}) J_\sigma \), the statement (2.7) is its straightforward consequence.

 Proposition 2.3. The matrices \( C_n \) for all \( n \) have the following properties:

(i) \( \det C_n = 1 \),

(ii) \( c_{11}^n \neq 0, c_{22}^n \neq 0 \),

(iii) \( c_{11}^n = \frac{c_{11}}{\sigma_{11}}, c_{22}^n = \frac{c_{22}}{\sigma_{22}}, c_{12}^n = -\sigma c_{21}^n \).

Proof. (i) Since \( \det L(n,z) = S_{11}(z)S_{22}(z) \) is a Wiener–Hopf factorization of the scalar Laurent polynomial, it follows that \( \det l_+(n,z) = \alpha_n S_{22}(z), \det l_-(n,z) = \alpha_n^{-1} S_{11}(z) \) for some constant \( \alpha_n \). Let us normalize the factorization \( L(n,z) = l_+(n,z)l_-(n,z) \) in the following manner
\[
L(n,z) = \tilde{\text{\( l_+(n,z) \)}}\text{\( \tilde{l}_-(n,z) \)} = l_+(n,z) \begin{pmatrix} \alpha_n^{-1} & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \alpha_n & 0 \\ 0 & 1 \end{pmatrix} l_-(n,z).
\]
Then \( \det \tilde{l}_+(z) = S_{22}(z), \det \tilde{l}_-(z) = S_{11}(z) \) and, thus, \( \det \tilde{A}_n = \det \tilde{l}_+(0) = S_{22}(0) = 1. \) Similarly \( \det \tilde{B}_n = \det l_-(\infty) = S_{11}(\infty) = 1 \), and \( \det C_n = \det \tilde{A}_n \det \tilde{B}_n = 1 \) for all \( n \).

(ii) It is clear that \( \det F_n(z) \neq 0 \) for \( z \neq 0 \). Let us represent \( F_n(z) \) in the form \( F_n(z) = \Phi_0 + \Phi_1 z \).
From the definition of \( F_n(z) \) it follows that
\[
\Phi_0 = A_{n+1}^{-1} \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} A_n \quad \text{and} \quad \Phi_1 = B_{n+1} \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} B_n^{-1}.
\]
Hence,
\[
A_{n+1} F_n(z) B_n = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} C_n + z C_{n+1} \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} c_{11}^{n+1} & c_{12}^{n+1} \\ c_{21}^{n+1} & c_{22}^{n+1} \end{pmatrix}.
\]
Since \( A_{n+1} F_n(z) B_n \) is invertible for any \( n \) and \( z \neq 0 \), we have \( c_{11}^{n+1} \neq 0, c_{22}^{n+1} \neq 0 \).
(iii) Now we will use factorization (2.7). We then have

\[ C_n = A_n B_n = \tilde{A}_n \tilde{B}_n = J_\sigma B_n^\sigma J_\sigma A_n J_\sigma, \]

where this result is equivalent to the statements in (iii).

**Proposition 2.4.** The matrix function \( L(n, z) \) admits the factorization \( L(n, z) = \tilde{l}_+(n, z) \tilde{l}_-(n, z) \) with the following two-point normalization

\[ \tilde{l}_+(n, 0) = \begin{pmatrix} \frac{1}{\sigma_{+}} & \frac{c_{+}^{0}}{\sigma_{+}} \\ 0 & 1 \end{pmatrix}, \quad \tilde{l}_-(n, \infty) = \begin{pmatrix} 1 & 0 \\ c_{-}^{0} & c_{-}^{1} \end{pmatrix}. \]

Here, \( c_{ij}^{0} \) are the entries of the matrix \( C_n \).

**Proof.** Since \( c_{22}^{0} \neq 0 \) and det \( C_n = 1 \), the matrix \( C_n \) admits the following UL-factorization:

\[ C_n = C_n^+ C_n^- = \begin{pmatrix} \frac{1}{\sigma_{+}} & \frac{c_{+}^{0}}{\sigma_{+}} \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ c_{-}^{0} & c_{-}^{1} \end{pmatrix}. \] (2.9)

If \( L(n, z) = l_+(n, z) l_-(n, z) \) is an arbitrary factorization and \( l_+(n, 0) = A_n, \ l_-(n, \infty) = B_n, \ C_n = A_n B_n, \) then we can define a matrix \( U_n = B_n (C_n^-)^{-1} \) and consider a new factorization

\[ L(n, z) = \tilde{l}_+(n, z) \cdot \tilde{l}_-(n, z) = (l_+(n, z) U_n) \cdot (U_n^{-1} l_-(n, z)). \]

It only remains to verify that \( \tilde{A}_n = A_n B_n (C_n^-)^{-1} = C_n^+ \) and \( \tilde{B}_n = C_n^- B_n B_n^{-1} = C_n^- \) and, thus, this last proposition statement has been proven.

A normalization at points \( z = 0 \) and \( z = \infty \) was first introduced in the paper [33], and this normalization is an obligatory step in the approach of Khabibullin & Shagalov [4].

**Proposition 2.5.** Let \( L(n, z) = l_+(n, z) l_-(n, z) \) be the factorization constructed in proposition 2.4. Then the matrix polynomial \( F_n(z) = \tilde{l}_+^{1}(n+1, z) \tilde{l}_-^{1}(n, z) = \tilde{l}_-(n+1, z) \tilde{l}_+^{1}(n, z) \) has the following form

\[ F_n(z) = \begin{pmatrix} z & \sigma c_{21}^{n+1} \\ z c_{21}^{n+1} & 1 \end{pmatrix}. \]

**Proof.** Let \( F_n(z) = \tilde{\Phi}_0 + \tilde{\Phi}_1 z \). Here the matrices \( \tilde{\Phi}_0, \tilde{\Phi}_1 \) can be found by formula (2.8). Since \( \tilde{A}_n = C_n^+, \ \tilde{B}_n = C_n^-, \ c_{12}^{n} = -\sigma c_{21}^{n} \), the calculation gives the following result:

\[ \tilde{\Phi}_0 = \begin{pmatrix} 0 & \sigma c_{21}^{n+1} \\ 0 & 1 \end{pmatrix} \quad \text{and} \quad \tilde{\Phi}_1 = \begin{pmatrix} 1 & 0 \\ c_{21}^{n+1} & 0 \end{pmatrix}. \]

Since the inverse scattering problem is uniquely solvable (see, for example, [34]), we have \( F_n(z) = f_n(z) \).

Now the final result in the reconstruction of the initial potential \( u_n = u_n(0) \) can be formulated in terms of an arbitrary factorization if we use the invariant \( C \). This is the main difference between our approach and the one in [4].

**Theorem 2.6.** Let \( L(n, z) = l_+(n, z) l_-(n, z) \) be an arbitrary factorization and \( C_n = l_+(n, 0) l_-(n, \infty) \). Then

\[ u_n = c_{21}^{n+1}, \quad n \in \mathbb{Z}. \] (2.10)

**Remark 2.7.** As we have already noted, if the initial data \( u_n \in \mathbb{Q}(i) \), then the factorization \( L(n, z) \) can be found exactly arithmetically and the potential \( u_n \) can be restored exactly.

In any Computer Algebra System a real number \( \alpha \) can be converted to a rational number with the help of the continued fraction representation of \( \alpha \). Hence, if the initial data is given in a floating point format, then by conversion into rational numbers with a given precision, we can further apply the ExactMPF package for error-free calculations.
3. The IST method for the discrete NLSE: the case of \( \tau > 0 \)

Within the previous section, we have restored the original (known) potential \( u_n(0) \). Simultaneously, we have demonstrated that any matrix factorization (independent of any specific normalization of the factors) functions equally well within the IST method. It is important to note that at \( \tau = 0 \) the problem of the Wiener–Hopf factorizations has been solved explicitly, if the initial data are known exactly, i.e., if \( u_n(0) \in \mathbb{Q}(i) \).

The following stage in the scheme (1.2) from Khabibullin & Shagalov [4] is to perform a time step, considering the Wiener–Hopf factorization of matrix functions from the following family

\[
r(n, z, \tau) = \frac{1}{S_{22}(z)} \left( \frac{1}{S_{21}(z) e^{-2i\tau} e^{irwz-n}} - \sigma S_{12}(z) e^{2ir} e^{-irwz-n} D \right),
\]

\[w = z + z^{-1}, \quad n \in \mathbb{Z}, \quad \tau > 0,
\]

and in accordance with the formulas (1.5), (1.6) and (2.5) from Khabibullin & Shagalov [4]. Similarly, as in the case of \( \tau = 0 \) above, instead of \( r(n, z, \tau) \), we consider the matrix functions

\[
L(n, z, \tau) = S_{22}(z) r(n, z, \tau)
\]

\[
= \left( \frac{1}{S_{21}(z) e^{-2i\tau} e^{irwz-n}} - \sigma S_{12}(z) e^{2ir} e^{-irwz-n} D \right), \quad w = z + z^{-1}.
\]

(3.1)

It is easy to see that \( L(n, z, \tau) \) also admits a left canonical factorization. Indeed, since the following identity holds true

\[
S_{12}(z) e^{2ir} e^{-irw(z-n)} = S_{21}(z^{-1}) e^{-2i\tau} e^{irw(z^{-1})}(z^{-1})^{-n},
\]

the matrix function \( L(n, z, \tau) \) has the same structure as \( L(n, z, 0) \) itself, consequently, all results of the previous subsection are retained. The most important of these is

**Theorem 3.1.** If \( L(n, z, \tau) = l_+(n, z, \tau) \cdot l_-(n, z, \tau) \) is an arbitrary factorization of the matrix function \( L(n, z, \tau) \) and \( C_n(\tau) = l_+(n, 0, \tau) \cdot l_-(n, \infty, \tau) \) are constant matrices defined in §2, then the potentials, \( u_n(\tau) \) at each spatial discretization point \( n \) are directly computed

\[
u_n(\tau) = c_{21}^{n+1}(\tau), \quad n \in \mathbb{Z}.
\]

(3.2)

Thus, the theorem shows that in order to find a solution of the Cauchy problem for (1.2) at the fixed time \( \tau \), we must find solutions to the factorization problems for the infinite family of matrix functions \( \{L(n, z, \tau)\}_{n=-\infty}^{\infty} \). This also highlights the fact that the output of the ICT method represents the solution in the entire spatial axis not only on the finite interval.

Let \([-N, K] \subset [-N_0, K_0] \) is the support of the finite initial potential \( u_n(0) \), i.e. support of the initial data for the Cauchy problem. If we know the solution of the factorization problems for the finite family of matrices \( \{L(n, z, \tau)\}_{n=-N}^{K} \), then, in accordance with the theorem, we can find the part of the solution, \( \{u_n(\tau)\}_{n=-K}^{K} \). If we would like to expand this interval by one point, say \( n = K \), there is no need to solve the factorization problems again for \( n = K + 1 \). It is enough to solve the additional factorization problem at the additional point \( n = K + 1 \). In general, if \([-N, K] \subset [-N_1, K_1] \) then the part of the solution on the interval \([-N_1, K_1] \) is a continuation of the part of the solution on the smaller interval \([-N, K] \). The result of a numerical verification of this fact is given in electronic supplementary material, table S13.

A crucial difference between the matrix \( L(n, z, 0) \) and \( L(n, z, \tau) \) is that the latter does not admit an explicit factorization. The matrices \( L(n, z, \tau) \) are analytic over the whole complex plane except at the point \( z = 0 \) and \( z = \infty \) where they have essential singularities. Unfortunately, for such classes of matrix functions, constructive methods for their factorization are still unknown (see [32,35,36]), and so we can only construct an approximate factorization. In the next subsection we construct the family \( \{L_s^r(n, z, \tau)\}_{n=-\infty}^{\infty} \) of Laurent matrix polynomials that approximate the matrix functions \( \{L(n, z, \tau)\}_{n=-\infty}^{\infty} \). Here \( s \) is some parameter that characterizes the order of approximation.
We construct the approximation in such a way that the polynomial $L^s(n, z, \tau)$ admits the exact factorization, which can be found using the package ExactMPF. The use of error-free calculations makes it possible to avoid the accumulation of errors which is inevitable when applying the Runge–Kutta method to a sufficiently large time. Thus, the methods are different not only in the essence but even in terms of their output.

(a) Reduction to the explicitly solvable factorization problem

Our goal is to approximate $L(n, z, \tau)$ by a rational matrix function in such a way that the approximant preserves the structure of $L(n, z, \tau)$. The obvious approach would be to replace $e^{i\tau w(z)}$ by its Taylor polynomial. However, this leads to a matrix function that does not satisfy our stated requirement. We suggest the replacement of the exponential $e^{i\tau w}$ by the function $\pi_s(i\tau w)$, where $\pi_s(z)$ is the diagonal Padé approximant of degree $s$ for the function $\exp z$. It is known (see [37], Ch. 2) that

$$\pi_s(z) = \frac{P_s(z)}{P_s(-z)}, \quad (3.3)$$

where $P_s(z)$ is a polynomial of degree $s$ with rational coefficients. While the approximant $\pi_s(z)$ is uniquely defined, its numerator $P_s(z)$ is determined up to a nonzero multiplicand. In what follows, we impose, unless stated otherwise, that the leading coefficient of the polynomial $P_s(z)$ is equal to $(-1)^s$. As a result, it has the following form [37]

$$P_s(z) = (-1)^s \sum_{j=0}^{s} \binom{s}{j} (s+1) \cdots (2s-j)z^j. \quad (3.4)$$

In particular, $P_s(0) = (-1)^s(s+1) \cdots (2s)$. As usual, the empty product is considered equal to 1.

Next we approximate $L(n, z, \tau)$ by a rational matrix function

$$L_s(n, z, \tau) = \begin{pmatrix} 1 & -\sigma S_{12}(z)z^n e^{2i\tau} & -\sigma S_{12}(z)z^n e^{2i\tau} \pi_s(-i\tau w) \\ S_{21}(z) & \frac{-\sigma S_{12}(z)z^n e^{2i\tau} \pi_s(-i\tau w)}{D} \end{pmatrix},$$

$$w = z + z^{-1}. \quad (3.5)$$

We must determine where the function $\pi_s(i\tau w)$ is continuous on the unit circle, that is $P_s(i\tau w) \neq 0$ for $|z| = 1$.

**Lemma 3.2.** If $s > \tau - 1$ then $P_s(i\tau w) \neq 0$ on the unit circle and $\min_{|z|=1} |P_s(i\tau w)| = (s+1) \cdots (2s)$.

**Proof.** Suppose that there exists $z_0$, $|z_0| = 1$, such that $P_s(i\tau (z_0 + z_0^{-1})) = 0$. Then $v_0 = 2i\tau \cos \phi_0$ ($\phi_0 = \text{Arg } z_0$) is a zero of the polynomial $P_s(v)$. The point $v = v_0$ belongs to the segment $[-2i\tau, 2i\tau]$ of the imaginary axis. If $\tau < s + 1$, then $[-2i\tau, 2i\tau] \subset (-2(s+1)i, 2(s+1)i)$. By the theorem of Saff & Varga (see [38], theorem 5.7.3), the approximant $\pi_s(v)$ of the function exp $v$ has no zeros inside the parabola $y^2 \leq 4(s+1)(x + s + 1)$, where $v = x + iy$. However, the interval $(-2(s+1)i, 2(s+1)i)$ lies inside this parabola. This contradiction proves the first statement of the lemma.

Now, for an arbitrary point $z$ from the unit circle, we define a real polynomial $G_2(\tau h)$ of degree $2s$ in the following manner

$$G_2(\tau h) = |P_s(i\tau h)|^2 = P_s(i\tau h)P_s(-i\tau h),$$

where $h = w(z) = 2\cos \phi \in [-2, 2]$. Note that all the odd coefficients of the polynomial $G_2(\tau h)$ vanish, that is $G_2(\tau h) = a_0 - a_2(\tau h)^2 + a_4(\tau h)^4 + \cdots$. Moreover, we can prove that $a_{4k+2} < 0$, $a_{4k} > 0$, for all $k$. Hence, all the coefficients remaining before the even terms $(\tau h)^{2k}$ are positive and, thus, $\min_{|h|\leq 2} |P_s(i\tau h)|^2 = a_0 = P_s^2(0)$. ■

**Remark 3.3.** The determination of the signs of the coefficients $a_j$ is carried out using rather cumbersome calculations involving the gamma function $\Gamma(x)$. We omit these calculations here,
since in reality we need Padé approximants for small values of $s$. In such cases, the polynomial $G_s(\tau h)$ can be found by a direct calculation. For example, for $s = 6$ we have for $x = \tau h$:

$$G_6(x) = x^{12} + 84x^{10} + 10080x^8 + 1209600x^6 + 127008000x^4 + 10059033600x^2 + 442597482400$$

and $\min_{|\tau| = 1} |P_6(\tau w)| = 6652807$.

Now we can estimate the error in approximating $e^{\tau hw}$ by $\pi_s(\tau hw)$.

**Lemma 3.4.** Denote $\gamma(s, \tau) = \left( (2\tau^{2s+1})/(2s)! \right) \int_0^1 (1 - t^2)^s \, dt$. Then for $s > \tau - 1$

$$|e^{\tau hw} - \pi_s(\tau hw)| \leq \gamma(s, \tau).$$

(3.6)

Here $\| \cdot \|_{\mathbb{C}(\mathbb{T})}$ is sup-norm on the unit circle $\mathbb{T}$.

**Proof.** Denote $R_s(v) = P_s(-v) e^v - P_s(v)$. We use the following formula for the residual $R_s(v)$ (see [37, ch.2, (2.12)]):

$$R_s(v) = \frac{v^{2s+1}}{s!} \int_0^1 t^s (1 - t)^s e^{\tau ht} \, dt.$$

For $v = \tau(z + z^{-1})$, we have on the unit circle $|z| = 1$

$$|e^{\tau hw} - \pi_s(\tau hw)| = \left\| \left( \frac{\tau h^{2s+1}}{s!} P_s(-\tau h) \right) \int_0^1 t^s (1 - t)^s e^{\tau ht} \, dt \right\|_{\mathbb{C}(\mathbb{T})}, \quad h \in [-2, 2].$$

Hence,

$$|e^{\tau hw} - \pi_s(\tau hw)| \leq \frac{(2\tau)^{2s+1}}{s! \min_{|\tau|\leq 2} |P_s(-\tau h)| \max_{|\tau|\leq 2} \left\{ \int_0^1 t^s (1 - t)^s e^{\tau ht} \, dt \right\}}.$$

We now compute the integral for the right-hand side of the latter estimation. By replacing the variable, we obtain

$$\int_0^1 t^s (1 - t)^s e^{\tau ht} \, dt = e^{\tau h/2} \int_{-1/2}^{1/2} \left( \frac{1}{4} - x^2 \right)^s e^{\tau hx} \, dx = 2 e^{\tau h/2} \int_0^{1/2} \left( \frac{1}{4} - x^2 \right)^s \cos \tau hx \, dx,$$

and then by making one more change in the variable of integration we finally have

$$\int_0^1 t^s (1 - t)^s e^{\tau ht} \, dt = \frac{e^{\tau h/2}}{4^s} \int_0^1 (1 - t^2)^s \cos \frac{\tau ht}{2} \, dt.$$

Consequently, we reach the required estimation:

$$|e^{\tau hw} - \pi_s(\tau hw)| \leq \left( \frac{(2\tau)^{2s+1}}{4^s (2s)!} \right) \int_0^1 (1 - t^2)^s \, dt.$$

Note that $\gamma(s, \tau)$ can be represented by the gamma function:

$$\gamma(s, \tau) = \frac{\tau^{2s+1} \Gamma(1/2) \Gamma'(1 + s)}{\Gamma(3/2 + s) \Gamma(2s + 1)}.$$

**Remark 3.5.** The estimate (3.6) also represents the relative error of the approximation.

Theorem 3.7 below provides us with a basic estimate of the approximation error $||L(n, z, \tau) - L_s(n, z, \tau)||$. Since the parameter $\gamma(s, \tau)$ is involved in the basic estimation result (theorem 3.7 below), it is important to analyse its dependence on its variables. In figure 2, we present a
Figure 2. Contour lines of the function $\gamma$ defined in (3.6) ($\gamma(s, \tau) = \epsilon$) for three different values $\epsilon = 10^{-2}, 10^{-4}, 10^{-6}$. The shadowed domain indicates the set of parameters $\tau$ and $s$ where the conditions of the lemma 3.4 hold true for $\epsilon = 10^{-4}$.

parametric space for the determination of the approximation parameter $s$ for a given time step $\tau$, which guarantees that the estimate $||e^{\tau w} - \pi_s(i\tau w)||_{C(T)} \leq \epsilon$ is valid. For example, for $\tau = 1$ the values $s = 2, 3, 4$ guarantee that the accuracy of the approximation is not worse than $\epsilon = 10^{-2}, 10^{-4}, 10^{-6}$, respectively. While for $\tau = 3$, we need to take values $s = 4, 5, 6$, respectively, to guarantee the same levels of accuracy.

Remark 3.6. It is possible to replace the rather cumbersome function $\gamma(\tau, s)$ with some simpler approximations that do not involve the Gamma function:

$$
\gamma_{\text{asymp}} = \left( \frac{e\tau}{2s+1} \right)^{2s+1} \sqrt{\frac{2s+1}{2s+2}}
$$

and

$$
\gamma_{\text{simple}} = \left( \frac{e\tau}{2s+1} \right)^{2s+1}.
$$

The first one, $\gamma_{\text{asymp}}(s, \tau)$, is obtained by using the Stirling asymptote, the third one, $\gamma_{\text{simple}}(s, \tau)$, is the further simplification, while the second function, $\gamma_{\text{best}}(s, \tau)$, is a man-made approximation. For their comparison see figure 3.

We can now establish the basic theorem for the approximant $L_s(n, z, \tau)$ (see (3.5)). For the matrix function $A(t) = (a_{ij}(t))_{i,j=1,2}$ we use the norm

$$
||A(t)|| = \max_{1 \leq j \leq 2} \sum_{i=1}^{2} ||a_{ij}(t)||_{C(T)}.
$$

By virtue of the estimate (3.6) from 3.4, we can conclude that the matrix function $L(n, z, \tau)$ can be well enough approximated on the unit circle, $|z| = 1$, by the rational matrix function $L_s(n, z, \tau)$.

Theorem 3.7. For $s > \tau - 1$, the matrix function $L_s(n, z, \tau)$ has the same structure as $L(n, z, \tau)$, admits a left canonical Wiener–Hopf factorization in explicit form and

$$
||L(n, z, \tau) - L_s(n, z, \tau)|| \leq ||S_{12}(z)||_{C(T)} \cdot \gamma(s, \tau).
$$

Proof. By lemma 3.2, for $s > \tau - 1$ the entries of the rational matrix function $L_s(n, z, \tau)$ do not have poles on the unit circle and $\det L_s(n, z, \tau) = \det L(n, z, \tau) = S_{22}(z) \neq 0$. Hence $L_s(n, z, \tau)$
admits a left factorization. Due to the properties of the diagonal Padé approximants of the exponential function we have $S_{21}(z^{-1}) e^{-2\tau w(z^{-1})} = S_{12}(z) e^{2\tau w(z)}$. Hence the matrix function $L_s(n, z, \tau)$ has the same structure as $L(n, z, \tau)$ (and $L(n, z, 0)$) and all the results of the previous section remain valid for $L_s(n, z, \tau)$ as well. Therefore, $L_s(n, z, \tau)$ admits a left canonical factorization. The Wiener–Hopf factorization of the rational matrix function $L_s(n, z, \tau)$ can be reduced to the factorizations of scalar polynomials and a Laurent matrix polynomial. Indeed,

$$L_s(n, z, \tau) = \frac{1}{P_s(\tau w)P_s(-\tau w)} \left( \begin{array}{cc} P_s(\tau w)P_s(-\tau w) & -\sigma S_{12}(z) z^n e^{2\tau w} P_s^2(-\tau w) \\ S_{21}(z) z^{-n} e^{-2\tau w} P_s^2(\tau w) & DP_s(\tau w)P_s(-\tau w) \end{array} \right).$$

For $s > \tau - 1$ the scalar Laurent polynomials $P_s(\pm \tau w)$ do not vanish on the unit circle $T$. Therefore, they admit the Wiener–Hopf factorization and the Laurent matrix polynomials $P_s(\tau w)P_s(-\tau w)L_s(n, z, \tau)$ (and, consequently, the matrix $L_s(n, z, \tau)$ itself) can be factorized in an explicit form.

The following estimate is straightforward

$$||L(n, z, \tau) - L_s(n, z, \tau)|| \leq \max\{||S_{12}(z)||_{C(T)}, ||S_{21}(z)||_{C(T)}\} \times ||e^{\tau w} - \pi_s(\tau w)||_{C(T)},$$

and, since $|S_{12}(z)| = |S_{21}(z)|$ on the unit circle, we can apply lemma 3.4 to prove the last statement. □

(b) Reduction to the exactly solvable factorization problem

We aim to perform a factorization of the matrix function $L_s(n, z, \tau)$ using the error-free calculations offered by the ExactMPF package [28]. For this reason, all entries of the Laurent matrix polynomial $P_s(n, z, \tau) =$

$$P_s(\tau w)P_s(-\tau w)L_s(n, z, \tau) = \left( \begin{array}{cc} P_s(\tau w)P_s(-\tau w) & -\sigma S_{12}(z) z^n e^{2\tau w} P_s^2(-\tau w) \\ S_{21}(z) z^{-n} e^{-2\tau w} P_s^2(\tau w) & DP_s(\tau w)P_s(-\tau w) \end{array} \right)$$

must be scalar Laurent polynomials over the field $\mathbb{Q}(i)$, and the Laurent polynomial $P_s(\tau w)$ must admit the exact Wiener–Hopf factorization with respect to the unit circle $T$.  

Figure 3. Ratios of the functions $\gamma_{\text{asymp}}$, $\gamma_{\text{best}}$ and $\gamma_{\text{simple}}$ and the function $\gamma$ defined in (3.7).
We can assume that \( \tau \) and the initial data, i.e. \( u_n(0) \), belong to the field \( \mathbb{Q}(i) \). Then \( S_{12}(z), S_{21}(z) \) and \( P_s(\pm i\tau w) \) are Laurent polynomials over \( \mathbb{Q}(i) \). If \( u_n(0), \tau \) are given in a floating point format, then we can convert the data into rational numbers with the desired precision.

To apply the ExactMPF package, it remains to approximate \( e^{2i\tau} \) by a rational number and to approximate \( P_s(i\tau w) \) by a Laurent polynomial over \( \mathbb{Q}(i) \) that admits the exact Wiener–Hopf factorization. Moreover, the entire approximation must preserve the structure of \( L_0(n, z, \tau) \).

First, we approximate the quantity \( e^{2i\tau} \) by the rational number \( E_{s, r} = \pi_s(2i\tau) \). Since \( |E_{s, r}| = 1 \), this approximation preserves the required structure of the matrix function \( L_0(n, z, \tau) \). For estimation of the error introduced, \( |e^{2i\tau} - E_{s, r}| \), we can use lemma 3.4. Thus,

\[
|e^{2i\tau} - E_{s, r}| \leq \gamma(s, \tau).
\]  

Now we consider the Padé approximant \( \pi_s(z) \), as already created in (3.3), and, for a fixed pair \( (s, \tau) \), try to construct another polynomial \( P_{s, r}(z) \) on the field \( \mathbb{Q} \), which we will define as the ‘modified’ Padé approximant

\[
\pi_{s, r}(z) = \frac{P_{s, r}(z)}{P_{s, r}(-z)}.
\]  

We require \( P_{s, r}(z) \) to satisfy the following two conditions:

(a) \( \pi_{s, r}(i\tau w) \) is close enough to \( \pi_s(i\tau w) \) on the unit circle \( T \);
(b) the Laurent polynomial \( P_{s, r}(i\tau w) \) admits the exact Wiener–Hopf factorization with respect to \( z \in T \).

**Proposition 3.8.** For any \( s, \tau (s > \tau - 1) \), there exists a polynomial \( P_{s, r}(z) \) over \( \mathbb{Q}(i) \) such that \( P_{s, r}(i\tau w) \) satisfies the aforementioned conditions (a) and (b).

**Proof.** Consider the polynomial \( P_s(v) \) from the Padé approximants \( \pi_s(v) \) defined in (3.4), which has a leading coefficient equal to \((-1)^s\). For the given \( s, \tau \), we find the roots of the equation

\[
P_s(i\tau(z + z^{-1})) = 0,
\]  

(3.11)
to an accuracy of \( 10^{-M} \), where we have a natural index \( M \in \mathbb{N} \). For implementation in MAPLE we define \( M = \text{DIGITS} \), using the user’s declared precision for computation (the option offered by Maple Software). If \( z_0 \) is a root of this equation, then \( z_0^{-1} \) is also a root of the same multiplicity. By virtue of the condition \( s > \tau - 1 \), the equation (3.11) does not have roots on the unit circle. Let \( \tilde{z}_1, \ldots, \tilde{z}_s \) be those roots of (3.11) such that \( |\tilde{z}_j| > 1 \), and \( 1/\tilde{z}_1, \ldots, 1/\tilde{z}_s \) be the roots in the interior of the unit disc. Now we can construct a polynomial \( \tilde{W}_{s, r}^+(z) = (z - \tilde{z}_1) \cdots (z - \tilde{z}_s) \) over the field \( \mathbb{C} \) and convert its coefficients into rational numbers with the same precision of \( 10^{-M} \). We denote the last polynomial as \( W_{s, r}^+(z) \). As a result, we have obtained a polynomial \( W_{s, r}^+(z) \) over the field \( \mathbb{Q}(i) \) that is sufficiently close to \( \tilde{W}_{s, r}^+(z) \).

Next, we define polynomial \( W_{s, r}(z) \) and the Laurent polynomial \( W_{s, r}(z) \) of degree \( s \) in \( z, z^{-1} \)

\[
W_{s, r}(z) = \frac{(i\tau)^s}{W_{s, r}^+(0)} W_{s, r}^+ \left( \frac{1}{z} \right) \quad \text{and} \quad W_{s, r}(z) = W_{s, r}^+(z) \cdot W_{s, r}(z).
\]  

Note that \( W_{s, r}(z) \) admits the exact Wiener–Hopf factorization and is close enough to \( P_s(i\tau(z + z^{-1})) \) by construction. It is straightforward to verify that \( W_{s, r}(z) = W_{s, r}(1/z) \), and, thus, the coefficients of the Laurent polynomial

\[
W_{s, r}(z) = \sum_{j=-s}^{s} a_jz^j
\]  

exhibit the following useful property \( a_j = a_{-j} \) for \( j = 1, \ldots, s \).
Next we search for a polynomial \( P_{s,r}(z) \) of degree \( s \) such that

\[
P_{s,r}(z) = \sum_{j=0}^{s} x_j z^j, \quad P_{s,r}(i\tau(z + z^{-1})) = W_{s,r}(z).
\] (3.12)

The conditions (3.12) to a linear system of equations with respect to the unknown constants \( x_j \)

\[
\sum_{j=0}^{s} \sum_{m=0}^{j} \left( \begin{array}{c} j \\ m \end{array} \right) x_j \cdot (i\tau)^j \cdot z^{2m-j} = \sum_{j=-s}^{s} \omega_j z^j.
\] (3.13)

We will show that the system has a unique solution. Due to its symmetry, it is sufficient to consider only the nonnegative indices \( j = 0, \ldots, s \). Suppose that \( s = 2\rho \) is even. We separate the terms on the left hand side of equation (3.13) into their even and odd powers of \( z \):

\[
\sum_{k=0}^{\rho} \sum_{m=0}^{2k} \left( \begin{array}{c} 2k \\ m \end{array} \right) x_{2k} \cdot (i\tau)^{2k} \cdot z^{2m-2k} + \sum_{k=1}^{\rho-1} \sum_{m=0}^{2k-1} \left( \begin{array}{c} 2k - 1 \\ m \end{array} \right) x_{2k-1} \cdot (i\tau)^{2k-1} \cdot z^{2m-2k+1}.
\]

By rewriting the indices setting \( l = m - k \), and taking into account only the nonnegative powers of \( z \), we can write (3.13) in the form

\[
\sum_{l=0}^{\rho} z^{2l} \sum_{k=0}^{\rho} \left( \begin{array}{c} 2k \\ l+k \end{array} \right) x_{2k} \cdot (i\tau)^{2k} + \sum_{l=0}^{\rho-1} z^{2l+1} \sum_{k=l}^{\rho-1} \left( \begin{array}{c} 2k + 1 \\ l+k+1 \end{array} \right) x_{2k+1} \cdot (i\tau)^{2k+1} = \sum_{j=0}^{s} \omega_j z^j.
\]

Consequently, (3.13) can be separated into two independent systems with triangular matrices:

\[
\sum_{k=l}^{\rho} \left( \begin{array}{c} 2k \\ l+k \end{array} \right) x_{2k} \cdot (i\tau)^{2k} = \omega_{2l}, \quad l = 0, 1, \ldots, \rho;
\]

and

\[
\sum_{k=l}^{\rho-1} \left( \begin{array}{c} 2k + 1 \\ l+k+1 \end{array} \right) x_{2k+1} \cdot (i\tau)^{2k+1} = \omega_{2l+1}, \quad l = 0, 1, \ldots, \rho - 1.
\]

These systems always have unique solutions. The case of odd integers \( s \) is considered in a similar manner.

Following proposition 3.8, a procedure modPadetau has been created in Maple and used in the remaining part of this paper for computations.

Further, it is convenient in computations to use the numerators \( \tilde{P}_{s}(z) \), \( \tilde{P}_{s,r}(z) \), that have been normalized by the conditions \( \tilde{P}_{s}(0) = 1, \tilde{P}_{s,r}(0) = 1 \).

**Remark 3.9.** The polynomial \( \tilde{P}_{s,r}(z) \) depends on the accuracy used in the calculation of the roots of equation (3.11), as well as the coefficients of \( \tilde{P}_{s,r}(z) \). It is difficult to obtain an explicit theoretical estimate of the error in approximating \( \tilde{P}_{s}(i\tau w) \) by \( \tilde{P}_{s,r}(i\tau w) \)

\[
\left\| \tilde{P}_{s}(i\tau w) - \tilde{P}_{s,r}(i\tau w) \right\|_{C(T)} \leq \sum_{k=0}^{s} |P_k^s - P_k^{s,r}| (2\tau)^k = \delta(s, \tau, M), \quad \text{(3.14)}
\]

where \( \tilde{P}_{s}(z) = \sum_{k=0}^{s} \tilde{P}_k^s z^k \) and \( \tilde{P}_{s,r}(z) = \sum_{k=0}^{s} \tilde{P}_k^{s,r} z^k \). The value of \( \delta = \delta(s, \tau, M) \) can be estimated only \textit{a posteriori} and can be improved by increasing the polynomial degree, \( s \), and the Maple precision, DIGITS = \( M \).

Let us estimate \( \left\| \pi_s(i\tau w) - \pi_{s,r}(i\tau w) \right\|_{C(T)} \), assuming we have an already known estimate (3.14). We first estimate \( \left\| \pi_s(i\tau w) \right\|_{C(T)} \) itself.

**Lemma 3.10.** Let \( s > \tau - 1 \), then \( \left\| \pi_s(i\tau w) \right\|_{C(T)} \leq 1 + \gamma(s, \tau) \).
Proof. By lemma 3.4 we immediately obtain
\[
||\pi_s(\delta) - \pi_s(\delta)||_{C(T)} \leq ||e^{i\tau\delta}||_{C(T)} + ||\pi_s(\delta) - e^{i\tau\delta}||_{C(T)} = 2 + \gamma(s, \tau).
\]
\[
\Box
\]

**Lemma 3.11.** Let \( s > \tau - 1 \) and \( ||\tilde{P}_s(\delta) - \tilde{P}_{s, r}(\delta)||_{C(T)} = \delta < 1 \) (see remark 3.9), then
\[
||\pi_s(\delta) - \pi_{s, r}(\delta)||_{C(T)} \leq \frac{\delta}{1 - \delta}(2 + \gamma(s, \tau)).
\]
\[
(3.15)
\]

**Proof.** First, let us note that under the assumptions, the following estimate is valid on the unit circle \( T \): \( ||\tilde{P}_{s, r}(\delta(\tau = -i\delta)) = ||\tilde{P}_{s, r}(\delta(\tau = -i\delta)) - \max_{|z| = 1} ||\tilde{P}_{s, r}(\delta(\tau = -i\delta)) - \tilde{P}_{s, r}(\delta(\tau = -i\delta))|| = 1 - ||\tilde{P}_{s, r}(\delta(\tau = -i\delta)) - \tilde{P}_{s, r}(\delta(\tau = -i\delta))||_{C(T)} \geq 1 - \delta. \) Thus, \( ||\tilde{P}_{s, r}(\delta(\tau = -i\delta)) - \tilde{P}_{s, r}(\delta(\tau = -i\delta))||_{C(T)} \leq (1 - \delta)^{-1} \).

On the other hand, it is not difficult to verify that
\[
\pi_s(\delta) - \pi_{s, r}(\delta) = \frac{\pi_s(\delta)}{\tilde{P}_{s, r}(\delta(\tau = -i\delta))} \left( \tilde{P}_{s, r}(\delta(\tau = -i\delta)) - \tilde{P}_s(\delta(\tau = -i\delta)) \right)
\]
\[
+ \frac{1}{\tilde{P}_{s, r}(\delta(\tau = -i\delta))} \left( \tilde{P}_s(\delta(\tau = -i\delta)) - \tilde{P}_{s, r}(\delta(\tau = -i\delta)) \right).
\]

As a result, the estimate (3.15) follows immediately from lemma 3.10.
\[
\Box
\]

Thus, for the given \( s, \tau \) we can verify empirically where and how \( \pi_{s, r}(\delta) \) is close enough to \( \pi_s(\delta) \) on the unit circle.

We are now ready to suggest another rational matrix function \( L^*_s(n, z, \tau) \) that: (a) is close enough to the matrix function \( L_s(n, z, \tau) \) defined in (3.5) and (b) allows for exact factorization. Specifically, let us define a rational matrix function
\[
L^*_s(n, z, \tau) = \left( \begin{array}{c}
1 \\
S_{21}(z)z^{-n}E_{s, r}\pi_{s, r}(\delta(\tau = -i\delta)) \\
s_{12}(z)z^{-n}E_{s, r}\pi_{s, r}(\delta(\tau = -i\delta)) \\
D
\end{array} \right).
\]
\[
(3.16)
\]

**Theorem 3.12.** Assume that \( \tau \) and the initial data \( u_n(0) \) belong to the field \( \mathbb{Q}(i) \), while \( s > \tau - 1 \) is an integer and \( ||\tilde{P}_{s, r}(\delta(\tau = -i\delta)) - \tilde{P}_s(\delta(\tau = -i\delta))||_{C(T)} = \delta < 1 \). Then the matrix function \( L^*_s(n, z, \tau) \) has the same structure as \( L_s(n, z, \tau) \), admits the exact Wiener–Hopf factorization, and the following estimate holds true:
\[
||L_s(n, z, \tau) - L^*_s(n, z, \tau)||_{C(T)} \leq ||S_{12}(z)||_{C(T)} \left[ \gamma(1 + \gamma(s, \tau)) + \frac{\delta}{1 - \delta}(2 + \gamma(s, \tau)) \right].
\]
\[
(3.17)
\]

**Proof.** Obviously, by construction, \( L^*_s(n, z, \tau) \) has the same structure as \( L_s(n, z, \tau) \). As before, we can prove that for \( s > \tau - 1 \) the rational matrix function \( L^*_s(n, z, \tau) \) admits the left canonical factorization. The Wiener–Hopf factorization of \( L^*_s(n, z, \tau) \) can be reduced to the factorization of a Laurent matrix polynomial
\[
P^*_s(n, z, \tau) = P_{s, r}(\delta(\tau = -i\delta))P_{s, r}(\delta(\tau = -i\delta))L^*_s(n, z, \tau)
\]
\[
= \left( \begin{array}{c}
P_{s, r}(\delta(\tau = -i\delta))P_{s, r}(\delta(\tau = -i\delta)) \\
S_{21}(z)z^{-n}E_{s, r}\pi_{s, r}(\delta(\tau = -i\delta)) \\
s_{12}(z)z^{-n}E_{s, r}\pi_{s, r}(\delta(\tau = -i\delta)) \\
D
\end{array} \right).
\]

The entries of this polynomial are scalar Laurent polynomials over the field \( \mathbb{Q}(i) \) and its determinant
\[
\det P^*_s(n, z, \tau) = P_{s, r}(\delta(\tau = -i\delta))P_{s, r}(\delta(\tau = -i\delta))S_{22}(z)
\]
admits the exact Wiener–Hopf factorization on the unit circle. Hence, \( P^*_s(n, z, \tau) \) (and the rational matrix function \( L^*_s(n, z, \tau) \)) admits the exact left Wiener–Hopf factorization that can be performed with the help of the ExactMPF package.
It remains to prove that \( L_s^*(n, z, \tau) \) and \( L_s(n, z, \tau) \) are close enough. From the definitions \( L_s^*(n, z, \tau) \) and \( L_s(n, z, \tau) \), taking into account that \( \|S_{21}\|_{C(\mathbb{T})} = \|S_{12}\|_{C(\mathbb{T})} \), we have
\[
\|L_s(n, z, \tau) - L_s^*(n, z, \tau)\| = \|S_{12}\|_{C(\mathbb{T})} \cdot \max[[|e^{-2i\tau} \pi_s(\tau w) - E_{s, \tau} \pi_s(-\tau w)|C(\mathbb{T})],[|e^{2i\tau} \pi_s(-\tau w) - E_{s, \tau} \pi_s(-\tau w)|C(\mathbb{T})]].
\]

Since
\[
\|e^{-2i\tau} \pi_s(\tau w) - E_{s, \tau} \pi_s(-\tau w)|C(\mathbb{T}) = \|e^{2i\tau} \pi_s(-\tau w) - E_{s, \tau} \pi_s(-\tau w)|C(\mathbb{T})],
\]
we get
\[
\|L_s(n, z, \tau) - L_s^*(n, z, \tau)\| = \|S_{12}\|_{C(\mathbb{T})} \cdot \|e^{2i\tau} \pi_s(-\tau w) - E_{s, \tau} \pi_s(-\tau w)|C(\mathbb{T})].
\]

The latter norm can be further estimated, thus
\[
\|e^{2i\tau} \pi_s(-\tau w) - E_{s, \tau} \pi_s(-\tau w)|C(\mathbb{T}) \leq |e^{2i\tau} - E_{s, \tau}| \cdot |\pi_s(\tau w) + \pi_s(\tau w)|C(\mathbb{T})|.
\]

By use of equation (3.9) and lemmas 3.10 and 3.11 we obtain the required estimate.

We are now in a position to summarize the results of this subsection concerning the approximation of the matrix function \( L(n, z, \tau) \) from (3.1). From theorems 3.7 and 3.12 we obtain

**Theorem 3.13.** Assume that \( \tau \) and the initial data \( u_\tau(0) \) belong to the field \( \mathbb{Q}(i) \), while \( s > \tau - 1 \) is an integer and \( \|\tilde{P}_s(\tau w) - \tilde{P}_{s, \tau}(\tau w)|C(\mathbb{T}) = \delta < 1 \). Then the matrix function \( L_s^*(n, z, \tau) \) has the same structure as \( L(n, z, \tau) \), admits the exact Wiener–Hopf factorization, and the following estimate holds true:
\[
\|L(n, z, \tau) - L_s^*(n, z, \tau)\| \leq \|S_{12}(z)|C(\mathbb{T})|2 + \gamma(s, \tau)|\gamma(s, \tau) + \frac{\delta}{1 - \delta} = \delta(s, \tau, M).
\]

Theorems 3.7–3.13 are a crucial element of this work. Indeed, the package ExactMPF cannot be directly applied to the matrix functions \( L(n, z, \tau) \). The factorization of the matrices can be constructed only approximately. The package is applied to the approximate Laurent matrix polynomials \( L_s^*(n, z, \tau) \). The theorems allow us to control the accuracy of calculations. In general, the theorems are instrumental in approximation of any given matrix function by a polynomial one that preserves several properties of the original matrix and simultaneously allows for exact factorization.

Thus, \( L_s^*(n, z, \tau) \) is close enough to \( L(n, z, \tau) \) and both the matrix functions admit the left canonical factorization. By virtue of the stability of the canonical factorization (see, for example, [39]), the normalized factorization factors \( l^*_s, l^*_s(n, z, \tau) \) and \( l_+(n, z, \tau) \) are also close enough [39, Ch. X, proposition 1.1]. Note that in some cases, it is even possible to effectively estimate a distance between these factors in the Wiener algebra \( W(\mathbb{T}) \) [40].

Hence, the potentials \( u_\tau(\tau) \) and \( u_\tau^*(\tau) \), that are found by the factorizations of \( L(n, z, \tau) \) and \( L_s^*(n, z, \tau) \), from the relationship (3.2), are also close enough and we can find \( u_\tau^*(\tau) \) via the ExactMPF package and its error-free calculations. As a result, the potential \( u_\tau(\tau) \) can be found to the desired accuracy. In the next section, we discuss how this fact can be practically verified.

If \( u_\tau(0) \) and \( \tau \) are given in floating point format, then we can convert them into rational numbers with the desired precision and replace \( L(n, z, \tau) \) by a close enough matrix function \( \tilde{L}(n, z, \tau) \) for which the conditions of the above theorem 3.13 are fulfilled.

In the following section, we consider examples which demonstrate that our approach permits the finding of a solution of the discrete NLSE to a prescribed accuracy.
4. Numerical experiment

In this section, we consider the Cauchy problem of the equation (1.2), with $\sigma = 1$ and a finite (initial) potential concentrated at the points $n = -2, \ldots, 2$:

$$u_n(0) = \begin{cases} 3/5, & |n| \leq 2, \\ 0, & |n| \geq 3. \end{cases} \quad (4.1)$$

First we define the scattering matrix $S(z)$ from (1.3)–(2.1) and, consequently, the matrix function $L(z)$ from (2.6)

$$L(z) = \begin{pmatrix} 1 & -\left(\frac{3}{5}z + \frac{156}{125}z^{-1} + \frac{42818}{3125}z^{-1} + \frac{2304}{15625}z^{-1} + \frac{1048576}{9765625}\right) \\ \frac{3}{5}z^2 + \frac{156}{125}z^{-2} + \frac{42818}{3125}z^{-2} + \frac{2304}{15625}z^{-2} + \frac{1048576}{9765625} & 0 \end{pmatrix}.$$ 

Note that $L_{12}(z) = -S_{12}(z)$ and $||S_{12}(z)||_{CT} \leq ||S_{12}(z)||_W = 16.368/3125 = 5.23776$. This floating number is exact and is used in the computations.

(a) Restoration of the initial potential

As has been discussed in §3, the problem of restoration of the original potential $u_n(0)$ can be solved with the help of the Wiener–Hopf factorizations of the sequence of matrix functions $L(n, z, 0) = L(z)$. We restrict ourselves to the points $-9 \leq n \leq 9$ only. As stated, the consequent factorization problems can be solved exactly with the assistance of the ExactMPF package. By theorem 2.6, to find $u_n(0)$ we can use an arbitrary factorization of $L(n + 1, z, 0)$ at only the point $n + 1$, in contrast with the work [4]. If $C_{n+1} = I_+(n + 1, 0)l_-(n + 1, \infty, 0)$ is the constant matrix defined around theorem 2.6, then $u_n = e_{21}^{n+1}$.

Our calculations have shown that the potential (4.1) is indeed then restored exactly.

As an example, we present here only the result of calculations determining $u_n(0)$ for $n = -1$. For this, we need the factorization of $L(n, z, 0)$ for $n = 0$. The ExactMPF package returns the following factorization of $L(0, z, 0) = L(z)$:

$$I_+(0, z, 0) = \begin{pmatrix} \frac{25}{16} & \frac{27}{26} & -\frac{3}{5} \\ \frac{9}{256} & \frac{15}{16} & -\frac{768}{3125} \\ \frac{129}{125} & \frac{27}{256} & \frac{1}{2} \end{pmatrix}, \quad I_-(0, \infty, 0) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad \text{and} \quad C_0 = \begin{pmatrix} \frac{25}{16} & -\frac{3}{5} \\ \frac{9}{256} & \frac{256}{625} \end{pmatrix}.$$ 

Hence, $u_{-1}(0) = e_{21}^0 = (C_0)_{21} = 3/5$.

(b) Approximate calculations of the potentials $u_n(\tau)$ for $\tau > 0$

Now we will compute the potential evolution $u_n(\tau)$ for $n = -9, \ldots, 9$, within the period $\tau \in (0, 5]$. Following the line of reasoning from the previous section, we approximate the matrix functions $L(n, z, \tau)$ by $L^*_n(n, z, \tau)$ (see theorem 3.13). The factorization of $L^*_n(n, z, \tau)$ can be found exactly with the help of the ExactMPF package, i.e. with error-free calculations. Further, we carry out all calculations in exact arithmetic, and then convert the results into floating point format.

We aim to guarantee the accuracy of the potential $u_n(\tau)$ at any point in space and time considered with a precision of at least four decimal places. Since the effective a priori estimations of the factors, $||l_{+s}^*(n, z, \tau) - l_+(n, z, \tau)||$, are still unknown, we first demonstrate how appropriate parameters for computations can be chosen. Note that increasing both $s$ and $M = \text{DIGITS}$ (see discussion in the previous section) leads to higher computational accuracy. On the other hand,
since we use exact computations, this dramatically increases the lengths of the numbers and consequently the computational times. Thus, we need to establish an optimal strategy to balance the values of $\gamma(s, \tau)$ and $\delta$ in (3.18) to deliver the minimal possible error.

If the value of $\gamma(s, \tau)$ can be easily computed (or estimated from (3.6)), the value of the parameter $\delta = \delta(s, \tau, M)$ is difficult to estimate analytically. Below, we present and discuss this issue only for a particular time $\tau = 1$. Specifically, we compute $\delta = \delta(s, \tau, M)$ for various values of $s = 3, 4, 5, 6, 7$ and $M = 6, 8, 10$. The respective results are collected below. First, in figure 4, we estimate the value of $\delta = \delta(s, \tau, M)$, numerically. In order to compute this parameter, we do not need to perform any factorization, but only to use the approximation procedure modPadetab to construct the Laurent polynomials. It is interesting to observe that, while increasing the value of $s$, the accuracy in the approximation remains, in fact, on the same level. This indicates that a sufficient accuracy can be achieved without additional increase in the value of $s$ chosen for the Padé approximation of $\pi_s(x)$. A more crucial quantity here is the value of the parameter $M = \text{DIGITS}$. From figure 4, we can also conclude that $\log(\delta) \simeq -M$ for $\tau = 1$.

In figures 5 and 6 we present results from numerical experiments to analyse the accuracy of the final approximation of the matrix function $L(n, z, \tau)$ by a close $L_s^\ast(n, z, \tau)$ that allows for exact factorization. It is clear from the presented results that, if we aim for accuracy of the order $\varepsilon = 10^{-4}$ for the approximation of the matrix function $L(n, z, \tau)$, and simultaneously fix $M = \text{DIGITS} = 6$ in the computations, there are two candidates for the choice of the parameter $s$. The choice $s = 5$ guarantees required accuracy while $s = 4$ can be sufficient for the purpose, but this can only be checked in the post-processing stage (comparing the results for the potential computed for both those choices). If we require more accurate computations, say of the order $\varepsilon = 10^{-6}$ or $\varepsilon = 10^{-8}$, we must choose the pairs $(s, M) = (6, 8)$ or $(s, M) = (7, 10)$, respectively.

If we aim to preserve the same computational accuracy $\varepsilon$ for all time steps under consideration, such an analysis should be performed at least for several points $\tau$ (and the smoothness of the initial data should also be taken into account, which we will show later). On the other hand, such analysis gives us only an upper bound set for the parameters. Conversely, since we exactly construct the factorization of the approximant $L_s^\ast(n, z, \tau)$ (see theorem 3.13), we can expect that this factorization also sufficiently approximates the factorization of $L(n, z, \tau)$. Unfortunately, an a priori estimate of the error from such a replacement of the factors is unknown. In reality, the numbers, $s$ and $M$, can be made even smaller. For this reason, we perform also a posteriori analyses for different values of the parameter $s$ with fixed $\text{DIGITS} = M = 6$. 

**Figure 4.** Accuracy ($\delta = \delta(s, \tau, M)$) of the representation of the polynomial $P_s(x)$ by the exactly factorizable $P_s^\ast(x)$ for $\tau = 1$, $s = 3, 4, 5, 6, 7$, and $M = 6, 8, 10$. 

![Graph showing accuracy of representation](https://royalsocietypublishing.org/doi/abs/10.1098/rspa.2022.0144)
Figure 5. Accuracy, $\varepsilon$, of the representation of the matrix functions $L(n, z, \tau)$ by the exactly factorizable matrix $L_s^*(n, z, \tau)$ from the estimate (3.18) for $\tau = 1, s = 3, 4, 5, 6, 7$, and DIGITS $= M = 6, 8, 10$.

Figure 6. Contour plot of the accuracy, $\varepsilon(s, M)$, of the representation of the matrix functions $L(n, z, \tau)$ by the exactly factorizable matrix $L_s^*(n, z, \tau)$ from the estimate (3.18) for $\tau = 1, s = 3, 4, 5, 6, 7$, and $M = 6, 8, 10$. The red arrow indicates an optimal direction for choosing the pair $(s, M)$.

Since our goal here is to only demonstrate whether and how computations can be performed, we restrict our analysis below by choosing a target $\varepsilon = ||L(n, z, \tau) - L_s^*(n, z, \tau)|| < 10^{-4}$ and using the same parameter $M = \text{DIGITS}$ for computations at all time steps. Then, to be able to control the computations not only by using a priori analysis using results of the theorem 3.13, but also a posteriori, we compute the potential $u_{n}(\tau)$ ($n = -9, \ldots, 9$) for three different consequent values of $s$ and compare the obtained results. To highlight how this is done, we refer the prospective reader to page 6 of electronic supplementary material, supplementary material 2. We can see that
Figure 7. Computations of the absolute values of the potential $|u_n(\tau)|$ using exact computations and $M = \text{DIGITS} = 6$, with a proper choice of the parameter $s$. Points represented by black stars have been additionally computed to estimate the accuracy of the cubic spline approximation between the given points in time. The accuracies of the approximations of the potential at those three additional points $\tau = 0.125, 0.3755$ and $1.125$ are given in Figure 8.

The stabilized digits in computations between the cases $s = 4$ and $s = 5$ indeed belong to the range dictated by the required accuracy ($10^{-4}$ in this case). The final accuracy of the potential $u_n$ for $\tau = 1$ coincides with the trends and the orders that have been discussed above.

In electronic supplementary material, supplementary material 2, we present results of the computations in the range $\tau \in (0, 5]$ using the ExactMPF package. Those results are also reproduced in graphical form in Figure 7 by markers, while the curves have been produced using cubic splines in time. On the time interval under consideration, we have used 16 points (with time step $\Delta \tau = 0.25$ over most of the interval). Note that the computational time grows with increase of both $n$ and $s$. Normalized computational time is presented in electronic supplementary material, figure 11 of the supplementary material 2. Since the time depends on the used computer we present a normalized time (normalized on the time to compute the smaller interval).
We have also computed potential $u_n(\tau)$ at three additional points $\tau = 0.125, 0.3755$ and 1.125 to estimate how close the extrapolated data are to the exact computations at those three points. The respective results are presented in figure 8. Unsurprisingly, the higher error corresponds to the points $(n=2,4)$ where we see the highest gradient in the initial data, and this feature decreases with time.

In figure 9, we present a few frames of $|u_n(\tau)|$ small times in the evolution process $(\tau = 0, 0.125, 0.25$ and $0.3755)$. In electronic supplementary material, supplementary material 1 (slide 1), we show full videos of the evolutions of the real and imaginary parts, and the modulus of the potential over time $\text{Re} u(\tau)$, $\text{Im} u_n(\tau)$ and $|u_n(\tau)|$, respectively.
Figure 10. Contour plot of the absolute value of the potential, $|u(\tau)|$, after reconstruction of the continuous potential.

Without the reconstruction of the continuous potential $u(\tau)$ at the intermediate spatial points, the respective movements of each particular discrete point from the interval under consideration ($n = -9, \ldots, 9$) are illustrated in electronic supplementary material, supplementary material 1 (slide 2 videos (a) and (c)) (separately for the real and imaginary part of $u_n(\tau)$) in the bar-graphic videos.

The contour plot of the absolute value of potential, $|u(\tau)|$, drawn in two-dimensional space with real and imaginary axes, obtained after reconstruction of the continuous potential, and shown in figure 10 indicates that the energy is redistributed without a concentration (no solitons are present) and that it spreads in time and space. Simultaneously, it is clear from this plot that the potential trajectories undergo circular movements. This circular movement in the trajectories can be seen in electronic supplementary material, video (b) in supplementary material 1 (slide 2), where the main argument of the potential, $\text{Arg } u_n(\tau), (-\pi \leq \text{Arg } u_n(\tau) < \pi)$ is drawn in the bar-style video. The jumps from $-\pi$ to $\pi$ (or vice versa) indicate completed circles of the corresponding points $n$. The movements of the potential, $u_n(\tau)$, at points ($n = 0, \ldots, 9$) are included in electronic supplementary material, video (c), and in one two-dimensional frame (Re $u$, Im $u$), both on slide 2. Finally, in electronic supplementary material, 1 (slide 3), we present each trajectory $u_n(\tau), (n = 0, \ldots, 9)$ on separate frames. We can observe there turning points and circling behaviour that we had expected to see by analysing figure 10 and from what had been predicted in [41].

(c) Discussions and conclusion

We have shown that with the use of the ExactMPF package, and with an additional procedure that allows for a proper approximation that reduces the matrix function under question into one that is sufficiently close, and that is exactly factorizable, we have been able to effectively solve the nonlinear discrete Schrödinger equation (1.2) and compute the potential $u_n(\tau)$. In the course of the analysis, we have proven an important theorem 3.13 allowing us to choose by rather simple preliminary computations (that do not involve the factorization itself) the values of the computational parameters $s$ and $M = \text{DIGITS}.

The following issues should be highlighted as a result of our analysis:

— The difference between this approach, based on the exact factorization of Laurent matrix polynomials, from the approach proposed in the work [4]. In this work, we proposed to
find a solution to the Riemann problem at a sufficiently remote point \( n_0 \), and then restore the solutions of boundary value problems for \( |n| < n_0 \) using recurrent formulae.

In the work [5], the authors proposed use of these recurrence relations not only for the reconstruction of the potential, but also simultaneously in finding an approximate solution of the problem of right canonical factorization of the invertible matrix functions \( r(z) \) with elements from the Wiener algebra \( W(T) \). The approach proposed here is applicable to the situation considered in [5].

In particular, we looked at an example from this work. By converting the initial data \( v(n), u(n) \), given in Table 1 of this work, into rational numbers, we solved all the Riemann problems by using the ExactMPF package exactly for points \( n = 0, 1, \ldots, 9 \).

Since the factorization problem arising from the analysis of this NLSE relates to the canonical factorization only (and, thus, the problem itself is stable), we were able to bypass some parts of the original ExactMPF package algorithm. However, since the ExactMPF package has been developed for a general case (for arbitrary sets of partial indices) and we did not want to interfere with the package itself, the computational time is not optimal, but it could be decreased further with appropriate package adjustment for this particular problem.

A specific procedure, modPadetau, had to be implemented in the package to correct the matrix function to be exactly factorizable.

If we need to reconstruct the solution for a long time interval, the best strategy is to fix the number \( \text{DIGITS} = M \), while controlling the accuracy by the proper choice of \( s = s_\ast(M) \) (taken from the theorem 3.13), and complementing the analyses by a posteriori comparison of the result with those computed additionally with use of the neighbouring values: \( s = s_\ast - 1, s_\ast + 1 \).

With increasing time, the demands on the values of the parameters \( s \) and \( M \) overreach the ability of the package to perform exact computations. For such values the package should be further developed to deliver not exact but approximate factorization. For the canonical factorization, this is a possible task and we also plan to develop our code in this direction. However, in a general case when the partial indices are not zeros, such a task still represents one of the hardest problems [28,36,42–45]. It is important to note that the most developed theory related to the factorization of matrix functions regardless of the set of their partial indices has also been summarized in the paper [42]. Interestingly, it requires (and allows for) simultaneous determination of both left and right partial indices and the respective left and right factorizations.

On the other hand, large time behaviour is more naturally deduced using asymptotic approaches (see [41,46–49]).

The results of this paper (for the case \( \sigma = 1 \)) can be directly applied for \( \sigma = -1 \) in the absence of the discrete spectrum. In the presence of the discrete spectrum, the algorithm should be modified (see [4]).

The ExactMPF package developed in [28] allows for use in various applications where the matrix Wiener–Hopf problems arise, such as, for example [35,50–52]. A number of such problems arising from various problems on discrete scattering in lattice structures have been collected in [53].

Data accessibility. The data are provided in electronic supplementary material [54].

Authors’ contributions. V.M.A.: conceptualization, investigation, methodology, project administration, software, supervision, writing—original draft; G.M.: conceptualization, investigation, methodology, software, supervision, visualization, writing—original draft.

Both authors gave final approval for publication and agreed to be held accountable for the work performed therein.

Conflict of interest declaration. We declare we have no competing interests.

Funding. V.A. was supported by RFBR grant no. 20-41-740024. The authors have been supported by funding from the European Union’s Horizon 2020 research and innovation programme under the Marie Sklodowska-Curie grant agreement EffectFact no. 101008140.
Acknowledgements. G.M. is thankful to the Royal Society for the Wolfson Research Merit Award and to the Welsh Government for the Future Generation Industrial Fellowship. The authors would like to thank Prof. I.T. Khabibullin for discussions and useful comments.

References

13. Li-Li W, En-Gui F, Yong C. 2021 Inverse scattering transform and high-order pole solutions for the NLS equation with quartic terms under vanishing/non-vanishing boundary conditions. [arXiv:2108.07404]
41. Novokshenov VY. 1985 Asymptotic behavior as $t \to \infty$ of the solution of the Cauchy problem for a nonlinear differential-difference Schrödinger equation. Differ. Urav. 21, 1915–1926. (in Russian), Differential Equations 21(11), 1288–1298 (in English)


