

# On the Accuracy of Some Absorbing Boundary Conditions for the Schrödinger Equation

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**Abstract.** A detailed analysis of absorbing boundary conditions for the linear Schrödinger equation is presented in this paper. It is focused on absorbing boundary conditions that are obtained by using rational functions to approximate the exact transparent boundary conditions. Different strategies are investigated for the optimal selection of the coefficients of these rational functions, including the Padé approximation, the  $L_2$  norm approximations of the Fourier symbol,  $L_2$  minimization of a reflection coefficient, and two error minimization techniques for the chosen benchmark problems with known exact solutions. The results of computational experiments are given and a detailed comparison of the efficiency of these techniques is presented.

**Keywords:** finite difference method, nonlocal boundary conditions, approximation, rational functions, Schrödinger equation, absorbing boundary conditions.

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## 1 Introduction

In this paper, as a basic mathematical model, we consider the initial-value problem for the linear one-dimensional Schrödinger equation

$$\begin{aligned}i \frac{\partial \tilde{u}}{\partial t} + \frac{\partial^2 \tilde{u}}{\partial x^2} &= 0, \quad -\infty < x < \infty, \quad t > 0, \\ \tilde{u}(x, 0) &= u_0(x).\end{aligned}\tag{1.1}$$

The Schrödinger equation is widely used for modelling quantum mechanics and non-linear optics problems. Usually, the equation is supplemented with an initial condition and only asymptotical behaviour of the solution at infinite boundaries is defined (the last requirement is equivalent to the boundedness of the solution in some specified norms). In order to solve this problem, a discretization must be performed and an infinite space domain must be reduced to a finite domain. Thus it is necessary to formulate correct artificial boundary conditions at the new boundaries of the selected domain.

In most cases, we are interested to find a solution of problem (1.1) only on a finite domain so a proper restriction of the infinite domain is well suited for most real world modelling applications. Thus it is a common practice to approximate the initial value problem (1.1) by some initial-boundary value problem.

$$\begin{aligned}
 i\frac{\partial \tilde{u}}{\partial t} + \frac{\partial^2 \tilde{u}}{\partial x^2} &= 0, \quad a < x < b, \quad t > 0, \\
 \tilde{u}(x, 0) &= u_0(x), \quad L_a \tilde{u} = g_a, \quad L_b \tilde{u} = g_b.
 \end{aligned}$$

However, these new boundary conditions must be carefully constructed, because they can perturb essentially the solution of the initial value problem. It is well known that if simple standard boundary conditions are formulated on the boundaries of the restricted domain (e.g. the homogeneous Dirichlet boundary conditions), the solution after reaching the boundary will be reflected back into the domain and will pollute the results of subsequent simulations. A simple and straightforward way to avoid such perturbations is to enlarge the domain of simulations and thus to delay the reflection of the wave from the artificial boundaries. However, for a long time modelling, this strategy is very inefficient – it forces calculations to be performed on a domain that is much bigger than the domain of interest.

Special artificial and transparent boundary conditions were developed and investigated in many papers, see [1, 2, 4, 5, 6, 9]. A good review on construction of transparent boundary conditions not only for differential problems but also for discrete finite difference schemes, as well as stability analysis and computational experiments are given in [2, 9]. The exact transparent boundary conditions are non-local in time and the full history of the solution at the boundary should be preserved during computations. We also mention papers where exact transparent boundary conditions are constructed and the stability of initial-boundary value problem is analysed for the differential Schrödinger equation [1, 2, 4]. A similar analysis for discrete unconditionally stable schemes for the one-dimensional Schrödinger equation is done in [2, 3]. The transparent boundary conditions for high-order finite difference schemes are constructed in [10, 16].

Non-local boundary conditions increase the computational costs and memory requirements of numerical algorithms and they are inefficient for long time modelling problems. Thus it is a challenge to construct appropriate local boundary conditions and to avoid the negative long memory effects included into the definition of the exact non-local transparent boundary conditions. A few approaches are proposed to construct such boundary conditions. Various

absorbing boundary conditions (ABCs) are constructed for this purpose (see, e.g. [9] and references therein). These boundary conditions absorb the energy of waves as they reach the boundary area and attempt to minimize the amount of energy reflected by the artificial boundaries.

Different techniques, such as polynomials, splines or finite elements, can be used as a basis for approximations. In this paper, we are interested in methods based on approximations by rational functions [5,9]. Our aim is to investigate the accuracy of a family of absorbing boundary conditions. Different objective functions are used to define the optimal values of coefficients and the convergence rate of the selected family of rational functions is tested. We start from the approximation of the Fourier symbol, which is defined by considering the Fourier transform of the exact transparent boundary conditions. The classical Padé method is considered as the first approach, where coefficients of the approximation can be computed in the explicit form. In the second method coefficients of the rational function are defined by solving the minimization problem and the Fourier symbol is approximated in the  $L_2$  norm.

The third method is based on minimization of the reflection coefficient [17], since the main aim of artificial boundary conditions is to avoid a reflection from the new boundaries. We note that the Nelder-Mead method [11] was used to find local minima in [17].

In the last part of computational experiments an adaptive strategy is applied. Two representative benchmarks are selected where the exact solutions of these problems are known. The coefficients of the rational functions are determined by minimizing the error of the approximate solution in the  $L_2$  and  $L_\infty$  norms. This part of computations enabled us to test the robustness of global optimization and estimate the possibilities/limitations of the rational functions technique when the order of polynomials is small.

The formulated minimization problems are black box problems of global optimization [18]. The search space is very large and therefore deterministic covering methods for global optimization are not applicable. We use multistart strategy for estimating the globally optimal solution. Derivative-free local optimization is applied since analytical expressions for gradients are not available and the objective functions are too computationally expensive for numerical estimation of the gradient. Starting points are generated randomly and local optimization by Nelder-Mead downhill simplex method [11] and Powell's method [14] is applied. This strategy is also favorable for parallelization since different runs of local optimization are independent and may be performed in parallel.

The rest of this paper is organized as follows. In Section 2, the initial value problem (1.1) is approximated by the initial-boundary value problem. Some general notations of finite difference schemes are introduced. A short review on exact transparent boundary conditions and discretizations is presented. In Section 3, approximate boundary conditions are constructed by using rational functions. Four different techniques are applied to define coefficients of the approximations. Three of them solve global minimization problems with different objective functions. Results of numerical experiments and theoretical analysis are given in Section 4. Final conclusions are presented in Section 5.

## 2 Transparent boundary conditions

To solve problem (1.1) we approximate it by an initial-boundary value problem formulated in a finite space domain:

$$\begin{cases} i \frac{\partial u}{\partial t} + \frac{\partial^2 u}{\partial x^2} = 0, & x \in (a, b), \quad t \in (0, T], \\ u(x, 0) = u_0(x), & x \in [a, b], \\ L_l u(a) = 0, \quad L_r u(b) = 0, & t \in (0, T], \end{cases} \tag{2.1}$$

where operators  $L_l, L_r$  define artificial boundary conditions. Let us assume that we are interested to find a solution only in the domain  $[A, B]$ . Then the operators  $L_l, L_r$  and the ends of the finite domain  $a, b$  must be such that

$$\int_0^T \int_A^B |\tilde{u} - u|^2 dx dt \leq \varepsilon, \quad a \leq A < B \leq b,$$

where  $\varepsilon$  is a selected accuracy of the approximation. The extended domains  $[a, A), (B, b]$  can be used to damp possible reflections and oscillations of the solution from the artificial boundaries. But in this paper, for simplicity we restrict to the case  $A = a, B = b$ .

### 2.1 Finite difference scheme

In this subsection we approximate equation (2.1) by the Crank-Nicolson method. We consider the domain  $[a, b] \times [0, T]$  and introduce the discretization  $\omega_h \times \omega_\tau$ , where  $\omega_h$  and  $\omega_\tau$  are discrete uniform grids,  $h$  and  $\tau$  are discrete steps:

$$\begin{aligned} \omega_h &= \{x_j : x_0 = a, x_J = b, x_k = x_{k-1} + h, k = 1, \dots, J\}, \\ \omega_\tau &= \{t^n : t^n = n\tau, n = 0, \dots, N, N\tau = T\}. \end{aligned}$$

We consider numerical approximations  $U_j^n$  of the exact solution  $u_j^n = u(x_j, t^n)$  at the grid points  $(x_j, t^n) \in \omega_h \times \omega_\tau$ . For functions defined on the grid we introduce the forward and backward difference quotients with respect to  $x$ :

$$\partial_x U_j^n = (U_{j+1}^n - U_j^n)/h, \quad \partial_{\bar{x}} U_j^n = (U_j^n - U_{j-1}^n)/h$$

and similarly the backward difference quotient and the averaging operator with respect to  $t$ :

$$\partial_{\bar{t}} U_j^n = (U_j^n - U_j^{n-1})/\tau, \quad U_j^{n-1+\theta} = \theta U_j^n + (1 - \theta)U_j^{n-1}.$$

We approximate the differential equation (2.1) by the Crank-Nicolson finite difference scheme [16]

$$i \partial_{\bar{t}} U_j^n + \partial_x \partial_{\bar{x}} U_j^{n-0.5} = 0, \quad x_j \in \omega_h, \quad n > 0. \tag{2.2}$$

Appropriate boundary conditions will be specified in the following sections.

### 2.2 Exact transparent boundary conditions

Following [1], for differential equation (2.1) we can write the exact transparent boundary conditions. To do this we factorize the Schrödinger equation (2.1)

$$\left(u_x - \sqrt{(-i)\partial_t}u\right)\left(u_x + \sqrt{(-i)\partial_t}u\right) = 0$$

and get the following boundary conditions

$$\partial_n u + e^{-i\frac{\pi}{4}} D_t^{1/2} u = 0, \quad x = a, b,$$

where  $\partial_n$  is the normal derivative and

$$D_t^{1/2} u(x, t) = \frac{1}{\sqrt{\pi}} \frac{\partial}{\partial t} \int_0^t \frac{u(x, s)}{\sqrt{t-s}} ds$$

is a nonlocal operator. There are many quadrature algorithms to approximate the integral in this boundary condition.

It is important to note, that a similar factorization can be done also for the discrete finite difference scheme (2.2) (see [1] for details), or for the high-order accuracy Numerov type finite difference scheme (see, e.g. [16] for details). Then specific discrete approximation algorithms are obtained and such finite difference schemes have the same stability properties as the original schemes formulated in the infinite domain.

A very simple and convenient approximation algorithm can be obtained if a semi-discrete finite difference scheme is considered, when the Crank-Nicolson approximation is applied only in time. Then after factorization, we get the following transparent boundary conditions [1]:

$$\partial_n U^{n+1} = -e^{i\pi/4} \sqrt{\frac{2}{\tau}} \sum_{k=0}^{n+1} \beta_k U^{n+1-k},$$

where  $\beta_k = (-1)^k \alpha_k$ ,  $\alpha_0 = 1$ ,  $\alpha_{2k} = \prod_{j=1}^k (2j-1)/2j = \frac{2k-1}{2k} \alpha_{2k-2}$ ,  $\alpha_{2k+1} = \alpha_{2k}$ ,  $k \geq 0$ :

$$(\alpha_0, \alpha_1, \alpha_2, \alpha_3, \dots) = \left(1, 1, \frac{1}{2}, \frac{1}{2}, \frac{3}{8}, \frac{3}{8}, \dots\right).$$

All these boundary conditions are non-local and for the implementation of them we must store the full history of the solution at the boundary points. Since the coefficients of discrete transparent boundary conditions (see, e.g.  $\beta_k$ ) decay very slowly it is impossible to reduce the complexity of the algorithm by summing only a small number of terms.

### 3 Approximation by rational functions

A very interesting approach to construct local artificial boundary conditions is based on the approximation of the transparent boundary condition

$$\partial_n u + e^{-i\frac{\pi}{4}} D_t^{1/2} u = 0$$

by rational functions. First, the Fourier transform is applied to get a spectral representation:

$$\partial_n \hat{u} + e^{-i\frac{\pi}{4}} \sqrt[4]{i\omega} \hat{u} = 0,$$

where  $\hat{u}(x, \omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} u(x, t) e^{-i\omega t} dt$ . Then the Fourier symbol  $\sqrt[4]{i\omega}$  is approximated by rational functions (see [17]):

$$\sqrt[4]{i\omega} \approx \frac{P_m(i\omega)}{Q_m(i\omega)} = a_0 + \sum_{k=1}^m \frac{a_k i\omega}{i\omega + d_k},$$

where the stability of finite difference schemes leads to the restrictions on coefficients  $a_k > 0, d_k > 0, k = 0, \dots, m$ .

The important advantage of this algorithm is that there exists an efficient implementation of the inverse transform proposed by Lindmann in [8], which leads to local boundary conditions. New functions

$$\hat{\varphi}_k(x, \omega) = \frac{1}{i\omega + d_k} \hat{u}(x, \omega)$$

are introduced for  $x = a, b$  and linear equations are obtained after simple computations

$$\hat{u}(x, \omega) = i\omega \hat{\varphi}_k(x, \omega) + d_k \hat{\varphi}_k(x, \omega), \quad k = 1, \dots, m.$$

Applying the inverse Fourier transform we get the initial value ODEs for  $\varphi_k(x, t)$  [1, 8, 17]:

$$\frac{d\varphi_k(x, t)}{dt} + d_k \varphi_k(x, t) = u(x, t), \quad \varphi_k(x, 0) = 0, \quad x = a, b, \quad k = 1, \dots, m.$$

Then the approximate boundary conditions can be written as

$$\partial_n u = -e^{-i\frac{\pi}{4}} \left( \left( \sum_{k=0}^m a_k \right) u - \sum_{k=1}^m a_k d_k \varphi_k \right), \quad x = a, b. \tag{3.1}$$

Below we formulate four algorithms to compute the coefficients  $a_k, d_k$ . Let us denote the set of coefficients  $S_m(a, d) = (a_0, a_1, \dots, a_m, d_1, \dots, d_m)$ , satisfying the stability requirements  $a_j \geq 0, d_j \geq 0$ .

### 3.1 Padé coefficients

First, we apply a well known algorithm to compute the Padé approximation [12] (Padé approximation is one of the approximations by rational functions). The coefficients are defined by [17]

$$a_0^m = 0, \quad a_k^m = \frac{1}{m \cos^2 \left( \frac{(2k+1)\pi}{4m} \right)}, \quad d_k = \tan^2 \left( \frac{(2k+1)\pi}{4m} \right). \tag{3.2}$$

Since the Padé approximation is based on a local information of the function it is approximating, the convergence can be slow and a sufficiently large  $m$  should be used. As a consequence, the memory requirements still can be quite large.

### 3.2 Approximation of the Fourier symbol in the $L_2$ norm

In this algorithm, we directly minimize the approximation error of the Fourier symbol (FS) in the  $L_2$  norm [8, 17]

$$R_F = \min_{S_m(a,d)} \frac{1}{\bar{\omega}} \int_0^{\bar{\omega}} \left| \sqrt{i\omega} - a_0 - \sum_{k=1}^m \frac{a_k i\omega}{i\omega + d_k} \right|^2 d\omega. \tag{3.3}$$

We consider only a part of the integral for positive  $\omega$ , since for negative values of  $\omega$  the values of square root and rational functions are equal to conjugate values for positive  $\omega$ . The selection of  $\bar{\omega}$  requires a special analysis. In all computations we use  $\bar{\omega} = 100$  without any proof of the optimality of such a choice.

### 3.3 Approximation of a reflection coefficient

An interesting approach is proposed in [17]. There a reflection coefficient

$$RC(\omega) = \frac{-\sqrt{\omega} - ia_0 - i \sum_{k=1}^m \frac{a_k(-\omega)}{-\omega + d_k}}{\sqrt{\omega} - ia_0 - i \sum_{k=1}^m \frac{a_k(-\omega)}{-\omega + d_k}},$$

$$\omega \in \mathbb{R}, \quad a_i > 0, \quad d_j > 0, \quad i = 0, 1, \dots, m, \quad j = 1, 2, \dots, m \tag{3.4}$$

is minimized. The coefficients of the optimal rational function are obtained by solving the following minimization problem

$$R = \min_{S_m(a,d)} \left( \int_{\delta t/2\pi}^{T/2\pi} \left| \frac{\sqrt{r} - a_0 r - \sum_{k=1}^m a_k r / (1 + d_k r)}{\sqrt{r} + a_0 r + \sum_{k=1}^m a_k r / (1 + d_k r)} \right|^2 \frac{dr}{1 + r^2} \right), \tag{3.5}$$

where  $r = -\frac{1}{\omega}$  and  $1/(1 + r^2)$  is the weight function. If  $m = 3$ , we get seven coefficients:  $a_0, a_1, a_2, a_3, d_1, d_2, d_3$ . It is noted in [17], that because  $\delta t$  is small, the reflection coefficient was optimized in the interval  $[0, T/2\pi]$  and the following values of coefficients were obtained:

$$a_0 = 0.7269284, \quad a_1 = 2.142767, \quad a_2 = 5.742223, \quad a_3 = 46.58032,$$

$$d_1 = 6.906263, \quad d_2 = 65.82243, \quad d_3 = 1124.376. \tag{3.6}$$

### 3.4 Minimization of adaptive errors in the $L_2$ and $L_\infty$ norms

In order to test the potential/limitations of the rational functions to approximate the non-local transparent boundary conditions and to investigate the robustness of the selected global optimization algorithms, we have included one more strategy for the selection of the objective functions. Two representative benchmark problems with the known exact solutions are selected and the

coefficients of rational functions are obtained by minimizing the errors of the discrete solutions in the  $L_2$  and  $L_\infty$  norms:

$$E_2 = \min_{S_m(a,d)} \left( \int_0^T \int_a^b |u - \tilde{u}|^2 dx dt \right)^{1/2} = \min_{S_m(a,d)} \|E\|_2,$$

$$E_\infty = \min_{S_m(a,d)} \left( \max_{x \in [A,B], t \in [0,T]} |u - \tilde{u}| \right) = \min_{S_m(a,d)} \|E\|_\infty,$$

where  $E = u - \tilde{u}$ .

We note that this technique adapts the coefficients to the selected benchmark problem. Thus the results for these objective functions may lack the universality, but analysis of them can show the limits of the approach based on rational functions.

In case of  $M$  problems with different solutions  $u_j, j = 1, 2, \dots, M$  we introduce a coupled adaptive strategy

$$E_\infty^c = \min_{S_m(a,d)} \left( \max_{1 \leq j \leq M} \left( \max_{x \in [A_j, B_j], t \in [0, T_j]} |u_j - \tilde{u}_j| \right) \right). \tag{3.7}$$

### 3.5 Global optimization

The formulated minimization problems (minimization of the reflection coefficient and minimization of the errors of approximations) are black box problems of global optimization [7, 13, 18]. Evaluation of values of these objective functions requires numerical integration or even numerical solution of PDE problems. Thus evaluation of the objective functions is computationally expensive. Moreover, properties of the objective functions of these problems are not known, unimodality or convexity of the objective functions may not be assumed and local optimization in the experimental investigation often results in different solutions. Moreover, intervals of possible values for variables (coefficients) are not known and the optimal values of different coefficients may differ by several orders of magnitude. Therefore, the search space may be very large and standard deterministic covering methods for global optimization are not applicable.

However, the initial investigation has shown that local optimization from different starting points sometimes finishes with the same optimal solution found. This substantiates the use of multistart strategy for estimating the globally optimal solution [18]. Random starting points are generated and a local optimization algorithm is applied from a number of random starting points. Since the objective functions are black boxes analytical expressions for gradients are not available. Moreover, since the objective functions are computationally expensive, numerical estimation of the gradient is also too expensive. Therefore, derivative-free methods for local optimization should be used. We applied two algorithms in our experimental investigations: the Nelder-Mead downhill simplex method [11] and the Powell’s method [14] available in Numerical Recipes [15]. Let us mention that the downhill simplex method was also used in [17].



Since the objective functions of the attacked global optimization problems are computationally expensive, experiments take considerable duration. Parallel computing may be applied to make experiments shorter. Multistart strategy for global optimization is favorable for parallelization. Separate runs of local optimization are independent and therefore may be performed in parallel. Another level of parallelization may be the evaluation of values of the objective function at different sample points. One more level is parallelization of numerical integration or numerical solution of the modelling problem.

The coefficients are restricted to non-negative values, but the downhill simplex method is a method for unconstrained optimization and sometimes negative values for the coefficients are computed. Therefore, we have modified the general version of the method to include the non-negativity constraints (3.4). After the reflection of a simplex is completed, the negative values of coefficients are changed to zero. When the expansion of a simplex is computed, if the expansion point is not feasible the simplex is shrank instead of expansion.

## 4 Numerical experiments

In this section we present results of numerical experiments. Our main aim is to estimate the accuracy of artificial boundary conditions by using results of selected computational experiments. The most important question is to investigate if it is possible to find a universal set of coefficients of rational functions which can be used for different cases of the one dimensional Schrödinger problems. As representative test problems we chose two examples presented in papers [17, 19].

**Example 1.** We use the explicit solution of (1.1) (see [17]):

$$u(t, x) = \frac{\exp(-i\pi/4)}{\sqrt{4t-i}} \exp\left(\frac{ix^2 - 6x - 36t}{4t-i}\right).$$

The problem is solved in the domain  $[-5, 5]$  for  $t \in [0, 0.8]$ . It can be noted that the solution has almost compact support in  $(-5, 5)$  at  $t = 0$  and crosses the boundary  $x = -5$  for some  $t < 1$ . In order to avoid the influence of discretization errors we take the uniform grid  $J \times N = 8000 \times 4000$ .

**Example 2.** We use the explicit solution of (1.1) (see [19]):

$$u(t, x) = \frac{1}{\sqrt[3]{1+it/\alpha}} \exp\left(ik(x-x^{(0)}-kt) - \frac{(x-x^{(0)}-2kt)^2}{4(\alpha+it)}\right),$$

where  $k = 100$ ,  $\alpha = 1/120$ ,  $x^{(0)} = 0.8$  presented in [19]. In this case we compute the numerical solutions in the domain  $[0, 1.5]$  for  $t \in [0, 0.04]$  and the uniform grid  $J \times N = 12000 \times 4000$  is used.

In all computations the finite difference scheme (2.2) is used and boundary conditions are approximated by (3.1). It was checked that the error values due to discretization are at least 10 times smaller than the errors due to boundary conditions approximations.

**Comparison of different approaches.** First, we obtain the coefficients of rational functions by using different approaches. The main aim is to compare the accuracy of approximations of the different objective functions. Second, we analyze the influence of the selected universal objective functions to the accuracy of solutions of the initial-boundary value problem (2.1) for two benchmark problems defined in Examples 1 and 2.

To solve the formulated global minimization problems local search from random starting points is used. For problems (3.3), (3.5) we use up to 10000 points. For each parameter the exponential distribution is applied with averages equal to the values defined by (3.6).

In the cases of adaptive strategy, the evaluation of the objective functions requires solution of the 1D non-stationary discrete problem for each sample point. This step is computationally quite costly. So we have restricted to 100 runs of local optimization even in the case of parallel computations.

The integration in (3.3) and (3.5) is done using the Gauss-Lobatto quadrature with adaptive refinement, the accuracy tolerance is equal to  $10^{-12}$ . According to [11], the following parameters are specified for the downhill simplex algorithm: reflection coefficient  $\alpha = 1$ , expansion coefficient  $\gamma = 2$ , contraction coefficient (used for both – single point and full contractions)  $\beta = 0.7$ , the tolerance parameter  $\varepsilon = 10^{-10}$  (for (3.5) we have used  $\varepsilon = 10^{-15}$ ).

In Table 1 we present optimal coefficients of the rational functions obtained applying different objective functions. It follows from the presented results that the coefficients vary a lot from one approach to another. We only note that adaptive techniques in different norms (for the same test problem) give similar coefficients. So it is hard to formulate any constructive conclusion about the distribution of these coefficients.

**Table 1.** Coefficients obtained with different approaches

Approach	$a_0$	$a_1$	$a_2$	$a_3$	$d_1$	$d_2$	$d_3$
Refl. coef. [17](3.5)	0.727	2.14	5.74	46.6	6.91	65.8	1124
Padé [12](3.2)	0	0.357	0.667	4.98	0.0717	1	13.9
FS (3.3)	0.602	1.78	3.53	23.1	4.94	38.0	364
Adapt. ( $E_\infty$ ) Ex. 1	1.01	2.11	3.30	24.5	10.4	51.3	413
Adapt. ( $E_2$ ) Ex. 1	1.07	2.11	3.48	26.9	10.9	53.5	470
Adapt. ( $E_\infty$ ) Ex. 2	9.30	29.3	7.20	229	0.437	1.01	28847
Adapt. ( $E_2$ ) Ex. 2	11.3	25.1	4.64	210	0.434	13.7	25567
Adapt. ( $E_\infty^c$ )	2.91	0	10.6	138	5.26	106	10329

The Padé coefficients presented in Table 1 are calculated by the explicit formulas (3.2). It is well known that the Padé approximation can be not accurate for small  $m$  but the accuracy is improved as  $m$  increases. Thus in order to test the potential of the Padé approximation we take bigger  $m$  to analyze the convergence rate. The results are presented in Table 2.

It follows from Table 2 that the convergence rate for Example 2 is significantly smaller than for Example 1. So the required value of  $m$  may be quite large depending on the problem and this can be computationally expensive. Therefore, alternative techniques to compute coefficients for small  $m$ , e.g.

**Table 2.** Padé test for two benchmark problems

Example 1			Example 2		
$m$	$\ E\ _\infty$	$\ E\ _2$	$m$	$\ E\ _\infty$	$\ E\ _2$
3	0.179	0.174	3	0.882	1.02e-2
9	1.41e-2	1.40e-2	15	0.627	7.17e-3
15	1.46e-3	1.36e-3	90	7.58e-2	8.30e-4

$m = 3$ , are needed.

In Table 1 values of the coefficients for the objective function defined by the reflection coefficient are taken from [17]. Our computations using  $\delta t = 0$ , as was recommended in [17], gave different optimal values of coefficients. So we have investigated in detail the dependence of the optimal coefficients on the parameter  $\delta t$ . The obtained results for Example 1 are presented in Table 3, where the optimal values of  $R$  are given for different parameters  $\delta t \in [0, 0.05]$ .

**Table 3.** Objective function (3.5), coefficients and errors for Example 1 are computed for different values of  $\delta t$

$\delta t$	$a_0$	$a_1$	$a_2$	$a_3$	$d_1$	$d_2$	$d_3$	$\ E\ _\infty$
0	1.1222	5.0569	28.777	450.63	23.606	634.82	55501	0.02680
0.0001	1.0572	4.3927	21.001	241.94	19.496	414.70	20779	0.02175
0.001	0.9498	3.4808	13.074	119.18	14.118	216.49	6255.0	0.01455
0.01	0.7868	2.4402	6.9552	56.046	8.4327	88.517	1611.7	0.00690
0.02	0.7277	2.1419	5.6515	44.817	6.9153	65.204	1065.1	0.00516
0.03	0.6913	1.9755	4.9984	39.405	6.0958	54.207	837.17	0.00435
0.04	0.6648	1.8617	4.5805	36.007	5.5475	47.436	706.46	0.00389
0.05	0.6458	1.7859	4.3173	33.868	5.1828	43.260	629.42	0.00366

We see from these results that for  $\delta t = 0.02$  the values of the coefficients are almost identical to the values given in (3.6). Therefore, in all further calculations we use the coefficients for the reflection coefficient  $R$  obtained with  $\delta t = 0.02$ . It is interesting to note that application of ABCs with such coefficients enabled us to solve the benchmark problems with much better accuracy than if the coefficients obtained with  $\delta t = 0$  are used. More details are provided in the last column of the table. As we see, the actual error becomes smaller as  $\delta t$  increases, however, it cannot be taken as a rule, since it depends on the example, i.e. initial conditions.

Using two selected universal (not depending on specific examples of solutions) approaches (3.5) and (3.3) we minimize the functionals that indirectly represent the errors due to artificial boundary conditions. However, these techniques cannot guarantee that the actual errors of the discrete solutions will be small. In order to estimate the suitability of the functionals (3.5) and (3.3), we use the obtained coefficients to define ABCs and solve two benchmark problems defined in Examples 1 and 2.

The problems (3.5) and (3.3) are global optimization problems. In our experiments we select a fixed number of starting points and use a local opti-

mization algorithm to descent to the minimum. Then the best local minimum point is used as an approximation of the global minimum point. This strategy is based on the assumption that a smaller value of the objective function means also a smaller error of the discrete solution of the Schrödinger problem. In order to analyze this assumption we have selected 7 random local minima for each functional  $R$  and  $R_F$  that were found during optimization. By using these coefficients we have solved Examples 1 and 2 and computed the errors of discrete solutions.

For Example 2 the  $L_2$  norm is scaled  $\|E\|_2^* = \|E\|_2 / \sqrt{T}$ . The results presented in Tables 4 and 5 show that for both examples the errors of discrete solutions monotonically decrease as the values of the functionals become smaller. But errors for Example 2 are quite large, so it is hard to make any conclusion on the convergence in this case.

**Table 4.** Monotonicity analysis of local minima using the reflection coefficient  $R$

$R$	Example 1		Example 2	
	$\ E\ _\infty$	$\ E\ _2$	$\ E\ _\infty$	$\ E\ _2^*$
7.29e-06	3.39e-2	3.35e-2	0.712	4.08e-2
7.14e-06	3.68e-2	3.61e-2	0.685	3.92e-2
2.66e-09	1.01e-2	9.74e-3	0.507	2.89e-2
2.41e-09	9.77e-3	9.42e-3	0.505	2.88e-2
2.25e-09	9.57e-3	9.23e-3	0.505	2.87e-2
2.61e-10	5.71e-3	5.36e-3	0.422	2.40e-2
1.40e-10	5.16e-3	4.89e-3	0.452	2.57e-2

**Table 5.** Monotonicity analysis of local minima using the Fourier symbol  $R_F$

$R_F$	Example 1		Example 2	
	$\ E\ _\infty$	$\ E\ _2$	$\ E\ _\infty$	$\ E\ _2^*$
0.446	5.08e-2	4.62e-2	0.738	4.24e-2
0.161	2.53e-2	2.26e-2	0.746	4.28e-2
8.20e-2	1.46e-2	1.22e-2	0.726	4.16e-2
5.81e-2	1.25e-2	1.08e-2	0.712	4.08e-2
4.27e-2	6.89e-3	6.95e-3	0.702	4.02e-2
3.54e-2	5.87e-3	6.06e-3	0.694	3.98e-2
3.18e-3	2.17e-3	1.56e-3	0.636	3.64e-2

Next, we present the results obtained by using all different techniques to define ABCs. The comparison of the obtained results (the optimization results for the universal functionals  $R$  and  $R_F$  and the solution errors in  $L_\infty$  and  $L_2$  norms) is presented in Table 6.  $R$  and  $R_F$  values for adaptive techniques are presented for Example 2, since it gives the biggest values.

The following main conclusions can be done. First, the heuristic for solving global optimization problems is quite robust. We have no guarantees that the global optimization problem is solved exactly, however, the smallest values for

**Table 6.** Values of all objective functions obtained with different approaches

Approach	$R$	$R_F$	Example 1		Example 2	
			$\ E\ _\infty$	$\ E\ _2$	$\ E\ _\infty$	$\ E\ _2^*$
Refl. coef. (3.5)	1.40e-10	2.15e-2	5.16e-3	4.89e-3	0.452	2.57e-2
FS (3.3)	4.62e-06	3.18e-3	2.18e-3	1.56e-3	0.636	3.64e-2
Adapt. ( $E_\infty$ )	0.106	1689	3.21e-4	2.75e-4	9.43e-3	6.13e-4
Adapt. ( $E_2$ )	0.100	1255	7.19e-4	2.58e-4	1.53e-2	4.09e-4
Padé	2.06e-3	16.2	0.179	0.173	0.882	5.07e-2

all objective functions are obtained when the global optimization algorithm has minimized the specified objective functional. So we have concluded that the obtained computational results are sufficient to formulate our main qualitative conclusions.

Second, considering both universal objective functions (reflection coefficient and Fourier symbol), the accuracy of both ABCs is similar: the errors of discrete solutions are small for Example 1 and much larger for Example 2. So we conclude that the presented two techniques are not universal, there is no guarantee that they are suitable for all initial conditions, at least with small  $m = 3$ . Moreover, from Table 6 we see that both functionals  $R$  and  $R_F$  obtain big values when adaptively strategy is used to find the coefficients for Example 2. Although  $m = 3$  is small so this result was expected – adaptive error minimization cannot guarantee small values of the universal functionals.

Third, the adaptive techniques for Example 2 defined coefficients leading to sufficiently small errors of the discrete solution. So even for this example an accurate approximation by rational functions is still possible. However, this technique adapts the coefficients to the selected example and the obtained optimal coefficients can give considerably bigger errors for other initial conditions.

Next we investigate the suitability of ABCs approximation by rational functions technique in general case. We already saw that it is possible to find accurate coefficients for different benchmarks separately. In Table 7 a cross-check of adaptive techniques for different examples is done, i.e. errors of discrete solutions are estimated for both examples using coefficients that were obtained applying adaptive techniques for both benchmarks.

**Table 7.** Cross-check of the accuracy for different examples

	Approach	Example 1		Example 2	
		$\ E\ _\infty$	$\ E\ _2$	$\ E\ _\infty$	$\ E\ _2^*$
Example 1	Adapt. ( $E_\infty$ )	3.21e-4	2.75e-4	0.600	3.43e-2
	Adapt. ( $E_2$ )	7.19e-4	2.58e-4	0.596	3.40e-2
Example 2	Adapt. ( $E_\infty$ )	0.594	0.560	9.43e-3	6.13e-4
	Adapt. ( $E_2$ )	0.576	0.542	1.53e-2	4.09e-4
coupled	Adapt. ( $E_\infty^c$ )	4.44e-2	3.73e-2	4.44e-2	2.64e-3

It follows from the results presented in Table 7, that the errors of the discrete solutions are small when the specific norm for the same solution is used as an objective function. The type of the norm is not very important in computation of optimal coefficients for the given benchmark problem. At the same time the errors of the discrete solution are big for the remaining test problem. In order to test the approximation accuracy of the family of rational functions with  $m = 3$  we have used one more objective function (3.7), when a coupling of the errors of both benchmark problems is considered. The results presented in Table 7 show that this objective function enables us to find the coefficients giving small enough errors for both benchmarks. Thus the coupled adaptive strategy allows us to find an efficient compromise among two discrete solutions.

In overall, we see that all analysed approaches can be used for calculation of coefficients of rational functions but only with some limitations.

## 5 Conclusions

Two test problems from the literature were used to investigate coefficients of rational functions to approximate the exact transparent boundary conditions. Two universal techniques for obtaining coefficients, approximation of the Fourier symbol and minimization of the reflection coefficient, resulted in small errors of the same order in the case of the first test problem. However, these techniques gave big errors for the second test problem. This means that these universal techniques do not suit all possible problems.

Minimization of the actual error gave a significant increase in the accuracy of calculations. However, this technique is tuned to the selected test problem only. The coupled adaptive technique to obtain the optimal values of coefficients showed that it is possible to find values that suit both test problems with the errors that are small enough for many modelling purposes. However, it is unclear if such values exist in a general case with any initial conditions. It is necessary to perform analysis using other test problems in order to generalize the results.

One more possibility how to increase the accuracy of ABC based on rational functions is to use the Laplace transform and instead of the Fourier symbol to approximate the Laplace symbol, when  $s$  is the general complex time covariable. It would be interesting to investigate this approach in the future.

It would also be useful to investigate advanced black box global optimization algorithms instead of multistart used. Another research direction is multi-level parallelization for obtaining coefficients in adaptive techniques what would make computations faster but also might allow us to find better values.

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