Weierstraß-Institut

für Angewandte Analysis und Stochastik

Leibniz-Institut im Forschungsverbund Berlin e. V.

Preprint ISSN 0946 – 8633

Compact high order finite difference schemes for linear Schrödinger problems on non-uniform meshes

Mindaugas Radziunas[1], Raimondas Čiegis[2], Aleksas Mirinavičius[2]

submitted: December 10, 2012

[1] Weierstrass Institute
Mohrenstr. 39
10117 Berlin, Germany
E-Mail: Mindaugas.Radziunas@wias-berlin.de

[2] Vilnius Gediminas Technical University
Saulėtekio al. 11
LT-10223 Vilnius, Lithuania
E-Mail: rc@vgtu.lt
amirinavicius@gmail.com

No. 1748

Berlin 2012

2010 *Mathematics Subject Classification.* 65M06, 65M20, 65M99, 35Q60, 65M12.

Key words and phrases. finite-difference schemes, high-order approximation, compact scheme, Schrödinger equation, transparent boundary conditions .

The work of M. R. was supported by DFG Research Center MATHEON “Mathematics for key technologies: Modelling, simulation, and optimization of real-world processes”.

Edited by
Weierstraß-Institut für Angewandte Analysis und Stochastik (WIAS)
Leibniz-Institut im Forschungsverbund Berlin e. V.
Mohrenstraße 39
10117 Berlin
Germany

Fax: +49 30 20372-303
E-Mail: preprint@wias-berlin.de
World Wide Web: http://www.wias-berlin.de/

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. Discrete transparent boundary conditions are constructed for the given high-order finite difference scheme. 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.

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 [1], optical frequency conversion [2], printing, marking materials processing [3], or pumping fiber amplifiers [4].

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 $E^{\pm}(z,x,t)$ [5], 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 $N(z,x,t)$ [6]:

$$\begin{aligned}
&\frac{\partial E^{\pm}}{\partial t} \pm \frac{\partial E^{\pm}}{\partial z} = -\frac{i}{2}\frac{\partial^2 E^{\pm}}{\partial x^2} - i\beta(N,\varepsilon|E^{\pm}|^2)E^{\pm} - i\kappa^{\mp}E^{\mp} - g_p(E^{\mp} - p^{\pm}),\\
&\frac{\partial p^{\pm}}{\partial t} = i\omega_p p^{\pm} + \gamma_p\big(E^{\pm} - p^{\pm}\big), \quad \frac{1}{\mu}\frac{\partial N}{\partial t} = \frac{\partial}{\partial x}\Big(D\frac{\partial N}{\partial x}\Big) + \Re e\,\mathcal{N}\big(N, E^{\pm}, p^{\pm}\big)\,.
\end{aligned}$$

Here, $t \in \mathbb{R}_+$, $z \in [0,L]$ and $x \in \mathbb{R}$ denote temporal, longitudinal and lateral coordinates, respectively, while optical field functions $E^{\pm}$ satisfy the following reflection-injection conditions at the longitudinal boundaries of the domain:

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

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 [6, 7, 8]. 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 ($0 \geq g_p/\gamma_p \ll 1$), 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) [9]. In our previous paper [10] we have investigated the performance of the standard Crank-Nicolson scheme supplemented with the exact discrete transparent boundary conditions (DTBCs) [11], with the approximate DTBCs suggested by Szeftel [12] 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.

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. Results of computational experiments are presented, which confirm the predicted accuracy of compact high-order schemes.

For the compact high-order finite difference scheme the corresponding exact DTBCs are derived in Section 3. Next, by using the technique from previous sections, we construct compact high-order approximations of the Robin type BCs, which can be interpreted as an approximation of the DTBCs suggested by Szeftel [12]. For Neumann type BCs, which are a particular case of Robin BCs, a stability analysis of the obtained compact 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 a 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:

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

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 $x \to \pm\infty$, 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:

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

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

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

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

$$
\omega_\tau = \big\{t^n : \ t^n = n\tau, \ n = 0 \cup \mathbb{N}\big\},
$$

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

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

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):

$$a_j U_{j-1} + c_j U_j + b_j U_{j+1} = V_j, \tag{4}$$

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 (4) 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

$$dV_j = f_j + \mathcal{B}_j U_j - i\frac{dU_j}{dt}, \tag{5}$$

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

$$-d\,\partial_x^2 U_j = f_j + \mathcal{B}_j U_j - i\frac{dU_j}{dt}. \tag{6}$$

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

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:

$$aU_{j-1} + \frac{2}{h^2}U_j + bU_{j+1} = \alpha V_{j-1} + \gamma V_j + \beta V_{j+1}. \tag{7}$$

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

$$\begin{aligned} U(x) &= \{1,\ \ (x-x_j),\ \ (x-x_j)^2,\ \ (x-x_j)^3,\ \ (x-x_j)^4\}, \\ V(x) &= \{0,\ \ 0,\ \ -2,\ \ -6(x-x_j),\ \ -12(x-x_j)^2\} \end{aligned} \tag{8}$$

would satisfy the discrete scheme (7) 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 (5), we derive the following semi-discrete scheme

$$-d\partial_x^2 U_j = A_h\Big(f_j + \mathcal{B}_j U_j - i\frac{dU_j}{dt}\Big), \tag{9}$$

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 [15].

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 (9) with $f \equiv 0$, as well as of corresponding high-order Crank-Nicolson finite difference scheme

$$-d\partial_x^2 U_j^{n+\frac{1}{2}} = \left(I + \frac{h^2}{12}\partial_x^2\right)\left(\mathcal{B}_j^{n+\frac{1}{2}} U_j^{n+\frac{1}{2}} - i\partial_t U_j^n\right). \tag{10}$$

For more results, see [9].

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* (9) *with $f \equiv 0$ and the finite difference scheme* (10) *preserve the discrete analogue of* (2) *in time*

$$\|U(t)\|^2 = \textit{const}, \quad t \geq 0, \qquad \|U^n\|^2 = \textit{const}, \quad n \geq 0. \tag{11}$$

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

$$
\begin{aligned}
&d\,\|\partial_x U(t)]|^2 - \mathcal{B}\|U(t)\|^2 = \textit{const}, \quad t \geq 0,\\
&d\,\|\partial_x U^n]|^2 - \mathcal{B}\|U^n\|^2 = \textit{const}, \quad n \geq 0.
\end{aligned}
\tag{12}
$$

Proof. First we consider the case $\mathcal{B}_j(t) = \mathcal{B}$. Doing the inner product on both sides of equation (9) 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. (9) 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 (11) and (12).

For a general case of mesh function $\mathcal{B}_j$ we use the technique from Ref. [16]. Since $I + \frac{h^2}{12}\partial_x^2 \geq \frac{2}{3}I > 0$, we can rewrite the semi-discrete scheme (9) with $f \equiv 0$ as follows:

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

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 (11) for the semi-discrete scheme (9).

The fully discrete version of conservation laws (11) and (12) are obtained after performing similar operations with difference scheme (10) and grid functions $-2iU_j^{n+\frac{1}{2}}$ or $2\tau\partial_t U_j^n$, $n = 0, 1, \ldots$ □

In general, the above derived scheme (9) is similar to that one presented in Ref. [14]

$$
-d\,\partial_x^2 U_j = C_h[1]f_j + C_h[\mathcal{B}]U_j - iC_h[1]\frac{dU_j}{dt}, \tag{13}
$$

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 (13) 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 (9) and (13) coincide, but for general non-constant $\mathcal{B}$, however, the approximation order of the scheme (13) 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 (8) as approximation order conditions and solving the obtained system of linear equations, we get the semi-discrete high-order finite difference scheme

$$-d\, \partial_x^2 U_j = \widetilde{A}_h \Big(f_j + \mathcal{B}_j U_j - i \frac{dU_j}{dt} \Big), \tag{14}$$

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

$$\begin{aligned} &\widetilde{A}_h \eta_j := \alpha_j \eta_{j-1} + (1 - \alpha_j - \beta_j) \eta_j + \beta_j \eta_{j+1}, \\ &\alpha_j = \frac{h^2_{j-\frac{1}{2}} + h_{j+\frac{1}{2}}(h_{j-\frac{1}{2}} - h_{j+\frac{1}{2}})}{12 h_j h_{j-\frac{1}{2}}}, \quad \beta_j = \frac{h^2_{j+\frac{1}{2}} + h_{j-\frac{1}{2}}(h_{j+\frac{1}{2}} - h_{j-\frac{1}{2}})}{12 h_j h_{j+\frac{1}{2}}}. \end{aligned}$$

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 (11) and (12). Computational experiments have also confirmed that the related Crank-Nicolson finite difference scheme

$$-d \partial_x^2 U_j^{n+\frac{1}{2}} = \widetilde{A}_h \left(\mathcal{B}_j^{n+\frac{1}{2}} U_j^{n+\frac{1}{2}} - i \partial_t U_j^n \right) \tag{15}$$

on the arbitrary non-uniform mesh is not conservative.

The finite difference scheme (14) on non-uniform mesh reminds the scheme presented in Ref. [14]:

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

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

$$\begin{aligned} &\widetilde{C}_h[w] \eta_j := \frac{h_{j-1/2}}{12 h_j} w_{j-1/2} \eta_{j-1} + \frac{10}{12} \widehat{w}_j \eta_j + \frac{h_{j+1/2}}{12 h_j} w_{j+1/2} \eta_{j+1}, \\ &\widehat{w}_j := \frac{h_{j-1/2}}{2 h_j} w_{j-1/2} + \frac{h_{j+1/2}}{2 h_j} w_{j+1/2}. \end{aligned} \tag{16}$$

It is noteworthy that this averaging operator is self-adjoint, and the difference scheme possesses discrete analogues of the conservation laws (11) and (12). However, even in the case of constant mesh function w the scheme (16) differs from the high-order approximation (14) and has approximation accuracy $\mathcal{O}(h^2)$.

3 DTBCs for compact high-order finite difference scheme

Let us consider the linear Schrödinger problem (1) with $f \equiv 0$ and a corresponding compact high-order finite difference scheme (15) 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 the truncated mesh

$$\begin{aligned} &\Omega_h^T = \omega_h^T \times \omega_\tau^T, \qquad \text{where} \qquad \omega_\tau^T := \omega_\tau \cap [0,T], \\ &\omega_h^T := \omega_h \cap [-X,X] = \{x_j \in \omega_h, j = J_l, \dots, J_r\}. \end{aligned} \tag{17}$$

Without loss of generality we can 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 (15) in these outer regions coincide with the Numerov scheme (10).

To close the system (15) 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 the rest of this section we will construct two different types of boundary conditions admitting nearly reflection-free field propagation through the boundary of the truncated domain.

3.1 Exact DTBCs

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

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

Following [13] we can prove the theorem:

Theorem 2 *Assume, that conditions* (19) *are satisfied. Then the exact DTBCs for the high-order compact finite difference scheme* (15) *considered on the truncated grid* Ω_h^T *are given by*

$$\eta_0^k U_{J_k}^n - U_{J_k+\nu_k}^n = \beta_k U_{J_k+\nu_k}^{n-1} - \sum_{s=0}^{n} \eta_{n-s}^k U_{J_k}^s, \quad k \in \{l, r\}, \tag{20}$$

where all parameters entering these conditions are defined as follows:

$$
\begin{aligned}
\eta_n^k &= \frac{6+5\sigma_k}{6-\sigma_k}\delta_n^0 + \frac{6+5\sigma_k^*}{6-\sigma_k}\delta_n^1 + \alpha_k\lambda_k^{-n}\frac{P_n(\mu_k)-P_{n-2}(\mu_k)}{2n-1},\\
\beta_k &= \frac{6-\sigma_k^*}{6-\sigma_k},\quad \sigma_k = \frac{(-\bar{\mathcal{B}}_k\tau+2i)h^2_{J_k+\nu_k/2}}{2d\tau},\quad \lambda_k = \frac{-\sigma_k(3+\sigma_k)}{|\sigma_k(3+\sigma_k)|},\\
\mu_k &= \frac{\Re e((3+\sigma_k^*)\sigma_k)}{|\sigma_k(3+\sigma_k)|},\quad \alpha_k = \frac{-\sqrt[+]{24\sigma_k(3+\sigma_k)}}{6-\sigma_k},\quad \nu_l=1,\ \ \nu_r=-1.
\end{aligned}
\tag{21}
$$

Proof. Taking into account the assumptions (18) and (19), the finite difference scheme (15) at the outer regions is of Numerov type and can be written as

$$
U_{j-1}^{n+1}+U_{j+1}^{n+1}+\beta_k\left(U_{j-1}^n+U_{j+1}^n\right)-2\left(\frac{6+5\sigma_k}{6-\sigma_k}U_j^{n+1}+\frac{6+5\sigma_k^*}{6-\sigma_k}U_j^n\right)=0,
$$

where $k=l$ for $j\le J_l$, $k=r$ for $j\ge J_r$, and constants β_k and σ_k are as defined in (21). Following [11, 13], for derivation of the DTBCs we apply the $\mathcal{Z}$-transformation

$$
\mathcal{Z}(f_n)=\hat{f}(z):=\sum_{n=0}^{\infty}f_nz^{-n},\quad z\in\mathbf{C},\quad |z|>R_f
$$

with respect to the time series $\{f_n\}_{n=0}^{\infty}$ representing the considered finite difference scheme at temporal grid points $t_n\in\omega_\tau$. Taking into account the assumption (19) on the initial conditions u_0, the resulting equation reads as

$$
\hat{U}_{j+1}(z)-2\frac{(6+5\sigma_k)z+6+5\sigma_k^*}{(6-\sigma_k)(z+\beta_k)}\hat{U}_j(z)+\hat{U}_{j-1}(z)=0.
$$

For all $j\le J_l$ ($k=l$) and $j\ge J_r$ ($k=r$) the solutions of this scheme are given by

$$
\hat{U}_j(z)=A_k^+(z)\hat{\chi}_k^{j-J_k}(z)+A_k^-(z)\hat{\chi}_k^{J_k-j}(z),
$$

where $\hat{\chi}_k\in\{\hat{\chi}_k^+,\hat{\chi}_k^-\},\ \hat{\chi}_k^-\hat{\chi}_k^+=1,\ |\hat{\chi}_k|=\max|\hat{\chi}_k^\pm|\ge 1$, and $\{\hat{\chi}_k^-,\hat{\chi}_k^+\}$ are two roots of the characteristic equation

$$
\hat{\chi}_k^2(z)-2\frac{(6+5\sigma_k)z+6+5\sigma_k^*}{(6-\sigma_k)(z+\beta_k)}\hat{\chi}_k(z)+1=0.
$$

In order to have a decaying solution $\hat{U}_j(z)$ outside of the computational domain, we should set $A_l^-(z)=0$ (or $A_r^+(z)=0$). These assumptions yield the boundary conditions

$$
\hat{U}_{J_k+\nu_k}(z)=\hat{\chi}_k(z)\hat{U}_{J_k}(z)\quad\Longrightarrow\quad\frac{z+\beta_k}{z}\hat{U}_{J_k+\nu_k}(z)=\hat{\eta}_k(z)\hat{U}_{J_k}(z),\tag{22}
$$

where $\hat{\eta}_k=\frac{z+\beta_k}{z}\hat{\chi}_k(z)\in\{\hat{\eta}_k^+(z),\hat{\eta}_k^-(z)\}$ and

$$
\begin{aligned}
\hat{\eta}_k^\pm(z) &= \tfrac{6+5\sigma_k}{6-\sigma_k}+\tfrac{6+5\sigma_k^*}{6-\sigma_k}z^{-1}\pm\alpha_k\left(2\mu_k\lambda_k^{-1}z^{-1}-1-\lambda_k^{-2}z^{-2}\right)\hat{F}(\lambda_kz,\mu_k),\\
\hat{F}(z,y) &:= \tfrac{1}{\sqrt[+]{1-2yz^{-1}+z^{-2}}}=\textstyle\sum_{n=0}^{\infty}P_n(y)z^{-n}\quad\text{for}\quad |z|>R_f,
\end{aligned}
$$

After performing an inverse $\mathcal{Z}$-transform we get

$$\eta_n^{k,\pm} = \mathcal{Z}^{-1}\hat{\eta}_k^{\pm}(z)\big|_n = \frac{6+5\sigma_k}{6-\sigma_k}\delta_n^0 + \frac{6+5\sigma_k^*}{6-\sigma_k}\delta_n^1$$
$$\pm\,\alpha_k \sum_{s=0}^{n} \left(2\mu_k\lambda_k^{-1}\delta_{n-s}^1 - \delta_{n-s}^0 - \lambda_k^{-2}\delta_{n-s}^2\right) \mathcal{Z}^{-1}\hat{F}(\lambda_k z, \mu_k)\big|_s$$
$$= \frac{6{+}5\sigma_k}{6{-}\sigma_k}\delta_n^0 + \frac{6{+}5\sigma_k^*}{6{-}\sigma_k}\delta_n^1 \pm \alpha_k\lambda_k^{-n}\left[2\mu_k P_{n-1}(\mu_k) - P_n(\mu_k) - P_{n-2}(\mu_k)\right].$$

Here and above $P_n(\mu)$ are the Legendre polynomials, δ_n^s are the Croneker symbols, λ_k, μ_k, ν_k, and α_k are the parameters defined in (21), and $\sqrt[+]{z} = \sqrt{|z|}e^{i\arg(z)/2}$ denotes the principal branch of square root of the complex number (i.e., $\arg(z) \in (-\pi,\pi]$). The numerical test has shown that $\hat{\eta}_k = \hat{\eta}_k^+$, and, therefore, the required $\mathcal{Z}^{-1}$-transformed sets $\{\eta_n^k\}|_{n=0}^{\infty} = \{\eta_n^{k,+}\}|_{n=0}^{\infty}$.

The inverse $\mathcal{Z}$-transform of the boundary conditions (22) together with the recurrence property

$$xP_{n-1}(x) = \frac{n}{2n-1}P_n(x) + \frac{n-1}{2n-1}P_{n-2}(x)$$

of the Legendre polynomials imply the discrete transparency boundary conditions (20). □

In the case if the solution u and the potential function $\mathcal{B}$ are smooth enough, the finite difference scheme (15) on the grid Ω_h^T together with the exact DTBCs (20) have a precision of order $\mathcal{O}(\tau^2 + h^4)$.

3.2 High-order approximation of transparent BCs

Being elegant and exact, the DTBCs (20) have, however, a serious drawback: with each consequent time step one needs to estimate convolution sums of growing length involving full history of the field function U at the boundaries of the domain. Due to slow convergence of these sums (truncation of the sums implies significant errors!), some less computationally demanding algorithms providing good approximation of DTBCs are still required.

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:

$$-\sqrt{d}\,\frac{\partial u(-X,t)}{\partial x} + ir_l u(-X,t) = \mu_l, \qquad \sqrt{d}\,\frac{\partial u(X,t)}{\partial x} + ir_r u(X,t) = \mu_r. \tag{23}$$

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 a 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

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

and solve the system of linear equations derived from approximation conditions. The compact semi-discrete approximation of boundary condition (23) is obtained:

$$\begin{aligned} d\frac{U_{J_k} - U_{J_k+\nu_k}}{h_{J_k+\frac{\nu_k}{2}}} + \sqrt{d}\,(ir_k U_{J_k} - \mu_k) = \frac{h_{J_k+\frac{\nu_k}{2}}}{3}\left(f_{J_k} + \mathcal{B}_{J_k}U_{J_k} - i\frac{dU_{J_k}}{dt}\right) \\ + \frac{h_{J_k+\frac{\nu_k}{2}}}{6}\left(f_{J_k+\nu_k} + \mathcal{B}_{J_k+\nu_k}U_{J_k+\nu_k} - i\frac{dU_{J_k+\nu_k}}{dt}\right), \qquad k \in \{l, r\}. \end{aligned} \tag{24}$$

The approximation error of (24) 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 (24):

$$\begin{aligned} & d\frac{U_{J_k} - U_{J_k+\nu_k}}{h_{J_k+\frac{\nu_k}{2}}} + \sqrt{d}\,(ir_k U_{J_k} - \mu_k) = \frac{h_{J_k+\frac{\nu_k}{2}}}{2}\left(f_{J_k} + \mathcal{B}_{J_k}U_{J_k} - i\frac{dU_{J_k}}{dt}\right), \\ & k \in \{l, r\}. \end{aligned} \tag{25}$$

The Robin type BCs are also important when considering nonlocal transparent BCs [9, 17] for the linear homogeneous ($f \equiv 0$) Schrödinger problem (1) in the laterally truncated domain Ω^T. In Ref. [12], 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 [10]:

$$\begin{aligned} & -\nu_s\sqrt{d}\,\frac{\partial u(-\nu_s X, t)}{\partial x} + i\left(\beta + \sum_{k=1}^{m} a_k\right)u(-\nu_s X, t) = i\sum_{k=1}^{m} a_k d_k \varphi_{k,s}(t), \\ & \frac{d\varphi_{k,s}}{dt} = iu(-\nu_s X, t) - i(\bar{\mathcal{B}}_s + d_k)\varphi_{k,s}(t), \quad t > 0, \\ & \varphi_{k,s}(0) = 0, \qquad k = 1, \ldots, m, \quad m \geq 1, \quad s \in \{l, r\}. \end{aligned} \tag{26}$$

Having a similar form as Robin BCs (23), these conditions can be approximated by the semi-discrete compact high-order scheme

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

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 [18]. The influence of compact approximations is taken into account through the generalized formulation of eigenvalue problem by using the nondiagonal eigenvalue operator.

$$\begin{aligned}
&-\partial_x^2 V_j = \lambda A_h V_j, \quad j = J_l+1,\dots,J_r-1, \quad J_r = J_l + J,\\
&\frac{V_{J_s} - V_{J_s+\nu_s}}{h} + i r_s V_{J_s} = \frac{h\lambda}{6}\Big(2V_{J_s} + V_{J_s+\nu_s}\Big),\ s\in\{l,r\},\ \nu_l = 1,\ \nu_r = -1.
\end{aligned} \tag{27}$$

Here we are interested to separate the influence of the compact approximation of boundary conditions. Thus we take $A_h = I$, as in the case of standard second-order scheme (6). 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

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

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 (15) we have solved a test problem from [9, 10]. Consider linear Schrödinger equation (1) with $\mathcal{B} \equiv 0$, $f \equiv 0$, $d = 0.5$, the exact solution is given as

$$u_1(x,t) = u_1(x,t) := \sqrt{\frac{i}{i+2t}}\exp\big[(-ix^2 + 4x - 8t)/(i+2t)\big]. \tag{28}$$

We simulate the movement of a soliton 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 (28):

$$u_0(x) = u_1(x,0), \qquad u(\pm X, t) = u_1(\pm X, t). \tag{29}$$

The computational grid (17) 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 ρ

$$\begin{aligned} &\epsilon_\alpha(|\omega_h^T|, N) := \max_{t^n \in \omega_\tau^T} \varepsilon_\alpha(|\omega_h^T|, t^n), \quad \varepsilon_\alpha(|\omega_h^T|, t^n) = \max_{x_j \in \omega_h^T} |u(x_j, t^n) - U_j^n|, \\ &\rho_\alpha(J) := \varepsilon_\alpha(J/2, N/4) \big/ \varepsilon_\alpha(J, N) \end{aligned} \tag{30}$$

for solution of high-order compact finite difference scheme (15) 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 ρ_α for solution of high-order compact finite difference scheme (15) with initial and boundary conditions (29).

J	N	$\epsilon_{0.1}$	$\rho_{0.1}$	$\epsilon_{0.25}$	$\rho_{0.25}$
200	100	1.29e-2	—	1.03e-2	—
400	400	8.09e-4	15.9	6.64e-4	15.5
800	1600	4.62e-5	17.5	3.85e-5	17.2
1600	6400	3.11e-6	14.8	2.50e-6	15.4

4.2 Example 2

In this case we have solved numerically the test problem of Example 1 with the BCs (23), where

$$\mu_l = -\sqrt{d}\,\frac{\partial u_1(-X,t)}{\partial x}, \qquad \mu_r = \sqrt{d}\,\frac{\partial u_1(X,t)}{\partial x}, \qquad r_l = r_r = 0. \tag{31}$$

We note, that these boundary conditions are of Neumann type and are exact once the initial function u_0 is given by (29).

In this example we have tested the accuracy of the new compact high-order finite difference approximation of BCs (24), and compared it with the standard second-order accuracy scheme (25). The linear Schrödinger equation is approximated by the high-order finite difference scheme (10) 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. (30). Crank-Nicolson time discretization of (24) and (25) are used to approximate boundary conditions of the problem.

Results of computational experiments confirm the conclusion that local approximation errors of BCs should dominate the global error and the observed convergence orders coincide with the approximation orders of finite difference schemes (24) and (25).

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 (10), when BCs (23), (31) are approximated by the third order accuracy scheme (24) and the standard second order accuracy scheme (25).

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

References

[1] P. Chazan, J.M. Mayor, S. Morgott, M. Mikulla, R. Kiefer, S. Müller, M. Walther, J. Braunstein and G. Weimann. High-power near difraction-limited tapered amplifiers at 1064 nm for optical intersatelite communications. *IEEE Phot. Techn. Lett.*, **10**(11):1542–1544, 1998.

[2] M. Maiwald, S. Schwertfeger, R. Güther, B. Sumpf, K.Paschke, C. Dzionk, G. Erbert and G. Tränkle. 600 mw optical output power at 488 nm by use of a high-power hybrid laser diode system and a periodically poled mgo:linbo$_3$. *Optics Letters*, **31**(6):802–804, 2006.

[3] W. Schultz and R. Poprawe. Manufacturing with nover high-power diode lasers. *IEEE J. Select. Topics Quantum Electron.*, **6**(4):696–705, 2000.

[4] M. Pessa, J. Näppi, P. Savolainen, M. Toivonen, R. Murison, A. Ovchinnikov and H. Asonen. State-of-the-art aluminum-free 980-nm laser diodes. *J. Ligthw. Technol.*, **14**(10):2356–2361, 1996.

[5] S. Balsamo, F. Sartori and I. Montrosset. Dynamic beam propagation method for flared semiconductor power amplifiers. *IEEE Journal of Selected Topics in Quantum Electronics*, **2**:378–384, 1996.

[6] M. Spreemann, M. Lichtner, M. Radziunas, U. Bandelow and H. Wenzel. Measurement and simulation of distributed-feedback tapered master-oscillators power-amplifiers. *IEEE J. of Quantum Electron.*, **45**(6):609–616, 2009.

[7] R. Čiegis, M. Radziunas and M. Lichtner. Numerical algorithms for simulation of multisection lasers by using traveling wave model. *Math. Model. Anal.*, **13**(3):327–348, 2008.

[8] I. Laukaitytė, R. Čiegis, M. Lichtner and M. Radziunas. Parallel numerical algorithm for the traveling wave model. In R. Ciegis, D. Henty, B. Kagström and J. Žilinskas(Eds.), *Parallel Linear Algebra and Optimization: Advances and Applications. Springer Optimization and Its Applications. ISBN: 978-0-387-09706-0*, volume 27, pp. 237–250, New-York, 2009. Springer.

[9] X. Antoine, A. Arnold, Ch. Besse amd M. Ehrhardt and A. Schädle. A review of transparent and artificial boundary conditions techniques for linear and nonlinear Schrödinger equations. *Commun. in Comput. Physics*, **4**(4):729–796, 2008.

[10] R. Čiegis and M. Radziunas. Effective numerical integration of traveling wave model for edge-emitting broad-area semiconductor lasers and amplifiers. *Math. Model. Anal.*, **15**(4):409–430, 2010.

[11] M. Ehrhardt and A. Arnold, Discrete transparent boundary conditions for the Schrödinger equation. *Riv. Mat. Univ. Parma*, **6**:57–108, 2001.

[12] J. Szeftel. Design of absorbing boundary conditions for Schrödinger equation in R^d. *SIAM J. Numer. Anal.*, **42**(4):1527–1551, 2004.

[13] C.A. Moyer, Numerov extension of transparent boundary conditions for the Schrödinger equation in one dimension. *Amer. J. Phys.*, **72**:351–358, 2004.

[14] B. Ducomet, A. Zlotnik and I. Zlotnik, On a family of finite-difference schemes with approximate transparent boundary conditions for a generalized 1d Schrödinger equation. *Kinetic and related models*, **2**(1):151–179, 2009.

[15] A.A. Samarskii. The theory of difference schemes. *Marcel Dekker, Inc., New York-Basel*, 2001.

[16] M. Schulte and A. Arnold. Discrete transparent boundary conditions for the Schrödinger equation – a compact higher order scheme. *Kinetic and Related Models*, **1**, 101–125, 2008.

[17] R. Čiegis, I. Laukaitytė and M. Radziunas. Numerical algorithms for Schrödinger equations with absorbing boundary conditions. *Nonlinear Functional Analysis and Optimization*, **30**(9-10):903–923, 2009.

[18] W. Hundsdorfer and J.G. Verwer. *Numerical Solution of Time-Dependent Advection-Difusion-Reaction Equations*, volume 33 of *Springer Series in Computational Mathematics*. Springer, Berlin, Heidelberg, New York, Tokyo, 2003.