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ON COMPACT HIGH ORDER FINITE DIFFERENCE SCHEMES FOR LINEAR SCHRÖDINGER PROBLEM ON NON-UNIFORM MESHES

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This paper is dedicated to Prof. Francisco Lisbona

Abstract. In the present paper a general technique is developed for construction of compact high-order finite difference schemes to approximate Schrödinger problems on nonuniform meshes. Conservation of the finite difference schemes is investigated. The same technique is applied to construct compact high-order approximations of the Robin and Szeftel type boundary conditions. Results of computational experiments are presented.

Key words. finite-difference schemes, high-order approximation, compact scheme, Schrödinger equation, Szeftel type boundary conditions.

1. Introduction

High power high brightness edge-emitting semiconductor lasers and optical amplifiers are compact devices and they can serve a key role in different laser technologies such as free space communication [3], optical frequency conversion [11], printing, marking materials processing [16], or pumping fiber amplifiers [13].

To simulate the generation and/or propagation of the optical fields along the cavity of the considered device one can use a 2+1 dimensional system of PDEs which is based on the traveling wave (TW) equations for slowly varying in time longitudinally counter-propagating and laterally diffracted complex optical fields $E^{\pm}(z,x,t)$ [2], which are nonlinearly coupled to the linear ODEs for the complex induced polarization functions $p^{\pm}(z,x,t)$ and to the diffusion equation for the real carrier density $N(z,x,t)$ [17]:

$$\frac{\partial E^{\pm}}{\partial t} \pm \frac{\partial E^{\pm}}{\partial z} = -\frac{i}{2}\frac{\partial^2 E^{\pm}}{\partial x^2} - i\beta(N,|E^{\pm}|^2)E^{\pm} - i\kappa^{\mp}E^{\mp} - g_p(E^{\pm}-p^{\pm}),$$

$$\frac{\partial p^{\pm}}{\partial t} = i\omega_p p^{\pm} + \gamma_p\big(E^{\pm}-p^{\pm}\big),\ \frac{1}{\mu}\frac{\partial N}{\partial t} = \frac{\partial}{\partial x}\Big(D\frac{\partial N}{\partial x}\Big) + \Re e\,\mathcal{N}\big(N,E^{\pm},p^{\pm}\big)\,.$$

Here, $t \in \mathbb{R}_+$, $z \in [0,L]$ and $x \in \mathbb{R}$ denote temporal, longitudinal and lateral coordinates, respectively. Functions β, $\mathcal{N}$ and parameters g_p, $\kappa^{\mp}$, ω_p, γ_p, D, μ represent the propagation factor, injected current and nonlinear carrier recombination, Lorentzian gain amplitude, field coupling coefficient, gain peak detuning, Lorentzian half-width at half maximum, carrier diffusion coefficient, photon/carrier life time relation, respectively. Optical field functions $E^{\pm}$ satisfy the following reflection-injection conditions at the longitudinal boundaries of the domain:

$$E^{+}(0,x,t) = r_0(x)E^{-}(0,x,t) + a_0(x,t),$$
$$E^{-}(L,x,t) = r_L(x)E^{+}(L,x,t) + a_L(x,t).$$

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The initial conditions (if properly stated) are not very important, since after some transients the simulated trajectories approach one of the existing stable attractors.

A large scale system implied by a discretization of the computational domain and an appropriate approximation of artificially imposed lateral boundary conditions can be solved effectively with the help of parallel computing [17, 4, 10]. However, for the precise dynamic simulations of long and broad devices and tuning/optimization of the model with respect to one or several parameters, a further speedup of computations is still desired.

Since, in general, the carrier dynamics is slow ($0 < \mu \ll 1$), and in the most cases the polarization equations have only a small impact on the overall dynamics of the optical fields ($0 \leq g_p/\gamma_p \ll 1$), a proper construction of numerical schemes for the diffractive field equations plays a decisive role. Here we note, that for the temporarily fixed distribution of the propagation factor β, neglected polarization and absent coupling between counter-propagating fields (vanishing distributed coupling $\kappa^{\pm} = 0$ as well as field reflectivities at the longitudinal boundaries $r_0 = r_L = 0$), the equation for the forward (backward) propagating field on the characteristic lines $t - z = t_0$ (or $t - (L - z) = t_0$) is given by a linear 1+1 dimensional Schrödinger equation

$$\frac{\partial u}{\partial \nu} = -\frac{i}{2}\frac{\partial^2 u}{\partial x^2} - i\mathcal{B}(\nu, x)u,$$

where the field $u(\nu, x) = E^{+}(z, x, t)$ (or $u(\nu, x) = E^{-}(L - z, x, t)$), and the initial condition $u(0, x)$ is defined by the optical injection function $a_0(x, t)$ (or $a_L(x, t)$). Thus, a construction of the effective numerical schemes for the full model is closely related to the construction of the schemes for above given linear Schrödinger problem. One of the main challenges in this case is an implementation of the appropriate boundary conditions (BCs) [1]. In our previous paper [6] we have investigated the performance of the standard Crank-Nicolson scheme supplemented with the exact discrete transparent boundary conditions (DTBCs) [8], with the approximate DTBCs suggested by Szeftel [18] as well as with simple Dirichlet boundary conditions.

The main goal of the present paper is to develop a general technique for construction of compact high-order finite difference schemes for approximation of Schrödinger problems on nonuniform meshes. All these schemes can be of practical interest when dealing with broad lasers having a relatively high regularity of transversal heterostructures. In this case, due to enhanced spatial approximation precision, we can use a relatively sparse mesh in the transversal spatial direction, and, nevertheless, obtain the numerical solutions with a required precision. We note that in the case of uniform meshes, for the compact high-order finite difference scheme the corresponding exact DTBCs are derived in [12, 15]. We note that using the same ideas exact DTBCs can be constructed for the compact high-order finite difference schemes on non-uniform meshes, but such BCs are non-local in time and are not very efficient for applied problems described above.

The rest of the paper is organized as follows. In Section 2 we construct compact finite difference schemes on uniform and nonuniform meshes. On uniform mesh this high-order finite difference scheme coincides with the Numerov approximation. The conservation laws of the constructed finite difference schemes are investigated. For non-uniform meshes these laws can be violated due to non-symmetrical approximation of the source terms.

In Section 3, by using the technique from the previous section, we construct compact high-order approximations of the Robin type BCs, which can be interpreted as an approximation of the DTBCs suggested by Szeftel [18]. For Neumann type BC, which is a particular case of the Robin BC, a stability analysis of the obtained compact high-order schemes is done. It is shown that the finite difference scheme is unconditionally stable in this case. Finally, in Section 4 we present several computational experiments which confirm the theoretical convergence rate of the compact high-order finite difference schemes and lateral boundary conditions.

2. Compact high-order finite difference schemes

We consider the following linear Schrödinger problem in the laterally unbounded domain:

$$\begin{aligned} &-d\frac{\partial^2 u}{\partial x^2} = f(x,t) + \mathcal{B}(x,t)u - i\frac{\partial u}{\partial t}, \quad (x,t) \in \mathbb{R}\times\mathbb{R}_+, \\ &u(x,0) = u_0(x), \qquad x \in \mathbb{R}, \end{aligned} \tag{1}$$

where coefficient d represents the field diffraction.

It is easy to show, that once $u_0(x) \in W^{1,2}(\mathbb{R})$, potential $\mathcal{B}(x,t)$ is real, and $\frac{\partial u(x,t)}{\partial x}$ or $u(x,t)$ are vanishing with $x \to \pm\infty$, then the homogeneous Schrödinger equation ($f \equiv 0$) preserves in time the following integral:

$$I_1(t) := \int_{\mathbb{R}} |u(x,t)|^2\, dx = \text{const}, \qquad t \geq 0. \tag{2}$$

If, in addition, function $\mathcal{B}(x,t)$ is globally bounded and independent on time, the following integral is also preserved:

$$I_2(t) := d\int_{\mathbb{R}} \left|\frac{\partial u(x,t)}{\partial x}\right|^2 dx - \int_{\mathbb{R}} \mathcal{B}(x)|u(x,t)|^2\, dx = \text{const}, \qquad t \geq 0. \tag{3}$$

In this section we describe very briefly the technique for derivation of compact high-order approximations to Eq. (1), investigating also the conservation of discrete analogues of the integrals (2) and (3).

In the first step we restrict to the Method of Lines (MOL), when PDE is discretized only in space and we get semi-discrete schemes. For this reason we introduce a non-uniform spatial mesh

$$\begin{aligned} &\omega_h = \{x_j :\ x_j = x_{j-1} + h_{j-\frac{1}{2}},\ j \in \mathbb{Z}\}, \\ &\min_{j\in\mathbb{Z}} |x_j| = x_0, \quad h_j = \frac{h_{j-\frac{1}{2}} + h_{j+\frac{1}{2}}}{2}, \quad h := \max_{j\in\mathbb{Z}}(h_j), \end{aligned}$$

and define the first and the second order difference operators for spatially discrete functions η_j

$$\partial_x \eta_j := \frac{\eta_j - \eta_{j-1}}{h_{j-\frac{1}{2}}}, \quad \partial_x^2 \eta_j := \frac{1}{h_j}\Big(\partial_x \eta_{j+1} - \partial_x \eta_j\Big),$$

as well as mesh counterparts of the inner product and norm in the complex space $L_2(\mathbb{R})$:

$$\begin{aligned} &(\eta,\zeta)_h = \sum_{j\in\mathbb{Z}} \eta_j \zeta_j^* h_j, \quad \|\eta\| = \sqrt{(\eta,\eta)_h}, \\ &(\partial_x\eta, \partial_x\zeta]_h = \sum_{j\in\mathbb{Z}} \partial_x\eta_j\, \partial_x\zeta_j^* h_{j-\frac{1}{2}}, \quad \|\partial_x\eta]| = \sqrt{(\partial_x\eta, \partial_x\eta]_h}. \end{aligned}$$

In the next step we perform a discretization of the resulting equations in time by using the Crank-Nicolson method. For this reason we introduce a uniform time mesh

$$\omega_\tau = \{t^n : t^n = n\tau, \ \ n \in \mathbb{N}^*\}, \quad \text{where } \mathbb{N}^* = \mathbb{N} \cup \{0\},$$

and define the forward difference quotient and symmetric averaging in time for spatially and temporarily discrete functions η_j^n

$$\partial_t \eta_j^n = \frac{\eta_j^{n+1} - \eta_j^n}{\tau}, \quad \eta_j^{n+\frac{1}{2}} = \frac{1}{2}\big(\eta_j^{n+1} + \eta_j^n\big).$$

Let us consider the linear Schrödinger problem (1) with $f \equiv 0$. The corresponding compact high-order finite difference schemes will be constructed on a spatially non-uniform mesh. In practical computations we should restrict our considerations to the truncated domain $(x,t) \in \Omega^T = [-X, X] \times [0, T]$ and therefore the truncated mesh Ω_h^T is defined

$$\begin{aligned} &\Omega_h^T = \omega_h^T \times \omega_\tau^T, \qquad \text{where} \qquad \omega_\tau^T := \omega_\tau \cap [0, T], \\ &\omega_h^T := \omega_h \cap [-X, X] = \{x_j \in \omega_h, j = J_l, \dots, J_r\}. \end{aligned} \tag{4}$$

2.1. Second order approximation on non-uniform mesh. The first example is selected to demonstrate the basic technique for derivation of finite difference schemes of high approximation order when a given stencil of the mesh is used. We consider the following family of three-point semi-discrete finite difference approximations to the Schrödinger equation (1):

$$a_j U_{j-1} + c_j U_j + b_j U_{j+1} = V_j, \tag{5}$$

where U_j, V_j are mesh functions approximating $u(x,t)$ and $v(x,t) = -\frac{\partial^2 u}{\partial x^2}$ at $x = x_j$, respectively. In order to find coefficients (a_j, b_j, c_j) we require that corresponding pairs of test functions $\big(U(x), V(x)\big)$

$$U(x) = \{1, \quad (x - x_j), \quad (x - x_j)^2\}, \quad V(x) = \{0, \quad 0, \quad -2\}$$

would satisfy the discrete scheme (5) exactly. Then we get a system of linear equations

$$\begin{cases} a_j + c_j + b_j = 0, \\ -h_{j-\frac{1}{2}} a_j + h_{j+\frac{1}{2}} b_j = 0, \\ h_{j-\frac{1}{2}}^2 a_j + h_{j+\frac{1}{2}}^2 b_j = -2. \end{cases}$$

By solving it and using the equality

$$dV_j = f_j + \mathcal{B}_j U_j - i\frac{dU_j}{dt}, \tag{6}$$

we get the standard Finite Volume Method (FVM) semi-discrete scheme of approximation order $\mathcal{O}(h^2)$:

$$-d\,\partial_x^2 U_j = f_j + \mathcal{B}_j U_j - i\frac{dU_j}{dt}. \tag{7}$$

Here $U_j(t)$ is an approximation to $u(x_j, t)$. It is easy to prove that for $f \equiv 0$ and real $\mathcal{B}$ the solution of this scheme satisfies the condition $\|U(t)\|^2 = \text{const}$, $t \geq 0$, which is the discrete analogue of Eq. (2). If, additionally, $\mathcal{B}$ is globally bounded and time-independent, then $d\|\partial_x U(t)]|^2 - (\mathcal{B}U(t), U(t))_h = \text{const}$, $t \geq 0$, i.e. the discrete analogue of Eq. (3) holds as well.

Let us introduce the discrete function U_j^n which is an approximation to $u(x_j, t^n)$. A corresponding Crank-Nicolson finite difference scheme

$$-d\,\partial_x^2 U_j^{n+\frac{1}{2}} = \mathcal{B}_j^{n+\frac{1}{2}} U_j^{n+\frac{1}{2}} - i\partial_t U_j^n$$

under the same assumptions on function $\mathcal{B}$ satisfies similar discrete conservation laws:

$$\|U^n\|^2 = \text{const}, \qquad d\|\partial_x U^n]|^2 - (\mathcal{B}U^n, U^n)_h = \text{const}, \qquad n \geq 0.$$

2.2. High-order approximation on uniform mesh. Now we consider a family of compact semi-discrete finite difference schemes, that are defined on the following three-point template:

$$aU_{j-1} + \frac{2}{h^2}U_j + bU_{j+1} = \alpha V_{j-1} + \gamma V_j + \beta V_{j+1}. \tag{8}$$

In order to find coefficients $(a, b, \alpha, \beta, \gamma)$ we require that the corresponding pairs of test functions

$$\begin{aligned} U(x) &= \{1,\ \ (x-x_j),\ \ (x-x_j)^2,\ \ (x-x_j)^3,\ \ (x-x_j)^4\}, \\ V(x) &= \{0,\ \ 0,\ \ -2,\ \ -6(x-x_j),\ \ -12(x-x_j)^2\} \end{aligned} \tag{9}$$

would satisfy the discrete scheme (8) exactly. Then we get a system of linear equations

$$\begin{cases} a + b = -2, \\ h(a-b) = 0, \\ h^2(a+b) = -2(\alpha + \gamma + \beta), \\ -h^3(a-b) = 6h(\alpha - \beta), \\ h^4(a+b) = -12h^2(\alpha + \beta). \end{cases}$$

By solving it and using equality (6), we derive the following semi-discrete scheme

$$-d\partial_x^2 U_j = A_h\Big(f_j + \mathcal{B}_j U_j - i\frac{dU_j}{dt}\Big), \tag{10}$$

where the averaging operator A_h is defined as

$$A_h\eta_j := \frac{1}{12}\eta_{j-1} + \frac{10}{12}\eta_j + \frac{1}{12}\eta_{j+1} = \left(I + \frac{h^2}{12}\partial_x^2\right)\eta_j.$$

This scheme coincides with the well-known Numerov scheme of higher order $\mathcal{O}(h^4)$, see also [14].

The conservation of a discrete approximation to Schrödinger equation, i.e., conservation of discrete analogues of integrals (2) and (3), is a desired property of any finite difference scheme. For a self-completeness of this paper, we present basic results on the conservation of the semi-discrete scheme (10) with $f \equiv 0$, as well as of corresponding high-order Crank-Nicolson finite difference scheme

$$-d\partial_x^2 U_j^{n+\frac{1}{2}} = \left(I + \frac{h^2}{12}\partial_x^2\right)\left(\mathcal{B}_j^{n+\frac{1}{2}} U_j^{n+\frac{1}{2}} - i\partial_t U_j^n\right). \tag{11}$$

For more results, see [1].

Theorem 1. *Let the real mesh function $\mathcal{B}_j(t)$ be bounded for all $t \geq 0$ and $x_j \in \omega_h$. Then the semi-discrete finite difference scheme* (10) *with $f \equiv 0$ and the finite difference scheme* (11) *preserve the discrete analogue of* (2) *in time*

$$\|U(t)\|^2 = const, \quad t \geq 0, \qquad \|U^n\|^2 = const, \quad n \geq 0. \tag{12}$$

If, additionally, function $\mathcal{B}$ is constant, then the discrete version of the second integral (3) *is also preserved*

$$
\begin{aligned}
&d\,\|\partial_x U(t)]|^2 - \mathcal{B}\|U(t)\|^2 = const, \quad t \geq 0, \\
&d\,\|\partial_x U^n]|^2 - \mathcal{B}\|U^n\|^2 = const, \quad n \geq 0.
\end{aligned} \tag{13}
$$

Proof. First we consider the case $\mathcal{B}_j(t) = \mathcal{B}$. Doing the inner product on both sides of equation (10) with $-2iU_j(t)$, using summation by parts and taking the real part, we obtain

$$\frac{d}{dt}\left(\|U(t)\|^2 - \frac{h^2}{12}\|\partial_x U(t)]|^2\right) = 0.$$

Similarly, when doing the same operations with Eq. (10) and $2\frac{d}{dt}U_j(t)$ we get

$$\frac{d}{dt}\left(\left(d + \frac{h^2}{12}\mathcal{B}\right)\|\partial_x U(t)]|^2 - \mathcal{B}\|U(t)\|^2\right) = 0.$$

From these two equalities we get

$$\frac{d}{dt}\|U(t)\|^2 = \frac{d}{dt}\|\partial_x U(t)]|^2 = 0,$$

what proves the first part of (12) and (13).

For a general case of mesh function $\mathcal{B}_j$ we use the technique from [15]. Since $I + \frac{h^2}{12}\partial_x^2 \geq \frac{2}{3}I > 0$, we can rewrite the semi-discrete scheme (10) with $f \equiv 0$ as follows:

$$i\frac{d}{dt}U_j(t) = \mathcal{B}_j(t)U_j(t) + dA_h^{-1}\,\partial_x^2 U_j(t), \quad A_h^{-1} := \left(I + \frac{h^2}{12}\partial_x^2\right)^{-1}.$$

After taking the inner product on both sides of this scheme with $-2iU_j(t)$, using summation by parts and taking the real parts we get

$$\frac{d}{dt}\|U(t)\|^2 = 2d\,\Im m\left(A\,\partial_x^2 U_j(t), U_j(t)\right).$$

Operators A and ∂_x^2 have a common system of eigenvectors, they commute and are self-adjoint. Thus, $A\,\partial_x^2$ is also a self adjoint operator and the right-hand side of the last equality vanishes. This completes the proof of (12) for the semi-discrete scheme (10).

The fully discrete version of conservation laws (12) and (13) are obtained after performing similar operations with difference scheme (11) and grid functions $-2iU_j^{n+\frac{1}{2}}$ or $2\tau\partial_t U_j^n$, $n = 0, 1, \ldots$ □

In general, the derived scheme (10) is similar to the scheme presented in [7]

$$-d\,\partial_x^2 U_j = C_h[1]f_j + C_h[\mathcal{B}]U_j - iC_h[1]\frac{dU_j}{dt}, \tag{14}$$

where the averaging operator C_h is given by

$$C_h[w]\eta_j := \frac{1}{12}w_{j-\frac{1}{2}}\eta_{j-1} + \frac{10}{12}\,\frac{w_{j-\frac{1}{2}} + w_{j+\frac{1}{2}}}{2}\eta_j + \frac{1}{12}w_{j+\frac{1}{2}}\eta_{j+1}.$$

We see that averaging operator $C_h[w]$ is self-adjoint for any w, and, therefore, the scheme (14) satisfies discrete analogues of conservation laws (2) and (3) even for non-uniform potential $\mathcal{B}$. Since $C_h[1] \equiv A_h$, for constant $\mathcal{B}$ both finite difference schemes (10) and (14) coincide, but for general non-constant $\mathcal{B}$, however, the approximation order of the scheme (14) is only $\mathcal{O}(h^2)$, since

$$C_h[\mathcal{B}]u - A_h\mathcal{B}u = h^2\Big(\frac{1}{24}\frac{\partial^2\mathcal{B}}{\partial x^2}\,u - \frac{\partial\mathcal{B}}{\partial x}\,\frac{\partial u}{\partial x}\Big).$$

2.3. High-order approximation on non-uniform mesh. In this section we apply the same technique to construct a high-order compact semi-discrete finite difference scheme on non-uniform mesh. It is defined on the same three-point template:

$$a_j U_{j-1} + \frac{2}{h_{j-\frac{1}{2}} h_{j+\frac{1}{2}}} U_j + b_j U_{j+1} = \alpha_j V_{j-1} + \gamma_j V_j + \beta_j V_{j+1}.$$

Applying corresponding pairs of test functions (9) as approximation order conditions and solving the obtained system of linear equations, we get the semi-discrete high-order finite difference scheme

$$-d\,\partial_x^2 U_j = \widetilde{A}_h \Big(f_j + \mathcal{B}_j U_j - i \frac{dU_j}{dt} \Big), \tag{15}$$

where the averaging operator $\widetilde{A}_h$ is defined as

$$\widetilde{A}_h \eta_j := \alpha_j \eta_{j-1} + (1 - \alpha_j - \beta_j)\eta_j + \beta_j \eta_{j+1},$$

$$\alpha_j = \frac{h^2_{j-\frac{1}{2}} + h_{j+\frac{1}{2}}(h_{j-\frac{1}{2}} - h_{j+\frac{1}{2}})}{12 h_j h_{j-\frac{1}{2}}}, \quad \beta_j = \frac{h^2_{j+\frac{1}{2}} + h_{j-\frac{1}{2}}(h_{j+\frac{1}{2}} - h_{j-\frac{1}{2}})}{12 h_j h_{j+\frac{1}{2}}}.$$

Since for non-uniform meshes the condition of self-adjoint operators $h_j \alpha_j^* = h_{j-1}\beta_{j-1}$ is, in general, not satisfied, we can not prove conservation estimates, similar to (12) and (13). Computational experiments have also confirmed that the related Crank-Nicolson finite difference scheme

$$-d\partial_x^2 U_j^{n+\frac{1}{2}} = \widetilde{A}_h \left(\mathcal{B}_j^{n+\frac{1}{2}} U_j^{n+\frac{1}{2}} - i\partial_t U_j^n \right) \tag{16}$$

on the arbitrary non-uniform mesh is not conservative.

The finite difference scheme (15) on non-uniform mesh reminds the scheme presented in [7]:

$$-d\,\partial_x^2 U_j = \widetilde{C}_h[1] f_j + \widetilde{C}_h[\mathcal{B}] U_j - i \widetilde{C}_h[1] \frac{dU_j}{dt},$$

where the averaging operator $\widetilde{C}_h[w]$ is defined as

$$\widetilde{C}_h[w]\eta_j := \frac{h_{j-1/2}}{12 h_j} w_{j-1/2} \eta_{j-1} + \frac{10}{12} \widehat{w}_j \eta_j + \frac{h_{j+1/2}}{12 h_j} w_{j+1/2} \eta_{j+1}, \tag{17}$$

$$\widehat{w}_j := \frac{h_{j-1/2}}{2h_j} w_{j-1/2} + \frac{h_{j+1/2}}{2h_j} w_{j+1/2}.$$

It is noteworthy that this averaging operator is self-adjoint, and the difference scheme possesses discrete analogues of the conservation laws (12) and (13). However, even in the case of constant mesh function w the scheme (17) differs from the high-order approximation (15) and has approximation accuracy $\mathcal{O}(h^2)$.

3. DTBCs for compact high-order finite difference scheme

In this section we consider the linear Schrödinger problem (1) with $f \equiv 0$. The corresponding compact high-order finite difference scheme (16) is constructed on a spatially non-uniform mesh. As was mentioned above, we should restrict to the truncated domain $(x,t) \in \Omega^T = [-X, X] \times [0, T]$ and the truncated mesh (4). Without loss of generality we assume, that outside of the computational domain

$[x_{J_l}, x_{J_r}]$ the spatial mesh ω_h is determined by the uniform steps $h_{J_l+\frac{1}{2}}$ and $h_{J_r-\frac{1}{2}}$

$$\omega_h = \begin{cases} x_j = x_{J_l} + (j - J_l)h_{J_l+\frac{1}{2}} & \text{if } j < J_l \\ x_j \in \omega_h^T & \text{if } j = J_l, \dots, J_r \ , \\ x_j = x_{J_l} + (j - J_r)h_{J_r-\frac{1}{2}} & \text{if } j > J_r \end{cases} \tag{18}$$

and the finite difference scheme (16) in these outer regions coincide with the Numerov scheme (11).

To close the system (16) defined on the inner part of the finite mesh Ω_h^T we need to define the boundary conditions for field function U_j^n at the left and right spatial boundary point x_{J_l} and x_{J_r}. In this section we will construct compact high-order discrete boundary conditions admitting nearly reflection-free field propagation through the boundary of the truncated domain.

Let us assume that outside of the computational bounds the initial function $u_0 = 0$ and the potential function $\mathcal{B}$ is constant:

$$u_0(x) \equiv 0 \quad \text{if} \quad x \in \mathbf{R} \setminus [x_{J_l+1}, x_{J_r-1}], \qquad \mathcal{B}(t,x) = \begin{cases} \bar{\mathcal{B}}_l, & \text{if } x \le x_{J_l+1} \\ \bar{\mathcal{B}}_r, & \text{if } x \ge x_{J_r-1} \end{cases}. \tag{19}$$

First of all, we construct a compact high-order approximation for the Robin type BCs at the lateral bounds $x = \pm X$ of the truncated domain Ω^T:

$$-\sqrt{d}\,\frac{\partial u(-X,t)}{\partial x} + ir_l u(-X,t) = \mu_l, \qquad \sqrt{d}\,\frac{\partial u(X,t)}{\partial x} + ir_r u(X,t) = \mu_r, \tag{20}$$

where r_l, r_r are the parameters defined from the special reflection function, μ_l, μ_r are the given fluxes of the solution on the boundary.

In order to derive a compact high-order approximation of BCs, we apply the same technique as in previous sections. In addition to functions u and $v = -\frac{\partial^2 u(x,t)}{\partial x^2}$, let us define $w = \frac{\partial u(x,t)}{\partial x}$. Now we use the following two-point template with the maximal number of free parameters:

$$a_k U_{J_k} + b_k U_{J_k+\nu_k} = W_{J_k} + \gamma_k V_{J_k} + \beta_k V_{J_k+\nu_k}, \quad k \in \{l,r\}, \ \ \nu_l = 1, \ \ \nu_r = -1.$$

Thus we can take the corresponding triples of test functions

$$\begin{aligned} U(x) &= \{1, \ \ x - x_j, \ \ (x - x_j)^2, \ \ (x - x_j)^3\}, \\ W(x) &= \{0, \ \ 1, \ \ 2(x - x_j), \ \ 3(x - x_j)^2\}, \\ V(x) &= \{0, \ \ 0, \ \ -2, \ \ -6(x - x_j)\}, \end{aligned}$$

and solve the system of linear equations derived from approximation conditions. The compact semi-discrete approximation of boundary condition (20) is obtained:

$$\begin{aligned} d\frac{U_{J_k} - U_{J_k+\nu_k}}{h_{J_k+\frac{\nu_k}{2}}} + \sqrt{d}\,(ir_k U_{J_k} - \mu_k) &= \frac{h_{J_k+\frac{\nu_k}{2}}}{3}\left(f_{J_k} + \mathcal{B}_{J_k} U_{J_k} - i\frac{dU_{J_k}}{dt}\right) \\ &+ \frac{h_{J_k+\frac{\nu_k}{2}}}{6}\left(f_{J_k+\nu_k} + \mathcal{B}_{J_k+\nu_k} U_{J_k+\nu_k} - i\frac{dU_{J_k+\nu_k}}{dt}\right), \qquad k \in \{l,r\}. \end{aligned} \tag{21}$$

The approximation error of (21) is of order $\mathcal{O}(h^3)$. By setting $\beta_k = 0$ one can also get a standard $\mathcal{O}(h^2)$-order approximation of (21):

$$d\frac{U_{J_k} - U_{J_k+\nu_k}}{h_{J_k+\frac{\nu_k}{2}}} + \sqrt{d}\,(ir_k U_{J_k} - \mu_k) = \frac{h_{J_k+\frac{\nu_k}{2}}}{2}\left(f_{J_k} + \mathcal{B}_{J_k} U_{J_k} - i\frac{dU_{J_k}}{dt}\right), \quad k \in \{l,r\}. \tag{22}$$

The Robin type BCs are also important when considering nonlocal transparent BCs [1, 5] for the linear homogeneous ($f \equiv 0$) Schrödinger problem (1) in the laterally truncated domain Ω^T. In [18], Szeftel proposed to approximate the nonlocal transparent BCs with a sequence of local operators. Assuming that the conditions (19) are satisfied, we can write these approximate transparent BCs for (1) at $x = \pm X$ as follows [6]:

$$(23)\qquad \begin{aligned} &-\nu_s\sqrt{d}\,\tfrac{\partial u(-\nu_s X,t)}{\partial x} + i\left(\beta + \sum_{k=1}^{m} a_k\right) u(-\nu_s X,t) = i\sum_{k=1}^{m} a_k d_k \varphi_{k,s}(t),\\ &\frac{d\varphi_{k,s}}{dt} = iu(-\nu_s X,t) - i(\bar{\mathcal{B}}_s + d_k)\varphi_{k,s}(t), \quad t>0,\\ &\varphi_{k,s}(0) = 0, \qquad k = 1,\dots,m, \quad m\ge 1, \quad s\in\{l,r\}. \end{aligned}$$

Having a similar form as Robin BCs (20), these conditions can be approximated by the semi-discrete compact high-order scheme

$$\begin{aligned} &d\tfrac{U_{J_s}-U_{J_s+\nu_s}}{h_{J_s+\frac{\nu_s}{2}}} + i\sqrt{d}\Big(\beta U_{J_s} + \sum_{k=1}^{m} a_k\big(U_{J_s} - d_k\Phi_{k,s}\big)\Big) =\\ &\tfrac{h_{J_s+\frac{\nu_s}{2}}}{3}\left(\bar{\mathcal{B}}_s U_{J_s} - i\tfrac{dU_{J_s}}{dt}\right) + \tfrac{h_{J_s+\frac{\nu_s}{2}}}{6}\left(\bar{\mathcal{B}}_s U_{J_s+\nu_s} - i\tfrac{dU_{J_s+\nu_s}}{dt}\right),\\ &\frac{d\Phi_{k,s}}{dt} = iU_{J_s} - i(\bar{\mathcal{B}}_s + d_k)\Phi_{k,s}(t), \quad \Phi_{k,s}(0)=0, \quad k=1,\dots,m,\ s\in\{l,r\}. \end{aligned}$$

The stability analysis of compact high-order BCs is a non-trivial task. It is important to see if the proposed approximations are A-stable. In the case of constant $\mathcal{B}$ and uniform mesh ω_h, a general technique of spectral analysis can be used. Since the operator defining the finite difference scheme together with BCs is not symmetric, we only can check whether it can be diagonalized and eigenvalues of the operator have positive real parts. Applying this method, we should find eigenvalues and eigenvectors of the generalized eigenvalue problem, defined by the appropriate discrete diffusion operator and the compact boundary conditions [9]. The influence of compact approximations is taken into account through the generalized formulation of eigenvalue problem by using the nondiagonal eigenvalue operator

$$(24)\qquad \begin{aligned} &-\partial_x^2 V_j = \lambda A_h V_j, \quad j = J_l+1,\dots,J_r-1, \quad J_r = J_l + J,\\ &\frac{V_{J_s} - V_{J_s+\nu_s}}{h} + ir_s V_{J_s} = \frac{h\lambda}{6}\Big(2V_{J_s} + V_{J_s+\nu_s}\Big), \ s\in\{l,r\},\ \nu_l = 1,\ \nu_r = -1. \end{aligned}$$

Here we are interested in separating the influence of the compact approximation of boundary conditions. Thus we take $A_h = I$, as in the case of standard second-order scheme (7). In order to simplify analysis, we restrict to the Neumann type boundary condition on boundary $x = x_{J_r} = X$, i.e. $r_r = 0$, and the Dirichlet boundary condition $V_{J_l} = 0$ at $x = x_{J_l} = -X$. Then it can be shown that $(J-1)$ eigenvectors V^k and corresponding eigenvalues λ_k are defined as

$$V_j^k = \sin\alpha_k(x_j + X), \quad \lambda_k = \frac{4}{h^2}\sin^2\frac{\alpha_k h}{2}, \quad k = 1,\dots,J-1,$$

where $0 < \alpha_k < \pi/h$ are $(J-1)$ roots of nonlinear equation

$$\sin\alpha Jh - \sin\alpha(J-1)h = \frac{2}{3}\sin^2\frac{\alpha h}{2}\big(2\sin\alpha Jh + \sin\alpha(J-1)h\big).$$

The remaining eigenvalue λ_J is computed numerically and it is shown that $\lambda_J > 4/h^2$. Thus the compact high-order approximation of boundary conditions is unconditionally stable in this case.

4. Numerical examples

4.1. Example 1. In order to test the accuracy of compact high-order scheme (16) we have solved a test problem from [1, 6]. Consider linear Schrödinger equation (1) with $\mathcal{B} \equiv 0$, $f \equiv 0$, $d = 0.5$, the exact solution is given as

$$u(x,t) := \sqrt{\frac{i}{i+2t}} \exp\left[(-ix^2 + 4x - 8t)/(i+2t)\right]. \tag{25}$$

We simulate the movement of a Gaussian wave for $(x,t) \in [-X, X] \times [0, T]$, where $X = 10$ and $T = 0.7$. The initial and boundary conditions are defined by the solution (25):

$$u_0(x) = u(x,0), \quad u(\pm X, t) = \sqrt{\frac{i}{i+2t}} \exp\left[(-iX^2 \pm 4X - 8t)/(i+2t)\right]. \tag{26}$$

The computational grid (4) is determined by the time step $\tau = 1/N$, and the truncated non-uniform spatial mesh ω_h^T having $|\omega_h^T| = J$ spatial steps

$$h_{j-\frac{1}{2}} = (\alpha + r_{j-\frac{1}{2}})\eta, \qquad j = J_l + 1, \dots, J_r = J_l + J$$

defined by the random number generator. Here, $0 < r_{j-\frac{1}{2}} \le 1$ are pseudo-random numbers, α is a regularization parameter and η is a scaling constant allowing to locate exactly J steps within computational interval $[-X, X]$.

In Table 1 errors in the maximum norm ε and convergence rates $\log_2 \rho$

$$\begin{aligned} &\epsilon_\alpha(|\omega_h^T|, N) := \max_{t^n \in \omega_\tau^T} \varepsilon_\alpha(|\omega_h^T|, t^n), \quad \varepsilon_\alpha(|\omega_h^T|, t^n) = \max_{x_j \in \omega_h^T} |u(x_j, t^n) - U_j^n|, \\ &\rho_\alpha(J) := \varepsilon_\alpha(J/2, N/4)/\varepsilon_\alpha(J, N) \end{aligned} \tag{27}$$

for solution of high-order compact finite difference scheme (16) are presented for a sequence of meshes and $\alpha = 0.1$ or $\alpha = 0.25$. Results of experiments show the discrete solution convergence with fourth order of accuracy even in the case of highly non-uniform space meshes.

TABLE 1. Errors ϵ_α and convergence rates $\log_2 \rho_\alpha$ for solution of high-order compact finite difference scheme (16) with initial and boundary conditions (26).

J	N	$\epsilon_{0.1}$	$\log_2 \rho_{0.1}$	$\epsilon_{0.25}$	$\log_2 \rho_{0.25}$
200	100	1.29e-2	—	1.03e-2	—
400	400	8.09e-4	3.991	6.64e-4	3.954
800	1600	4.62e-5	4.129	3.85e-5	4.104
1600	6400	3.11e-6	3.888	2.50e-6	3.945

4.2. Example 2. In this case we have solved numerically the test problem of Example 1 with the BCs (20), where

$$\mu_l = -\sqrt{d}\,\frac{\partial u(-X,t)}{\partial x}, \qquad \mu_r = \sqrt{d}\,\frac{\partial u(X,t)}{\partial x}, \qquad r_l = r_r = 0. \tag{28}$$

We note, that these boundary conditions are of Neumann type and are exact conditions once the initial function u_0 is given by (26).

In this example we have tested the accuracy of the new compact high-order finite difference approximation of BCs (21), and compared it with the standard second-order accuracy scheme (22). The linear Schrödinger equation is approximated by the high-order finite difference scheme (11) on a uniform mesh. The results were computed using a very small time step τ, to make temporal errors negligible. Table 2 gives maximum norm errors $\varepsilon_0(J,T)$ at time $T = 1.8$ for a sequence of space mesh points J, and the observed orders of convergence $\log_2 \rho_0(J)$

defined in Eq. (27). Crank-Nicolson time discretization of (21) and (22) are used to approximate boundary conditions of the problem.

TABLE 2. Errors $\varepsilon_0(J,T)$ and orders of convergence $\log_2 \rho_0(J)$ for solution of high-order compact finite difference scheme (11), when BCs (20), (28) are approximated by the third order accuracy scheme (21) and the standard second order accuracy scheme (22).

FDS		$J = 250$	$J = 500$	$J = 1000$	$J = 2000$
(21)	ε_0	1.41E-3	1.26E-4	1.47E-5	1.76E-6
(21)	$\log_2 \rho_0$	—	3.48	3.10	3.06
(22)	ε_0	8.75E-3	2.02E-3	4.99E-4	1.24E-4
(22)	$\log_2 \rho_0$	—	2.11	2.01	2.01

Results of computational experiments confirm the conclusion that local approximation errors of BCs should dominate the global error, since the differential equation is approximated by the high-order finite difference scheme. The observed experimental convergence orders coincide with the theoretical approximation orders of discrete boundary conditions (21) and (22), i.e. the third and second orders, respectively.

5. Conclusions

The presented analysis shows that high-order approximations of the linear Schrödinger equations and the Robin type BCs increase the efficiency of solvers targeted for this type of problems. In [4, 6], we have constructed effective numerical algorithms for simulation of multisection lasers by using the traveling wave model, which is described briefly in the Introduction of this paper. These algorithms are derived by using two ideas: splitting techniques are used to separate the linear Schrödinger equation and the complicated nonlinear interaction of waves, and special absorbing boundary conditions are applied to restrict computations only to a finite truncated computational domain. As it is shown in [5], very efficient artificial absorbing BCs of the Robin type can be constructed by using the Szeftel method, see (23). For both subproblems we can apply the high-order finite difference schemes, proposed in this paper. The analysis of the accuracy and efficiency of the obtained finite difference schemes for the full traveling wave model will be done in a separate paper.

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