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Exponential fourth order schemes for direct Zakharov-Shabat problem

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Abstract: Nowadays, improving the accuracy of computational methods to solve the initial value problem of the Zakharov-Shabat system remains an urgent problem in optics. In particular, increasing the approximation order of the methods is important, especially in problems where it is necessary to analyze the structure of complex waveforms. In this work, we propose two finite-difference algorithms of fourth order of approximation in the time variable. Both schemes have the exponential form and conserve the quadratic invariant of Zakharov-Shabat system. The second scheme allows applying fast algorithms with low computational complexity (fast nonlinear Fourier transform).

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1. Introduction

Recently, there has been great interest in the so-called nonlinear Fourier transform (NFT), which is a generalization of the ordinary linear Fourier transform (FT) in the sense that it allows one to decompose a field obeying a class of integrable nonlinear equations (by the inverse scattering transform method – IST) [1,2] into a special nonlinear basis that takes into account the contribution of solitons to the field distribution. In the limiting case, for fields with low power, the NFT coincides with the linear FT. The NFT makes it possible to find exact solutions for integrable nonlinear equations, such as the nonlinear Schrödinger equation (NLSE) and the Korteweg de Vries (KdV) equations. For the first time, this idea for the NLSE was proposed by Zakharov and Shabat in 1971 [1]. They showed that the NLSE can be integrated by the IST method, previously applied to the KdV equations. The NLSE describes the envelope for wave beams, therefore it is used in many areas of physics where there are wave systems [3,4].

Also, the NLSE has found wide application in telecommunication applications, since it allows one to describe the propagation of pulses in an optical fiber. In the past few years, some new NFT-based approaches have been actively explored to compensate for fiber nonlinearity and to exceed the limitations of nonlinearity-imposed limits of linear transmission methods [5–10].

Despite a large number of articles [11–15] devoted to NFT, the development of the accurate and fast numerical algorithms for NFT still remains an actual mathematical problem. A set of algorithms named fast nonlinear Fourier transform (FNFT) offers a new approach for numerical scheme construction having a low computational complexity $O(M \log^2 M)$, where M is the number of samples per signal [16–20]. Similarly to the fast Fourier transform (FFT) this type of algorithms can significantly increase a computational speed in comparison with traditional approaches with a complexity $O(M^2)$. Despite this, there remains a need to improve the accuracy of computational methods, including by increasing their approximation order, especially in problems where it is necessary to analyze the structure of complex wave forms in the lack of data to describe their shape [21].

In this paper, we consider a numerical method for solving the initial value problem for the Zakharov-Shabat (ZS) system in order to solve the direct spectral problem. The integration of

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this system is the first step in the general scheme of NFT. In addition, we focus on constructing one-step finite-difference schemes for solving the ZS system.

We present the general necessary conditions for the transition operator for fourth order one-step difference schemes for linear systems of first order differential equation. Then we give two examples of such schemes. Both schemes are the exponential fourth order ones, and we show their connection with the Magnus decomposition. The main property of such schemes is to conserve the quadratic form for real spectral parameters. Such conservation property allows calculating precisely by numerical schemes the reflection coefficient, that is valuable for various telecommunication problems related to information coding (for example, NFDM [5] and b-modulation [8,9]). The second scheme contains the spectral parameter only in the exponent. This property allows one to apply fast algorithms (FNFT) for the numerical solution of the ZS system [22,23].

The final part of the article presents comparisons of numerical computations using the proposed schemes and other well-known schemes: the Boffetta- Osborne second order scheme [11], Runge-Kutta fourth order scheme [12] and the fourth order conservative scheme [24].

In our work, we do not touch on numerical methods for solving the direct problem of the ZS system, which can be called nonlocal. However, for completeness, we will mention these methods and give a very brief overview. A more detailed overview of the methods for the direct ZS problem is available in [14]. First of all, such methods include the method based on the solution of the Gelfand-Levitan-Marchenko integral equations. These methods require the inversion of large matrices. Speedup of computations is achieved by using the Töplitz symmetry of the matrix and an "inner bordering" procedure [25]. The second method is based on a class of commutator-free quasi-Magnus (CFQM) exponential integrators [26]. The schemes of this method are given by compositions of several exponentials that comprise certain linear combinations of the values of the defining operator at specified nodes. Since the matrix of the system (in the case of the ZSP, the matrix is given by the potential and the spectral parameter) is usually given on a uniform grid, for applying CFQM it is necessary to compute multiple non-equispaced points within each subinterval. One can use neighboring points for this, but in practice, the schemes use cubic-spline based interpolation to obtain the non-equispaced points from the mid-points of each subinterval. One can also apply interpolation based on the Fourier transform [20]. Therefore, such schemes can be attributed to conditionally nonlocal. These schemes also conserve the quadratic form for real spectral parameter, and the fast algorithm (FNFT) can be applied to them to solve the direct ZSP [20], but they fundamentally depend on the method of interpolation.

2. Direct Zakharov-Shabat problem

The standard NLSE is a basic model for the pulse propagation along an ideally lossless and noiseless fiber

$$i\frac{\partial q}{\partial z} + \frac{\sigma}{2}\frac{\partial^2 q}{\partial t^2} + |q|^2 q = 0, \tag{1}$$

where $q = q(t, z)$ is a slow-varying complex optical field envelope which decays rapidly for $t \to \pm\infty$, the variable z is the distance along the optical fiber, t is a time variable; $\sigma = -1$ and $\sigma = 1$ corresponds to the normal and anomalous dispersion, respectively [3]. Equation (1) is written in the moving coordinate system and describes the propagation of pulses $q(t, z)$ in optical fibers. The Cauchy problem is solved with the initial conditions as follows:

$$q(t, z)|_{z=z_0} = q_0(t).$$

The mathematical method suggested by Zakharov and Shabat [1] allows to integrate the NLSE. The method, widely known as the Nonlinear Fourier Transform (NFT), allows transforming signal into nonlinear Fourier spectrum, which is defined by the solution of the Zakharov-Shabat problem (ZSP).

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Equation (1) can be written as a condition of compatibility

$$\frac{\partial L}{\partial z} = ML - LM \tag{2}$$

of two linear equations

$$L\Psi = \zeta\Psi, \quad \frac{\partial \Psi}{\partial z} = M\Psi, \tag{3}$$

where $\Psi(t)$ is a complex vector function of a real argument t,

$$L = i\begin{pmatrix} \partial_t & -q \\ -\sigma q^* & -\partial_t \end{pmatrix}, \quad M = i\begin{pmatrix} \sigma\frac{\partial^2}{\partial t^2} + \frac{1}{2}|q|^2 & -\sigma q\frac{\partial}{\partial t} - \frac{1}{2}\sigma\frac{\partial q}{\partial t} \\ -q^*\frac{\partial}{\partial t} - \frac{1}{2}\frac{\partial q^*}{\partial t} & -\sigma\frac{\partial^2}{\partial t^2} - \frac{1}{2}|q|^2 \end{pmatrix}. \tag{4}$$

2.1. ZS system

The first equation in Eq. (3) is the eigenvalue problem for the operator L. For $\sigma = -1$ the operator L is Hermitian ($L = L^\dagger \equiv (L^*)^T$, * denotes complex conjugation, ^{T} denotes transposition), therefore the complex spectral parameter $\zeta = \xi + i\eta$ becomes real $\zeta = \xi \in \mathbb{R}$. There is no such restriction for $\sigma = 1$. In this case the problem has the continuous and discrete spectra. The continuous spectrum lies on the real axis and the discrete spectrum is in the upper half plane $\mathrm{Im}(\zeta) > 0$.

Also the first Eq. in Eq. (3) can be rewritten as an evolutionary system

$$\frac{d\Psi(t)}{dt} = Q(t)\Psi(t), \tag{5}$$

where $q = q(t, z)$ and

$$\Psi(t) = \begin{pmatrix} \psi_1(t) \\ \psi_2(t) \end{pmatrix}, \quad Q(t) = \begin{pmatrix} -i\zeta & q \\ -\sigma q^* & i\zeta \end{pmatrix}.$$

Here z is a parameter, that we will skip further.

The system Eq. (5) can be written in a gradient form as follows:

$$\begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}_t = J\begin{pmatrix} \psi_1 \\ \sigma\psi_2 \end{pmatrix} = J\begin{pmatrix} \frac{\partial H}{\partial \psi_1^*} \\ \frac{\partial H}{\partial \psi_2^*} \end{pmatrix}, \quad J = \begin{pmatrix} -i\zeta & \sigma q \\ -\sigma q^* & i\sigma\zeta \end{pmatrix} \tag{6}$$

where $H = |\psi_1|^2 + \sigma|\psi_2|^2$. For real spectral parameters $\zeta = \xi$ the matrix J is skew-Hermitian $J = -J^\dagger$ for any $\sigma = \pm 1$ and, consequently, the system Eq. (6) conserves the quadratic form H. The invariant H and the matrix Q can be written using Pauli matrices σ_0 and σ_3 (see Appendix) as follows:

$$H = \begin{cases} (\Psi^*, \sigma_0\Psi), & \text{for} \quad \sigma = 1 \\ (\Psi^*, \sigma_3\Psi), & \text{for} \quad \sigma = -1 \end{cases}, \quad Q = \begin{cases} J\sigma_0, & \text{for} \quad \sigma = 1 \\ J\sigma_3, & \text{for} \quad \sigma = -1 \end{cases}, \tag{7}$$

where the curved bracket indicate the scalar product of the complex vectors.

Assuming that $q(t)$ decays rapidly when $t \to \pm\infty$, the specific solutions (Jost functions) for ZSP Eq. (5) can be derived as:

$$\Psi = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = \begin{pmatrix} e^{-i\zeta t} \\ 0 \end{pmatrix}[1 + o(1)], \quad t \to -\infty, \tag{8}$$

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and

$$\Phi = \begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix} = \begin{pmatrix} 0 \\ e^{i\zeta t} \end{pmatrix} [1 + o(1)], \quad t \to \infty, \tag{9}$$

Taking into account the boundary conditions Eq. (8), we get the condition $H = 1$ for real spectral parameters. Then we obtain the Jost scattering coefficients $a(\xi)$ and $b(\xi)$ as follows:

$$a(\xi) = \lim_{t\to\infty} \psi_1(t,\xi)\, e^{i\xi t}, \quad b(\xi) = \lim_{t\to\infty} \psi_2(t,\xi)\, e^{-i\xi t}. \tag{10}$$

The functions $a(\xi)$ and $b(\xi)$ can be extended to the upper half-plane $\xi \to \zeta$ [27], where ζ is a complex number with the positive imaginary part $\eta = \mathrm{Im}\zeta > 0$. The spectral data of ZSP Eq. (5) are determined by $a(\zeta)$ and $b(\zeta)$ in the following way:

(1) K zeros of $a(\zeta) = 0$ define the discrete spectrum $\{\zeta_k\}$, $k = \overline{0, K-1}$ of ZSP Eq. (5) and phase coefficients

$$r_k = \left.\frac{b(\zeta)}{a'(\zeta)}\right|_{\zeta=\zeta_k}, \quad \text{where} \quad a'(\zeta) = \frac{da(\zeta)}{d\zeta};$$

(2) the continuous spectrum is determined by the reflection coefficient $r(\xi) = b(\xi)/a(\xi)$, $\xi \in \mathbb{R}$.

These spectral data were defined using the "left" boundary condition Eq. (8). Both conditions Eqs. (8) and (9) can be used to calculate the coefficient $b(\zeta_k)$ of the discrete spectrum:

$$\Psi(t,\zeta_k) = \Phi(t,\zeta_k) b(\zeta_k). \tag{11}$$

In addition, the following trace formula is valid [2]:

$$C_n = -\frac{1}{\pi}\int_{-\infty}^{\infty} (2i\xi)^n \ln|a(\xi)|^2\, d\xi + \sum_{k=0}^{K-1} \frac{1}{n+1}\left[(2i\zeta_k^*)^{n+1} - (2i\zeta_k)^{n+1}\right], \tag{12}$$

which connects the NLSE integrals C_n with the coefficient $a(\xi)$ and the discrete spectrum ζ_k. The first integrals have the form

$$C_0 = \int_{-\infty}^{\infty} |q|^2 dt,\ C_1 = \int_{-\infty}^{\infty} q q_t^* dt,\ C_2 = \int_{-\infty}^{\infty} (q q_{tt}^* + |q|^4) dt,$$
$$C_3 = \int_{-\infty}^{\infty} (q q_{ttt}^* + 4|q|^2 q q_t^* + |q|^2 q^* q_t) dt.$$

Equation (12) for $n = 0$ gives

$$C_0 = -\frac{1}{\pi}\int_{-\infty}^{\infty} \ln|a(\xi)|^2 d\xi + \sum_{k=0}^{K-1} \left[2i\left(\zeta_k^* - \zeta_k\right)\right] \tag{13}$$

is called the Parseval nonlinear equality and is used to verify the numerical calculations and the consistency of the continuous and discrete spectra found. The first term on the right-hand side of Eq. (13) refers to the continuous spectrum energy:

$$E_c = -\frac{1}{\pi}\int_{-\infty}^{\infty} \ln|a(\xi)|^2 d\xi. \tag{14}$$

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2.2. Features of computational problem

We solve the system Eq. (5). The matrix $Q(t)$ linearly depends on the complex function $q(t)$ which is given in the whole nodes of the uniform grid with a step τ on the interval $[-L, L]$. Let us note main features of the discrete problem:

1. Since the matrix Q is defined on a uniform grid, the unknown function Ψ must also be computed on a uniform grid with the same step τ. Therefore, the Runge-Kutta methods (RK) cannot be used on such grid. If, for example, we use an explicit 4th order RK scheme [12], then we need to take the computational grid with a double step 2τ. In this case, values of Q_n will be used unequally.
2. For small values of the potential $|q(t)| << |\zeta|$ and $\mathrm{Im}\,\zeta > 0$, ZSP has exponentially growing and decreasing solutions, thus A-stability of finite-difference methods is required [28]. The method is called A-stable if all solutions of the equation $\partial x/\partial t = \lambda x$ tend to zero at $\mathrm{Re}\,\lambda < 0$ and fixed step τ. The second barrier of Dahlquist restricts the use of multi-step methods [29]. It means that there are no explicit A-stable multi-step methods for the Eq. (5), and the 2nd order of convergence is maximal for implicit multi-step methods.
3. The ZSP has a matrix of size 2, therefore, the inverse matrices and the matrix exponential (see Eq. (72) in Appendix) can be easily calculated. This allows us to include practically any functions of the matrix Q in the difference schemes.
4. In order to calculate the spectral data for a given spectral parameter ζ, it is necessary to solve the ZS system once. When solving the NLSE by the IST, the direct problem is only the first step. In this method, it is also necessary to solve the inverse problem, which requires to use the spectral data for a large number of spectral parameter values. This number approximately equal to the number of samples for the continuous spectrum and the finite number of spectral data necessary to find the discrete spectrum. Therefore, it is necessary to solve the ZS system for a large number of spectral parameter values ζ at a fixed potential $q(t)$. This should be taken into account when implementing the algorithms.

3. General theory of one-step schemes

In this section, we consider a one-step algorithm for solving the Zakharov-Shabat system and determine the necessary and sufficient condition for the transition matrix to have a fourth order of accuracy. These conditions are obtained in terms of the Taylor series for the transition matrix.

Let us consider the problem Eq. (5) in a general case. We need to solve the equation

$$Dx = Q(t)x, \quad D = \frac{d}{dt}, \tag{15}$$

where $x = x(t) \in \mathbb{C}^n$, using a one-step algorithm

$$x_{n+1} = Tx_n, \tag{16}$$

where T is the transition operator, $x_n = x(t_n)$, $t_n = n\tau$, τ is a step of the uniform grid.

We differentiate Eq. (15) and get the expressions for the derivatives $D^k x$ up to 5-th order as follows:

$$\begin{aligned}
&Dx = Qx,\\
&D^2x = (DQ)x + QDx,\\
&D^3x = (D^2Q)x + 2(DQ)(Dx) + QD^2x,\\
&D^4x = (D^3Q)x + 3(D^2Q)(Dx) + 3(DQ)(D^2x) + QD^3x,\\
&D^5x = (D^4Q)x + 4(D^3Q)(Dx) + 6(D^2Q)(D^2x) + 4(DQ)(D^3x) + QD^4x.
\end{aligned} \tag{17}$$

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Let us introduce the notation for the right-hand side of Eq. (17) and derivatives $Q^{(k)} = D^k Q$

$$D^k x = Q_k x, \quad Q_1 = Q. \tag{18}$$

Using Eqs. (17) and (18) we find recurrence relations for Q_k as follows:

$$\begin{aligned}
&Q_2 = Q^{(1)} + Q^2,\\
&Q_3 = Q^{(2)} + 2Q^{(1)}Q + QQ^{(1)} + Q^3,\\
&Q_4 = Q^{(3)} + 3Q^{(2)}Q + QQ^{(2)} + 3(Q^{(1)})^2 + 3Q^{(1)}Q^2 + 2QQ^{(1)}Q + Q^2Q^{(1)} + Q^4,\\
&Q_5 = Q^{(4)} + 4Q^{(3)}Q + QQ^{(3)} + 6Q^{(2)}Q^{(1)} + 4Q^{(1)}Q^{(2)} + 6Q^{(2)}Q^2 + 3QQ^{(2)}Q + Q^2Q^{(2)} +\\
&+8(Q^{(1)})^2Q + 4Q^{(1)}QQ^{(1)} + 3Q(Q^{(1)})^2 + 4Q^{(1)}Q^3 + 3QQ^{(1)}Q^2 + 2Q^2Q^{(1)}Q + Q^3Q^{(1)} + Q^5.
\end{aligned}$$

Let us derive the Taylor series of $x(t)$ at the point t, such that $t_n = t + \bar{s}\tau$, $t_{n+1} = t + s\tau$, $\bar{s} = s - 1$:

$$x(t_{n+1}) = x + s\tau Dx + \frac{(s\tau)^2}{2!}D^2x + \frac{(s\tau)^3}{3!}D^3x + \frac{(s\tau)^4}{4!}D^4x + \frac{(s\tau)^5}{5!}D^5x + O(\tau^6), \tag{19}$$

$$x(t_n) = x + \bar{s}\tau Dx + \frac{(\bar{s}\tau)^2}{2!}D^2x + \frac{(\bar{s}\tau)^3}{3!}D^3x + +\frac{(\bar{s}\tau)^4}{4!}D^4x + \frac{(\bar{s}\tau)^5}{5!}D^5x + O(\tau^6). \tag{20}$$

Then we denote the terms of Eqs. (19) and (20):

$$L_k = \frac{s^k}{k!}Q_k, \quad R_k = \frac{\bar{s}^k}{k!}Q_k \tag{21}$$

and write the expansion of Eq. (16) up to 5-th order

$$(E + L_1 + L_2 + L_3 + L_4 + L_5) = (T_0 + T_1 + T_2 + T_3 + T_4 + T_5)(E + R_1 + R_2 + R_3 + R_4 + R_5), \tag{22}$$

where E is a unit matrix and $T_0, \ldots, T_5$ are the series coefficients of T. After equating the terms of the same order we get

$$L_1 = R_1 + T_1, \tag{23}$$

$$L_2 = R_2 + T_1R_1 + T_2, \tag{24}$$

$$L_3 = R_3 + T_1R_2 + T_2R_1 + T_3, \tag{25}$$

$$L_4 = R_4 + T_1R_3 + T_2R_2 + T_3R_1 + T_4, \tag{26}$$

$$L_5 = R_5 + T_1R_4 + T_2R_3 + T_3R_2 + T_4R_1 + T_5. \tag{27}$$

Now we can derive recurrence relations for T_k. Obviously $T_0 = E$. From Eq. (23) we get

$$T_1 = L_1 - R_1 = sQ - \bar{s}Q = Q. \tag{28}$$

Therefore, for first order approximation, the expansion of transition operator T must begin with $T \approx E + \tau Q$ and we need to know the value of Q at the point t.

From Eq. (24) we get

$$T_2 = L_2 - R_2 - T_1R_1 = \frac{s^2 - \bar{s}^2}{2!}Q_2 - \bar{s}Q^2 = \frac{2s - 1}{2!}Q_2 - \bar{s}Q^2. \tag{29}$$

To find T_2 we need to know the values of Q^2 and $Q^{(1)}$ at the point t. If we do not have the analytical expression of $Q(t)$, we need to know the value of Q at two different points to use finite

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differences to calculate $Q^{(1)}$. Otherwise, we can set $s = 1/2$ and zero the coefficient at Q_2. Then we only need to know the value of Q^2 at the point t.

From Eq. (25) we get

$$\begin{aligned} T_3 &= L_3 - R_3 - T_1R_2 - T_2R_1 = \frac{s^3 - \bar{s}^3}{3!}Q_3 - Q\frac{\bar{s}^2}{2!}Q_2 - \bar{s}T_2Q = \\ &= \frac{3s^2 - 3s + 1}{3!}Q_3 - \frac{\bar{s}^2}{2!}QQ_2 - \frac{(2s-1)\bar{s}}{2!}Q_2Q + \bar{s}^2Q^3. \end{aligned} \tag{30}$$

Equation

$$s^3 - \bar{s}^3 = 3s^2 - 3s + 1 = 0$$

has no real roots, therefore we cannot zero the factor in front of Q_3 using s. It means that to use any scheme of order higher then 2 we must know $Q^{(2)}$ or values of Q at three different points.

From Eq. (26) we get

$$T_4 = L_4 - R_4 - T_1R_3 - T_2R_2 - T_3R_1 = \frac{s^4 - \bar{s}^4}{4!}Q_4 - \frac{\bar{s}^3}{3!}QQ_3 - \frac{\bar{s}^2}{2!}T_2Q_2 - \bar{s}T_3Q. \tag{31}$$

Since Eq.

$$s^4 - \bar{s}^4 = (2s-1)(2s^2 - 2s + 1) = 0$$

has only one real root $s = 1/2$, this is the only way to get rid of Q_4, that contains $Q^{(3)}$.

From Eq. (27) we get

$$T_5 = L_5 - R_5 - T_1R_4 - T_2R_3 - T_3R_2 - T_4R_1 = \frac{s^5 - \bar{s}^5}{5!}Q_4 + \cdots. \tag{32}$$

Since Eq.

$$s^5 - \bar{s}^5 = 0$$

has no real roots, we can not zero this coefficient varying s.

Thus we formulate

Theorem. Any one-step finite-difference Eq. (16) approximates Eq. (15) with a fourth order of accuracy on the interval $[t + \bar{s}\tau, t + s\tau]$, where τ is the length of the interval, $s \in (0, 1)$ and $\bar{s} = 1 - s$, if and only if the expansion of the transition operator T at t for the fixed s has a form

$$T = E + \tau Q + \tau^2 T_2 + \tau^3 T_3 + \tau^4 T_4 + O(\tau^5), \tag{33}$$

where

$$T_2 = \frac{2s-1}{2!}Q_2 - \bar{s}Q^2, \tag{34}$$

$$T_3 = \frac{3s^2 - 3s + 1}{3!}Q_3 - \frac{\bar{s}^2}{2!}QQ_2 - \frac{(2s-1)\bar{s}}{2!}Q_2Q + \bar{s}^2Q^3, \tag{35}$$

$$T_4 = \frac{(2s-1)(2s^2 - 2s + 1)}{4!}Q_4 - \frac{\bar{s}^3}{3!}QQ_3 - \frac{\bar{s}^2}{2!}T_2Q_2 - \bar{s}T_3Q \tag{36}$$

and the coefficients Q_k are expressed through the matrix Q and its derivatives

$$Q_2 = Q^{(1)} + Q^2, \tag{37}$$

$$Q_3 = Q^{(2)} + 2Q^{(1)}Q + QQ^{(1)} + Q^3, \tag{38}$$

$$Q_4 = Q^{(3)} + 3Q^{(2)}Q + QQ^{(2)} + 3(Q^{(1)})^2 + 3Q^{(1)}Q^2 + 2QQ^{(1)}Q + Q^2Q^{(1)} + Q^4. \tag{39}$$

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4. Examples of schemes

Let us consider examples of constructing fourth order schemes that satisfy the conditions of the theorem.

4.1. Constant matrix Q

Corollary 1. If the matrix Q is constant, then $Q_n = Q^n$ and the expansion of the matrix T does not depend on s and has the form

$$T = E + \tau Q + \frac{\tau^2}{2!}Q^2 + \frac{\tau^3}{3!}Q^3 + \frac{\tau^4}{4!}Q^4 + O(\tau^5). \tag{40}$$

It is clear that Eq. (40) is the expansion of the matrix exponential $\exp(\tau Q)$. Since it is an exact solution for the system with a constant matrix, then the one-step scheme with the exponential form has the infinity order of approximation for transition operator $T = \exp(\tau Q)$.

4.2. Symmetrical case

As mentioned before, the second order scheme does not contain the derivative $Q^{(1)}$ if and only if $s = 1/2$. It means that the transition matrix T depends only on $Q(t_n + \tau/2)$. Such choice of s corresponds to the center of the interval and will be called the symmetrical case. The expansion of the matrix T for the fourth order schemes in the symmetrical case gets rid of some terms and has only the dependence on $Q^{(1)}$ and $Q^{(2)}$. Therefore, it is necessary to use Q at least at three points for the fourth order scheme.

Corollary 2. The expansion Eq. (33) of the matrix T in the symmetrical case has the form as follows:

$$\begin{aligned} T = E + \tau Q + \frac{1}{2}\tau^2 Q^2 + \frac{\tau^3}{3!}Q^3 + \frac{\tau^3}{24}Q^{(2)} + \frac{\tau^3}{12}\left(Q^{(1)}Q - QQ^{(1)}\right) + \\ + \frac{\tau^4}{4!}Q^4 + \frac{\tau^4}{48}\left(QQ^{(2)} + Q^{(2)}Q\right) + \frac{\tau^4}{24}\left(Q^{(1)}Q^2 - Q^2Q^{(1)}\right). \end{aligned} \tag{41}$$

Approximating the derivatives in Eq. (41) by central finite differences of the second order

$$Q^{(1)}_{n+\frac{1}{2}} = \frac{Q_{n+\frac{3}{2}} - Q_{n-\frac{1}{2}}}{2\tau} + O(\tau^2), \quad Q^{(2)}_{n+\frac{1}{2}} = \frac{Q_{n+\frac{3}{2}} - 2Q_{n+\frac{1}{2}} + Q_{n-\frac{1}{2}}}{\tau^2} + O(\tau^2). \tag{42}$$

we retain the fourth order of accuracy of the operator

$$\begin{aligned} T_{n+\frac{1}{2}} &= E + \tau Q_{n+\frac{1}{2}} + \frac{\tau^2}{2}Q^2_{n+\frac{1}{2}} + \frac{\tau^3}{3!}Q^3_{n+\frac{1}{2}} + \frac{\tau^4}{4!}Q^4_{n+\frac{1}{2}} + \\ &+ \frac{\tau^3}{12}\left(Q^{(1)}_{n+\frac{1}{2}}Q_{n+\frac{1}{2}} - Q_{n+\frac{1}{2}}Q^{(1)}_{n+\frac{1}{2}}\right) + \frac{\tau^3}{24}Q^{(2)}_{n+\frac{1}{2}} + \\ &+ \frac{\tau^4}{48}\left(Q_{n+\frac{1}{2}}Q^{(2)}_{n+\frac{1}{2}} + Q^{(2)}_{n+\frac{1}{2}}Q_{n+\frac{1}{2}}\right) + \frac{\tau^4}{24}\left(Q^{(1)}_{n+\frac{1}{2}}Q^2_{n+\frac{1}{2}} - Q^2_{n+\frac{1}{2}}Q^{(1)}_{n+\frac{1}{2}}\right) + O(\tau^5). \end{aligned} \tag{43}$$

In the next two sections, we will show how to use Eqs. (41) and (42) to construct other schemes.

4.3. Exponential form

It is straightforward to verify that the Eq. (41) is an expansion of the exponent

$$T = \exp\left\{\tau F_1 + \tau^3 F_3\right\} + O(\tau^5), \tag{44}$$

where

$$F_1 = Q, \quad F_3 = \frac{1}{24}Q^{(2)} + \frac{1}{12}\left(Q^{(1)}Q - QQ^{(1)}\right), \quad F_2 = F_4 = 0. \tag{45}$$

Replacing the derivatives by the finite differences Eq. (42) we get the exponential scheme with the fourth order of accuracy (ES4). The advantage of this scheme is that for the skew-Hermitian

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matrix Q, the matrix T becomes unitary. The scheme Eq. (43) does not possess this property, although it also has the fourth order of accuracy. The scheme ES4 is the first of two schemes that are the main results of our article.

Exponential form Eq. (44) of the scheme allows approximating it by the Padé approximation [30] and apply to multidimensional systems. Also it should be noted that fast techniques (FNFT) cannot be applied directly to the transmission matrix Eq. (44), but it is possible to construct fast schemes using Eq. (41). These results will be presented in the future elsewhere.

4.4. Magnus expansion

Exponential form of Eq. (44) follows from the Magnus expansion [31,32]. It provides an exponential representation of the exact evolution operator of the system Eq. (5)

$$\Psi(t) = U(t,0)\Psi(0), \quad U(t,0) = e^{\Omega(t)},$$

which is constructed as a series expansion referred to as Magnus expansion: $\Omega(t) = \sum_{k=0}^{\infty} \Omega_k(t)$. First terms of this series have forms as follows:

$$\Omega_1(t) = \int_0^t dt_1 Q(t_1), \quad \Omega_2(t) = \frac{1}{2}\int_0^t dt_1 \int_0^{t_1} dt_2 \, [Q(t_1), Q(t_2)],$$

$$\Omega_3(t) = \frac{1}{6}\int_0^t dt_1 \int_0^{t_1} dt_2 \int_0^{t_3} dt_3 \, \left([Q(t_1), [Q(t_2), Q(t_3)]] + [Q(t_3), [Q(t_2), Q(t_1)]]\right).$$

Square brackets $[A, B] = AB - BA$ are the matrix commutator of A and B.

If we represent a matrix $Q(t)$ at the center of the integration interval $t/2$ by Taylor series and keep the main terms with respect to the small parameter t, then we get

$$\Omega_1 = tQ + \frac{t^3}{24}Q^{(2)} + O(t^5), \quad \Omega_2 = \frac{t^3}{12}\left[Q^{(1)}Q - QQ^{(1)}\right] + O(t^5), \quad \Omega_3 = O(t^5). \tag{46}$$

For $t = \tau$ Eq. (46) coincide with Eqs. (44)–(45). For the Schrödinger Eq. with a time-dependent operator, decomposition was obtained in a series of papers [33–35], but the authors decomposed the matrix Q in the Galerkin series and did not use difference schemes to find derivatives of Q.

The Magnus expansion for the ZS problem and the problem of splitting the operators was first considered in [36]. However, only the first term of the expansion was considered and the midpoint rule was used to approximate the integral. While this paper being reviewed an article appeared in which the formulas for the sixth order scheme were announced [37]. However, we consider independently only fourth order schemes and provide the alternative way of constructing such a scheme on a rigorous mathematical basis [38].

4.5. Triple-exponential scheme

Equation (41) can be continued in a different way:

$$T = e^{\tau Q} + \frac{\tau^2}{12}\left[Q^{(1)}e^{\tau Q} - e^{\tau Q}Q^{(1)}\right] + \frac{\tau^3}{48}\left[e^{\tau Q}Q^{(2)} + Q^{(2)}e^{\tau Q}\right] + O(\tau^5). \tag{47}$$

We can continue the Eq. (47) to the triple-exponential fourth order scheme (TES4)

$$T = \exp\left\{\frac{\tau^2}{12}Q^{(1)} + \frac{\tau^3}{48}Q^{(2)}\right\} \exp\{\tau Q\} \exp\left\{-\frac{\tau^2}{12}Q^{(1)} + \frac{\tau^3}{48}Q^{(2)}\right\}, \tag{48}$$

which contains a spectral parameter ζ only at the exponential $e^{\tau Q}$. The exponential can be split [22], so the fast techniques (FNFT) can be applied to this scheme. The Eq. (48) conserves the

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quadratic invariant H. If we use splitting in the form of a single product of exponential [23] then the Eq. (48) still conserves the quadratic invariant H.

The scheme TES4 is the second of two schemes that are the main results of our article.

If Q is skew-Hermitian, then $Q^{(1)}$ and $Q^{(2)}$ are also skew-Hermitian. All exponentials in Eq. (48) are unitary matricies and, therefore, they conserve the quadratic invariant H. The Maclaurin series of T Eq. (48) in τ gives exactly the decomposition of fourth order schemes for the symmetric case.

Note that an approximate solution of system Eq. (5) can be represented through the product of three exponentials using the Wilcox method [32,39]. In this case, each exponential depends on the matrix Q and its derivatives.

5. Numerical experiments

5.1. Numerical algorithms

We solve the system Eq. (5) on the uniform grid $t_n = -L + \tau n$ with a step τ on the interval $[-L, L]$, $L = 30$ unless otherwise stated. If the total number of points is $2M + 1$, then the grid step is $\tau = L/M$. We replace the original system Eq. (5) on the interval $(t_n - \frac{\tau}{2}, t_n + \frac{\tau}{2})$ with an approximate system with constant coefficients

$$\Psi_{n+\frac{1}{2}} = T\Psi_{n-\frac{1}{2}}. \tag{49}$$

The transition matrix T from the layer $n - \frac{1}{2}$ to the layer $n + \frac{1}{2}$ can be found using different numerical algorithms. Here we compared the numerical results for two new schemes presented above: the exponential scheme ES4 Eq. (44) and triple-exponential scheme TES4 Eq. (48). Then we tried the fourth order conservative transformed scheme (CT4) with the transition operator

$$T = e^{\frac{\tau}{2}Q_n}\left[I - \frac{\tau}{48}(M_{n+1} + M_{n-1})\right]^{-1}\left[I + \frac{\tau}{48}(M_{n+1} + M_{n-1})\right]e^{\frac{\tau}{2}Q_n} \tag{50}$$

where

$$M_{n+1} = e^{-\tau Q_n}(Q_{n+1} - Q_n)e^{\tau Q_n}, \quad M_{n-1} = e^{\tau Q_n}(Q_{n-1} - Q_n)e^{-\tau Q_n}.$$

The CT4 scheme was introduced recently in [24]. Here we present new and more detailed numerical results for this scheme.

Among the well known algorithms we chose the Boffetta-Osborne second order scheme (BO) [11] and the Runge-Kutta fourth order algorithm (RK4). Following [12] for RK4 scheme we solve the system for the envelope $\chi_1 = \psi_1 e^{i\zeta t}$, $\chi_2 = \psi_2 e^{-i\zeta t}$. Unlike the above schemes, RK4 does not require computing the transition matrix T. Note also that the conventional Runge-Kutta algorithm uses half-steps in its description. Here we set this half-step equal τ, where τ is a grid step for the potential $q(t)$.

The spectral data are finally defined by

$$a(\zeta) = \psi_1(L - \tau/2, \zeta)\, e^{i\zeta(L-\tau/2)}, \quad b(\zeta) = \psi_2(L - \tau/2, \zeta)\, e^{-i\zeta(L-\tau/2)}. \tag{51}$$

5.2. Computation of the derivative of $a(\zeta)$

To calculate the phase coefficients r_k we need to find the derivatives

$$\frac{da}{d\zeta} = \frac{d\psi_1}{d\zeta}e^{i\zeta(L-\tau/2)} + i(L - \tau/2)a(\zeta). \tag{52}$$

From Eq. (49) we get

$$\frac{d}{d\zeta}\Psi_{n+\frac{1}{2}} = T'_\zeta\Psi_{n-\frac{1}{2}} + T\frac{d}{d\zeta}\Psi_{n-\frac{1}{2}}, \tag{53}$$

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where initial value is defined from Eq. (8)

$$\frac{d}{d\zeta}\Psi(-L-\tau/2,\zeta)=\begin{pmatrix}-i(-L-\tau/2)\psi_1(-L-\tau/2,\zeta)\\0\end{pmatrix}. \tag{54}$$

For the exponential scheme ES4 Eq. (44) the transition matrix T can be represented as $T=\exp(A)$ and calculated using Pauli matrices Eq. (72) from the Appendix. Hence, we can find the derivative

$$T'_{(\mathrm{ES4})}=e^{a_0}\begin{pmatrix}c'+s'a_3+sa'_3 & s'a_1+sa'_1-is'a_2-isa'_2\\ s'a_1+sa'_1+is'a_2+isa'_2 & c'-s'a_3-sa'_3\end{pmatrix}, \tag{55}$$

where

$$\begin{aligned}
&c=\cos(\omega),\quad s=\frac{\sin(\omega)}{\omega},\quad \omega=\sqrt{-a_1^2-a_2^2-a_3^2},\\
&c'=-\sin(\omega)\omega',\quad s'=\frac{\omega'}{\omega}(c-s),\quad \omega'=-\frac{1}{\omega}(a_1a'_1+a_2a'_2+a_3a'_3),\\
&a'_1=i\frac{\tau^2}{24}(d_{12}-d_{21}),\quad a'_2=-\frac{\tau^2}{24}(d_{12}+d_{21}),\quad a'_3=-i\tau,\\
&d_{12}=q_{n+1}-q_{n-1},\quad d_{21}=-\sigma(q^*_{n+1}-q^*_{n-1}).
\end{aligned}$$

For the triple-exponential scheme TES4 Eq. (48) we obtain the derivative of the transition matrix T

$$T'_{(\mathrm{TES4})}=\exp\left\{\frac{\tau^2}{12}Q^{(1)}+\frac{\tau^3}{48}Q^{(2)}\right\}D\exp\left\{-\frac{\tau^2}{12}Q^{(1)}+\frac{\tau^3}{48}Q^{(2)}\right\}, \tag{56}$$

where $D=\left(e^{\tau Q_n}\right)'$ can be found from

$$\left(e^{\tau Q_n}\right)'=-\frac{\tau\zeta}{\omega_n}\sin(\omega_n\tau)I+\frac{\zeta}{\omega_n^3}\left[\tau\omega_n\cos(\omega_n\tau)-\sin(\omega_n\tau)\right]Q_n-i\frac{\sin(\omega_n\tau)}{\omega_n}\sigma_3, \tag{57}$$

where σ_3 is a Pauli matrix Eq. (71).

For CT4 scheme the transition matrix T Eq. (50) can be represented as a fraction $T=A^{-1}B$, therefore

$$T'_{(\mathrm{CT4})}=\left(A^{-1}B\right)'=A^{-1}Q'-A^{-1}A'A^{-1}B, \tag{58}$$

where

$$\begin{aligned}
A&=\left[I-\frac{\tau}{48}(M_{n+1}+M_{n-1})\right]e^{\frac{\tau}{2}Q_n}=A_1e^{\frac{\tau}{2}Q_n},\\
B&=\left[I+\frac{\tau}{48}(M_{n+1}+M_{n-1})\right]e^{\frac{3\tau}{2}Q_n}=B_1e^{\frac{3\tau}{2}}.
\end{aligned}$$

$$A'=-\frac{\tau}{48}\left(\left(e^{2\tau Q_n}\right)'(Q_{n-1}-Q_n)e^{-2\tau Q_n}+e^{2\tau Q_n}(Q_{n-1}-Q_n)\left(e^{-2\tau Q_n}\right)'\right)e^{\frac{\tau}{2}Q_n}+A_1\left(e^{\frac{\tau}{2}Q_n}\right)'.$$

$$B'=\frac{\tau}{48}\left(\left(e^{2\tau Q_n}\right)'(Q_{n-1}-Q_n)e^{-2\tau Q_n}+e^{2\tau Q_n}(Q_{n-1}-Q_n)\left(e^{-2\tau Q_n}\right)'\right)e^{\frac{3\tau}{2}Q_n}+B_1\left(e^{\frac{3\tau}{2}Q_n}\right)'.$$

We find the derivative of matrix exponential using Eq. (57).

For BO scheme the derivative of the transition matrix can be found in [11]. For RK4 scheme the derivative of $a(\zeta)$ can be computed using Romberg algorithm [12,40].

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5.3. Model signals

We considered a model signal in the form of a chirped hyperbolic secant

$$q(t) = A[\mathrm{sech}(t)]^{1+iC}. \tag{59}$$

For $C = 0$ it is a well-known Satsuma-Yajima signal. The detailed numerical results for this potential are presented in [15].

Here we consider two test potentials: $A = 5.25$, $C = 0$ for anomalous dispersion $\sigma = 1$ and $A = 5.2$, $C = 4$ for both anomalous and normal dispersion $\sigma = \pm 1$.

The analytical expressions of the spectral data of the potential Eq. (59) for anomalous dispersion are presented in [41]. But they can be obtained similarly for normal dispersion ($\sigma = -1$). Here we present general formulas using the Euler Gamma function Γ:

$$\begin{aligned} a(\xi) &= \frac{\Gamma[1/2 - i(\xi + C/2)]\,\Gamma[1/2 - i(\xi - C/2)]}{\Gamma[1/2 - i\xi - D]\,\Gamma[1/2 - i\xi + D]}, \\ b(\xi) &= \frac{1}{2^{iC}A}\frac{\Gamma[1/2 - i(\xi + C/2)]\,\Gamma[1/2 + i(\xi - C/2)]}{\Gamma[-iC/2 - D]\,\Gamma[-iC/2 + D]}, \quad D = \sqrt{\sigma A^2 - C^2/4}. \end{aligned} \tag{60}$$

The discrete spectrum ζ_k, $k = \overline{0, K-1}$ is determined by the zeros of the coefficient $a(\zeta)$ and exists only for anomalous dispersion ($\sigma = 1$):

$$\zeta_k = i\left(\sqrt{A^2 - C^2/4} - 1/2 - k\right), \quad k = 0, \ldots, [\sqrt{A^2 - C^2/4} - 1/2], \tag{61}$$

where square brackets denote the integer part of the expression.

To compute the phase coefficients r_k we need to know the derivative $a'(\zeta)$ only at points ζ_k of the discrete spectrum. Let us write the coefficient $a(\zeta)$ in the following form:

$$a(\zeta) = \frac{f(\zeta)}{\Gamma[1/2 - i\zeta - D]}, \quad \text{where} \quad f(\zeta) = \frac{\Gamma[1/2 - i(\zeta + C/2)]\,\Gamma[1/2 - i(\zeta - C/2)]}{\Gamma[1/2 - i\zeta + D]}.$$

The function $f(\zeta)$ and its derivative $f'(\zeta)$ have no singularities, so we have at the points of the discrete spectrum:

$$a'(\zeta)|_{\zeta=\zeta_k} = -if(\zeta_k)\varphi_k, \tag{62}$$

where the function φ_k is defined at the points of the discrete spectrum by a recurrence relation

$$\varphi_{k+1} = -(k+1)\varphi_k, \quad \varphi_0 = 1. \tag{63}$$

Thus we have a formula to compute the phase coefficients

$$r_k = \left.\frac{b(\zeta)}{a'(\zeta)}\right|_{\zeta=\zeta_k} = \left.\frac{b(\zeta)}{f(\zeta)}\right|_{\zeta=\zeta_k}\frac{i}{\varphi_k}. \tag{64}$$

To calculate energy of the discrete and continuous spectra E_d, E_c, we use the Eq. (13): $C_0 = E = E_c + E_d$. Full energy of the potential Eq. (59) is easily computed as $E = 2A^2$.

Let us denote $K = \left\lfloor \sqrt{A^2 - C^2/4} + 1/2 \right\rfloor$ as an integer part of the expression in square brackets and $\delta = \left\{ \sqrt{A^2 - C^2/4} + 1/2 \right\}$ as its fractional part. Then the discrete spectrum energy is

$$E_d = 4\sum_{k=0}^{K-1} \eta_k = 2\,(K + \delta - 1/2)^2 - 2\,(\delta - 1/2)^2\,. \tag{65}$$

and the continuous spectrum energy is

$$E_c = E - E_d = 2\left(C^2/4 + (\delta - 1/2)^2\right). \tag{66}$$

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5.4. Approximation order

The following formula was used to calculate the approximation order m:

$$m = \log_{\frac{\tau_1}{\tau_2}} \frac{\left\|\text{error}_{\tau_1}(\Psi)\right\|_2}{\left\|\text{error}_{\tau_2}(\Psi)\right\|_2} = \frac{\log_2 \frac{\left\|\text{error}_{\tau_1}(\Psi)\right\|_2}{\left\|\text{error}_{\tau_2}(\Psi)\right\|_2}}{\log_2(\tau_1/\tau_2)}, \tag{67}$$

where τ_i, $i = 1, 2$ are the steps of computational grids for two calculations with one spectral parameter ζ and $\tau_1 > \tau_2$; $\text{error}_{\tau_i}(\Psi) = \Psi_{\tau_i}(L) - \Psi_{exact}(L)$ is a deviation of the value $\Psi(L)$ calculated on a gris with a step τ_i from the exact analytical value at the boundary point $t = L$. The calculations were carried out for different p-norms and showed close values for the approximation orders. However, for the Euclidean 2-norm, the graphics were the smoothest.

Figure 1 confirms the approximation order $m = 4$ of the schemes with respect to a spectral parameter $\xi \in [-20, 20]$. Each line was calculated by the Eq. (67) using two embedded grids with a doubled grid step $\tau = L/M$, $L = 30$, where coarse and fine grids were defined by $M = 2^{10}$ and $M = 2^{11}$. Let us remind that the total number of points in the whole domain $[-L, L]$ is $2M + 1$.

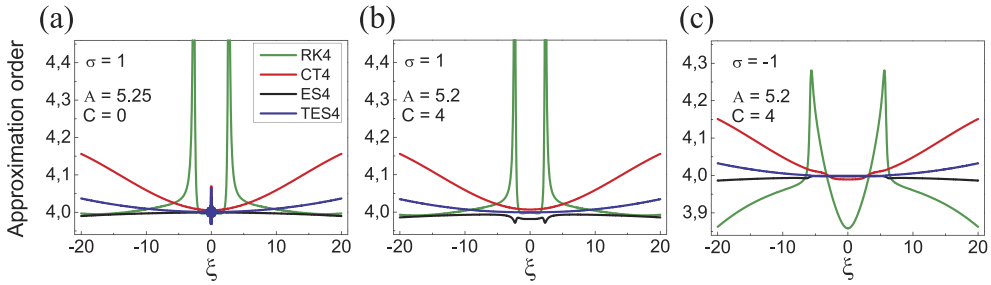

Fig. 1. The approximation order with respect to the spectral parameter ξ.

5.5. Formulas for errors

We present the numerical errors of calculating the spectral data for continuous and discrete spectrum. To find the calculation errors of the continuous spectrum energy E_c, residuals r_k, and the coefficients $a(\zeta)$, $b(\zeta)$ at fixed ζ we use formula

$$\text{error}[\phi] = \frac{|\phi^{comp} - \phi^{exact}|}{|\phi_0|}, \quad \phi_0 = \begin{cases} \phi^{exact}, \text{ if } |\phi^{exact}| > 1 \\ 1, \text{ otherwise,} \end{cases} \tag{68}$$

where ϕ can represent E_c, r_k, $a(\zeta)$ or $b(\zeta)$ at fixed ζ.

For the continuous spectrum we calculate the normalized mean squared error

$$NMSE[\phi] = \frac{1}{N}\sum_{j=1}^{N} \frac{|\phi^{comp}(\xi_j) - \phi^{exact}(\xi_j)|^2}{|\phi_0(\xi_j)|^2}, \quad \phi_0 = \begin{cases} \phi^{exact}(\xi_j), \text{ if } |\phi^{exact}(\xi_j)| > 1 \\ 1, \text{ otherwise,} \end{cases} \tag{69}$$

where ϕ can represent $a(\xi)$ or $b(\xi)$. Here we suppose the spectral parameter $\xi \in [-20, 20]$ with the total number of points $N = 2M + 1 = 1025$.

5.6. Numerical results for continuous spectrum

Figures 2 and 3 present the continuous spectrum errors for the potential Eq. (59) with two sets of parameters: $A = 5.25$, $C = 0$ for anomalous dispersion $\sigma = 1$ and $A = 5.2$, $C = 4$ for both anomalous and normal dispersion $\sigma = \pm 1$.

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Figure 2 shows the normalized mean squared error Eq. (69) of the coefficients $a(\xi)$ and $b(\xi)$ with respect to the number of grid nodes M. The total number of points in the whole domain $[-L, L]$ is $2M + 1$. Dashed vertical lines mark the minimum number of grid nodes $M_{\min}$ that guarantee a good approximation [24]. Actually, when calculating the continuous spectrum, it is necessary to choose a time step $\tau = L/M$ to describe correctly the fastest oscillations. For a fixed value of ξ, the local frequency $\omega(t;\xi) = \sqrt{\xi^2 + |q(t)|^2}$ of the system Eq. (5) varies from $\omega_{\min} = |\xi|$ to $\omega_{\max} = \sqrt{\xi^2 + q_{\max}^2}$, where $q_{\max} = \max_t |q(t)|$ is the maximum absolute value of the potential $q(t)$. Therefore, step τ cannot be arbitrary. In order to describe the most rapid oscillations, it is necessary to have at least 4-time steps for the oscillation period, so the inequality must be satisfied: $4\tau = 4L/M \le 2\pi/\omega_{\max}$. Therefore, any difference schemes will approximate the solutions of the original continuous system Eq. (5) if the inequality is fulfilled for the number of points $M \ge M_{\min} = 2\,L\,\omega_{\max}/\pi$.

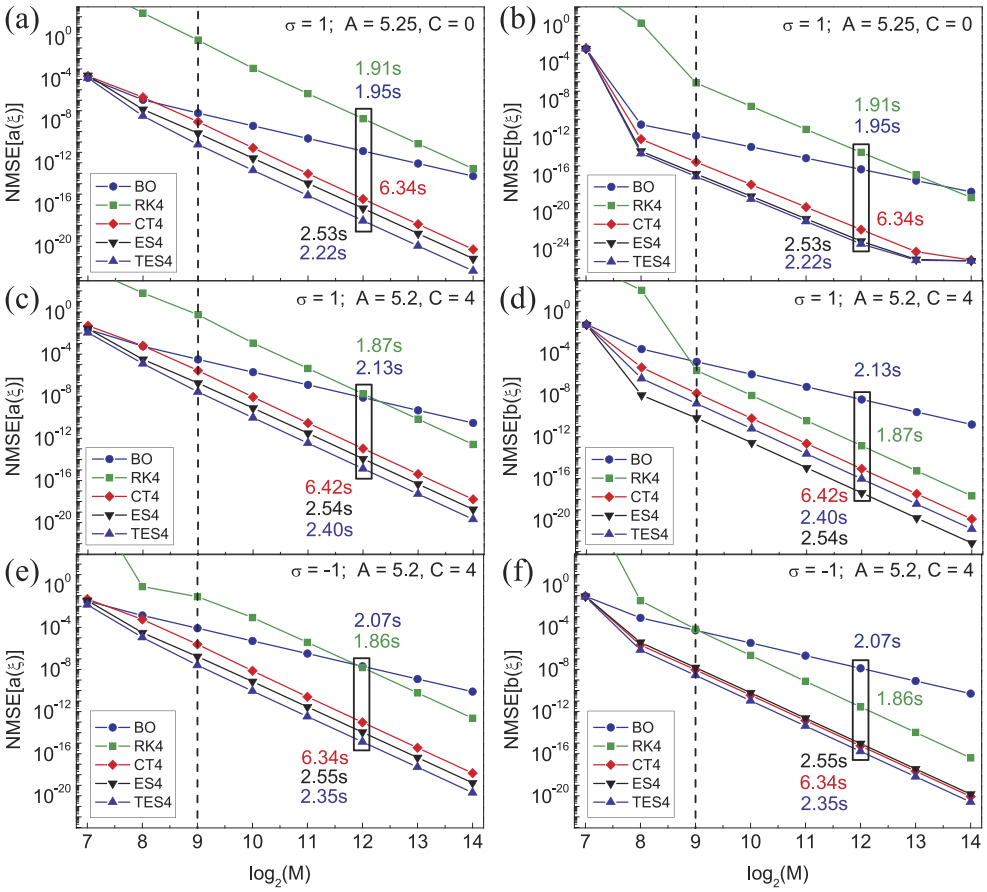

Fig. 2. Continuous spectrum normalized mean squared errors Eq. (69) of $a(\xi)$ and $b(\xi)$.

Figure 2 also demonstrates a comparison of the computational time. CT4, ES4 and TES4 show the comparebale accuracy, while TES4 demonstrates the best speed. In 5 out of 6 figures the accuracy of TES4 is slightly better.

The algorithms are implemented in C++. The numerical experiments are performed on a Intel(R) Core(TM) i7-7700HQ CPU 2.80GHz. Figure 3 shows how the numerical schemes conserve energy. The numerical errors Eq. (68) for the continuous spectrum energy Eq. (14)

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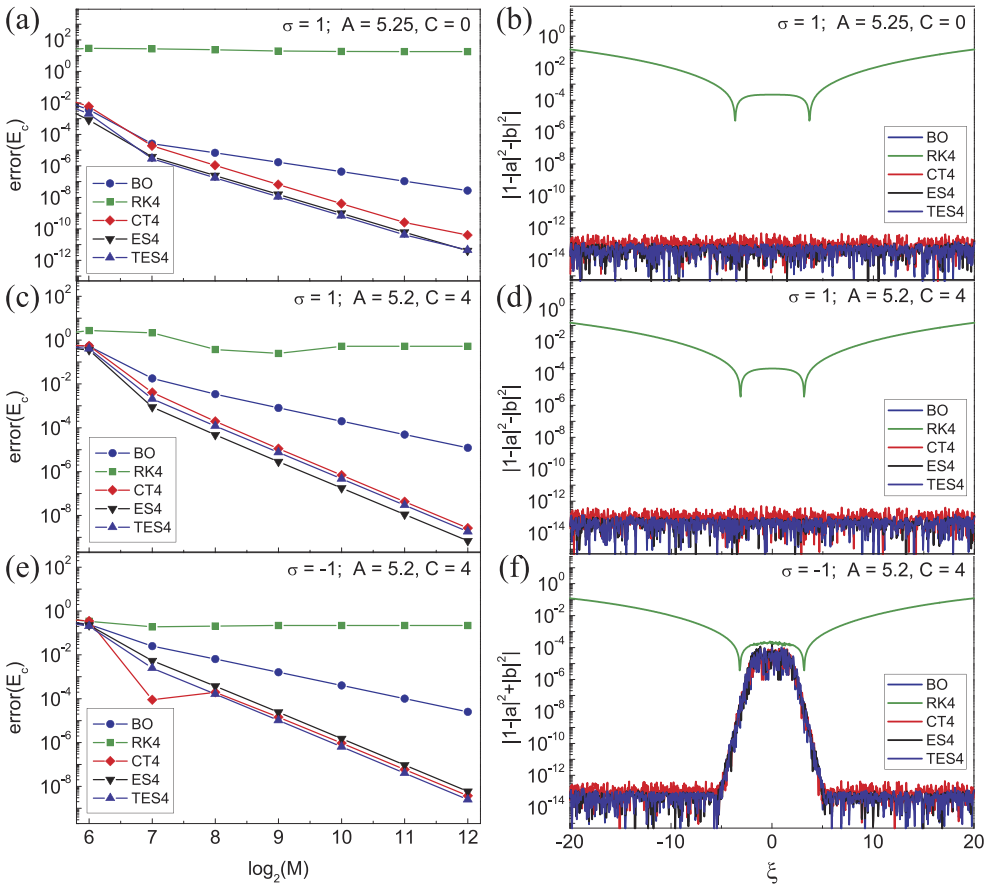

Fig. 3. (a, c, e) Errors Eq. (68) of continuous spectrum energy. (b, d, f) Absolute errors of quadratic invariants.

are compared in Figs. 3(a),(c), and (e). The integral was computed using the trapezoid rule. To calculate the continuous spectrum energy it is important to define the size of the spectral domain L_ξ and the corresponding grid step $d\xi$ [24]. According to the conventional discrete Fourier transform, we take the same number of points $N_\xi = N$ in the spectral domain and define a spectral step as $d\xi = \pi/(2L)$. So the size of the spectral interval is

$$L_\xi = \pi/(2\tau). \tag{70}$$

Figures 3(b), (d), and (f) demonstrates the deviation of the quadratic invariant $H = |a|^2 + \sigma|b|^2$ from unit with respect to the real spectral parameter ξ. Here the number of nodes is $M = 2^{10}$.

If the matrix Q is skew-Hermitian, then the matrix $\exp(\tau Q)$ is unitary and the quadratic invariant conserves. For the direct ZSP this corresponds to anomalous dispersion ($\sigma = 1$) with a real spectral parameter $\zeta = \xi$.

Let us consider a more general system with a matrix $Q = KD$, where $K(t)$ is anti-Hermitian matrix depending on t, D is a constant Hermitian matrix. The system Eq. (5) conserves the

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quadratic value $H = (\Psi^*, D\Psi)$. Indeed, we have this result from the chain of equalities

$$\frac{d}{dt}(\Psi^*, D\Psi) = \left(\frac{d\Psi^*}{dt}, D\Psi\right) + \left(\Psi^*, D\frac{d\Psi}{dt}\right) = (K^*D^*\Psi^*, D\Psi) + (\Psi^*, DKD\Psi) =$$
$$= \left(\Psi^*, (D^*)^T(K^*)^T D\Psi\right) + (\Psi^*, DKD\Psi) = \left(\Psi^*, D(K^\dagger + K)D\Psi\right) = 0.$$

For one-step exponential methods $\Psi_{n+\frac{1}{2}} = e^{R_n D}\Psi_{n-\frac{1}{2}}$, where R_n is skew-Hermitian matrix, the quadratic invariant also conserves. It follows from the chain of equalities

$$(\Psi^*_{n+\frac{1}{2}}, D\Psi_{n+\frac{1}{2}}) = (e^{\tau R_n^* D^*}\Psi^*_{n-\frac{1}{2}}, De^{\tau R_n D}\Psi_{n-\frac{1}{2}}) = (e^{\tau R_n^* D^*}\Psi^*_{n-\frac{1}{2}}, e^{\tau D R_n}D\Psi_{n-\frac{1}{2}}) =$$
$$= (\Psi^*_{n-\frac{1}{2}}, e^{-\tau R_n D}e^{\tau D R_n}D\Psi_{n-\frac{1}{2}}) = (\Psi^*_{n-\frac{1}{2}}, D\Psi_{n-\frac{1}{2}}).$$

Here we used the formula $De^{\tau R_n D} = e^{\tau D R_n}D$, because for any natural p the equality is valid: $D(R_nD)^p = (DR_n)^pD$.

From this result follows, that Boffetta-Osborne scheme BO [11], exponential scheme ES4 Eq. (44), and triple-exponential scheme TES4 Eq. (48) are conservative for normal and anomalous dispersion. Similarly the scheme CT4 Eq. (50) also conserves the quadratic invariant, because it is the function of R_nD.

Figure 3 confirms that RK4 scheme does not conserve the continuous spectrum energy and quadratic invariant for the real spectral parameters.

Figure 3(f) corresponds to the case of normal dispersion, therefore in the center of the spectral interval the parameters $a(\xi)$ and $b(\xi)$ have large values. This leads to the higher computational error in this zone. At the same time the quadratic invariant in this case equally conserves for all schemes considered here. However, RK4 scheme again shows the worst results at the edges of the spectral interval.

5.7. Numerical results for discrete spectrum

Figures 4 and 5 present the discrete spectrum errors Eq. (68). The parameters $a(\zeta_k)$, $b(\zeta_k)$ and r_k were computed for the analytically known eigenvalues Eq. (61). Here we did not use any numerical algorithm to find the eigenvalue but computed spectral data at the exact point $\zeta = \zeta_k$ right away. It was made intentionally to estimate the error of the scheme itself and to avoid the influence of the other numerical algorithm errors. The review of the approaches for finding the eigenvalues can be found in recent papers [15,20].

There are well known problems with the computation of the coefficient $b(\zeta_k)$. We used the bi-directional algorithm [42] to find $b(\zeta_k)$ by the Eq. (11).

Figure 5 presents the errors Eq. (68) of computing the phase coefficients for the maximum eigenvalue ζ_0 Eq. (61) with respect to the amplitude A of the potential Eq. (59). Here $L = 20$, $M = 2^{11}$.

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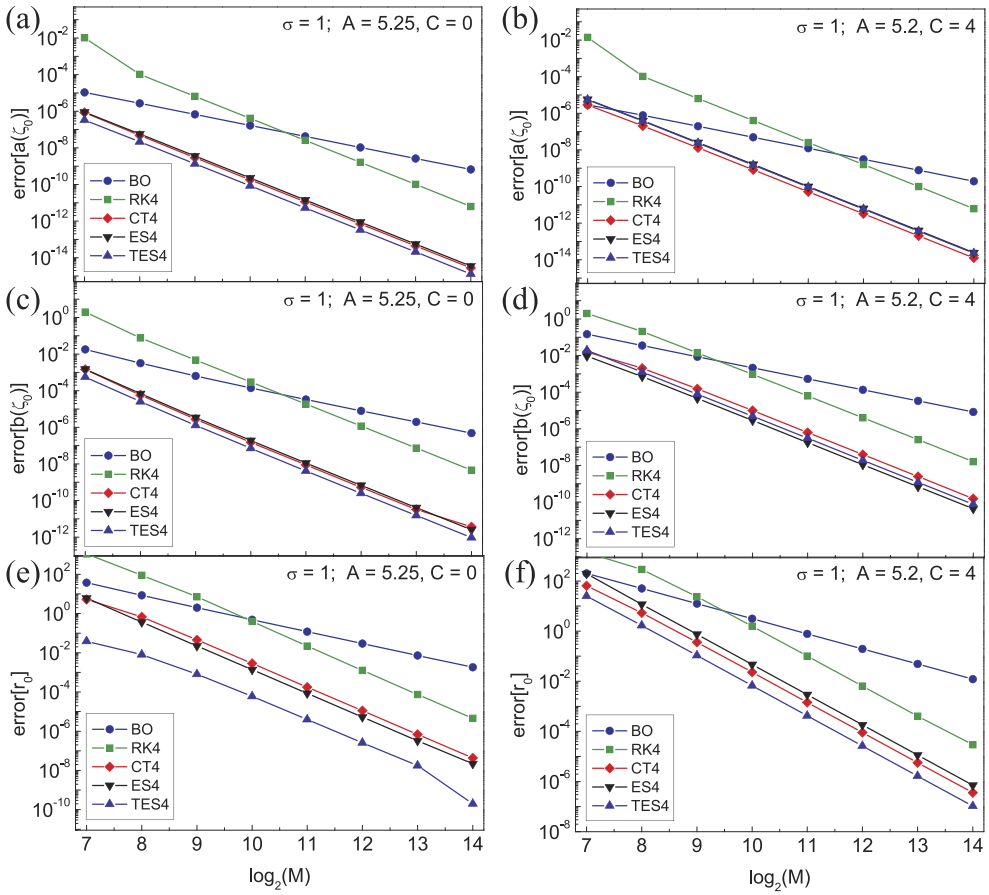

Fig. 4. Discrete spectrum errors for the maximum eigenvalue ζ_0.

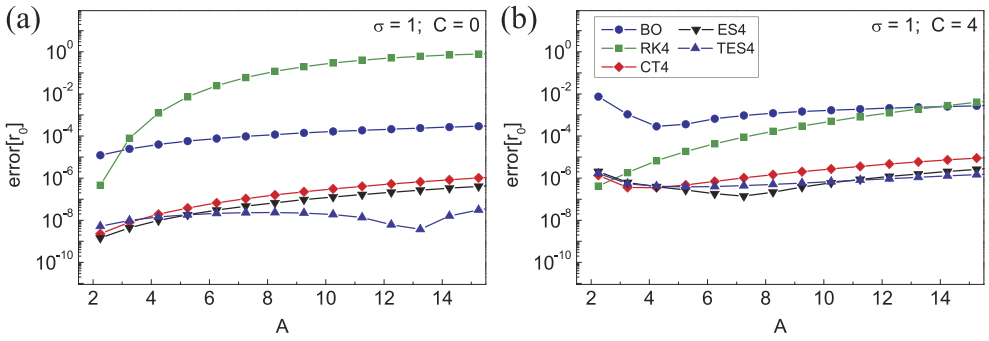

Fig. 5. The errors Eq. (68) of phase coefficients for the maximum eigenvalue ζ_0 Eq. (61).

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6. Conclusion

Two new forth order exponential schemes for the numerical solution of the direct Zakharov-Shabat problem were presented and compared with the known ones. The ES4 scheme demonstrates the excellent computational speed and accuracy, but has difficulties with the direct application of the FNFT algorithms. The TES4 scheme shows almost the same accuracy and even better speed than ES4. One can expect that a three-exponentials scheme should work at least 3 times longer than a one-exponential scheme. The speed of TES4 is explained by the fact, that two exponentials do not depend of the spectral parameter, while the third one $\exp(\tau Q)$ is calculated by the simplified explicit formula [11]. The exponential in ES4 requires the general form of Eq. (72). However the main advantage of TES4 scheme is that FNFT algorithms can be applied to it [23].

The CT4 scheme also shows good accuracy comparable with two exponential schemes mentioned above, but it works about $2.5-3$ times longer than ES4. In the recent paper [43] CT4 scheme was compared with NFT algorithms based on exponential integrators, namely, the integrators based on the classical fourth order (explicit) Runge-Kutta method, the three-stage Lobatto IIIA (implicit) Runge-Kutta method, as well as the standard and commutator-free Magnus methods. In addition the multi-step implicit Adams method was considered. In terms of accuracy, CT4 outperforms every other method examined in [43].

The CT4 scheme does not allow the direct application of the FNFT algorithms. However the FNFT algorithms can be applied to the CT4 and ES4 schemes after exponential approximation [22].

All the schemes ES4, TES4 and CT4 have an advantage over RK4 because they conserve the energy for the continuous spectrum parameter.

As already mentioned in the introduction, the CFQM schemes also conserve the quadratic form and have a high order of accuracy. Of course, they depend fundamentally on the interpolation method, but comparing our one-step schemes with such CQFM schemes is of interest and will be done carefully in subsequent works.

Appendix

The Pauli matrices can be used to calculate the matrix exponential in Eq. (44). A 2×2 complex matrix A can be presented as $A = a_0\sigma_0 + a_1\sigma_1 + a_2\sigma_2 + a_3\sigma_3$, where σ_j are Pauli matrices:

$$\sigma_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{71}$$

Then the matrix exponential can be found as

$$e^A = e^{a_0}\left[c\sigma_0 + is\left(a_1\sigma_1 + a_2\sigma_2 + a_3\sigma_3\right)\right] = e^{a_0}\begin{pmatrix} c + sa_3 & s(a_1 - ia_2) \\ s(a_1 + ia_2) & c - sa_3 \end{pmatrix}, \tag{72}$$

where $\omega = \sqrt{-a_1^2 - a_2^2 - a_3^2}$, $c = \cos(\omega)$, $s = \dfrac{\sin(\omega)}{\omega}$.

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