# Weierstraß-Institut
## für Angewandte Analysis und Stochastik

im Forschungsverbund Berlin e.V.

Preprint ISSN 0946 – 8633


# Implementing exact absorbing boundary condition for the linear one-dimensional Schrödinger problem with variable potential by Titchmarsh-Weyl theory


Matthias Ehrhardt [1] , Chunxiong Zheng [2]



submitted: June 22, 2009



[1] Weierstrass Institute for Applied Analysis and Stochastics, Mohrenstrasse 39, 10117 Berlin, Germany
email: ehrhardt@wias-berlin.de

[2] Department of Mathematical Sciences, Tsinghua University, Beijing 100084, P.R. China
email: czheng@math.tsinghua.edu.cn



No. 1426
Berlin 2009

2000 *Mathematics Subject Classification.* 65M99, 81-08.

*Key words and phrases.* absorbing boundary conditions, variable potential, Schrödinger equation, Titchmarsh-Weyl m-function, unbounded domain.

Edited by
Weierstraß-Institut für Angewandte Analysis und Stochastik (WIAS)
Mohrenstraße 39
10117 Berlin
Germany

Fax: + 49 30 2044975
E-Mail: preprint@wias-berlin.de
World Wide Web: http://www.wias-berlin.de/

**Abstract**

A new approach for simulating the solution of the time-dependent Schrödinger equation with a general variable potential will be proposed. The key idea is to approximate the Titchmarsh-Weyl m-function (exact Dirichlet-to-Neumann operator) by a rational function with respect to a suitable spectral parameter. With the proposed method we can overcome the usual high-frequency restriction for absorbing boundary conditions of general variable potential problems. We end up with a fast computational algorithm for absorbing boundary conditions that are accurate for the full frequency band.

## 1. Introduction

We consider in this paper the Schrödinger problem of the following form

$$\begin{aligned} iu_t + \partial_x^2 u &= V(x)u, \quad (x,t) \in \mathbb{R} \times (0,T], \\ u(x,0) &= u_0(x), \quad x \in \mathbb{R}, \end{aligned} \tag{1}$$

where $T$ denotes the finite evolution time, and $u_0$ is an initial wave packet supported in a finite interval $\Omega_{\text{int}} = [x_-, x_+]$ with $x_- < x_+$. It is well–known that under mild conditions the Cauchy problem (1) has a unique solution $u \in C(\mathbb{R}^+, L^2(\mathbb{R}))$, cf. [30], e.g.:

**Theorem 1.** *Let $u_0 \in L^2(\mathbb{R})$ and $V \in L^\infty(\mathbb{R})$. Then the problem (1) has a unique solution $u \in C(\mathbb{R}^+, L^2(\mathbb{R}))$. Moreover, the "energy" is preserved, i.e.*

$$\|u(.,t)\|_{L^2(\mathbb{R})} = \|u_0\|_{L^2(\mathbb{R})}, \forall\, t \geq 0. \tag{2}$$

The Schrödinger problem (1) is defined on an unbounded domain $x \in \mathbb{R}$. In order to numerically simulate its solution, it is a common practice to truncate the computational domain to a bounded one, say $\Omega_{\text{int},T} = \Omega_{\text{int}} \times (0,T]$. *Absorbing boundary conditions* (ABCs) are thus necessary for well–posedness at the two artificially introduced boundaries, $\Sigma_{\pm,T} = \{x_\pm\} \times (0,T]$.

Numerical simulation of the linear Schrödinger equation on unbounded domains with an external potential has been a hot research area for nearly thirty years, cf. the concise review article [7]. An ABC is called *exact* if the solution of truncated domain problem remains the same as that of the original unbounded domain problem. The exact ABC is guaranteed to exist due to the well-posedness of the linear Schrödinger problem (1), but it can only be formulated analytically for some special potentials, such as constant potential [17], linear potential [18], symmetric periodic potential [20], isotropic free particle potential, Morse potential, harmonic potential, and Bargeman potential, cf. e.g. [31]. In the more general case, i.e. for general variable potential problems, one is led to design approximate analytical ABCs for a specific frequency regime in terms of some a-priori criterion. Methods in this category includes the pseudo-differential calculus method [5, 6, 8], the perfectly matched layer (PML) method [39] and the operator splitting method [37]. To the authors' knowledge all of them are in essence based on the *high frequency approximations*. For low frequency problems, the ABCs by these methods would be less accurate.

In this paper, a new approach for designing ABCs for the Schrödinger problem will be proposed. Inspired by the work of Alpert, Greengard and Hagstrom [2] on the fast evaluation of nonreflecting boundary kernels for time-domain wave propagation, we approximate the *Titchmarsh-Weyl m-function* (equivalently exact DtN operator) in the frequency domain by a rational function with respect to an appropriate spectral parameter. In the time domain, the nonreflecting boundary kernels are thus approximated by a sum of exponentials, which makes the approximate ABCs easy to implement. The rationality of the above treatment is due to the analyticity property and asymptotic behavior of the m-function. Since our approximation is made in the whole frequency regime, the proposed ABCs are expected to be more versatile and more accurate, especially in the low-frequency regime and thus overcoming the typical high-frequency restriction. We remark that the Titchmarsh-Weyl m-function is nothing else but the so–called *total symbol* in the microdifferential calculus, which is treated by an asymptotic expansion to get a hierarchy of ABCs, cf. [5, 6, 8]. Also note that Titchmarsh-Weyl theory is already used in practical applications in the fields of quantum mechanics [14, 24] and for option pricing in mathematical finance [28].

This work is organized as follows. In Section 2 we review for the ease of later reference the basic facts of the Titchmarsh-Weyl theory for Schrödinger operators in one dimension. Then, in Section 3 we discuss the Titchmarsh-Weyl m-function (i.e. the exact Dirichlet-to-Neumann operator) and explain the used algorithm to compute the m-function numerically. Hence, at least from a numerical point of view, the exact ABC is explicitly known, see Section 3. However, when simulating the Schrödinger equation (1), the difficulty does not lie in the computation of the m-function in a frequency domain method that is presented Section 4, but in its inverse Laplace transformation which is too much costly. For this reason we introduce in Section 5 a rational approximation of the m-function in the frequency domain to obtain an approximate ABC that can be calculated efficiently using a fast evaluation technique [38] in the time-domain. We discuss practical implementation issues and finally in Section 6 we conclude with numerical results illustrating that our new approach leads to an efficient and reliable algorithm for the time-dependent Schrödinger equation with a general variable potential.

## 2. The Titchmarsh–Weyl theory

We will review here for convenience of the later work the essentials of the *Titchmarsh–Weyl (TW) theory* for Schrödinger operators in one dimension. The interested reader may consult [23, Section 2] for a more detailed presentation.

To start with, we consider the Schrödinger operator $L$ on the real line given by

$$L = -\partial_x^2 + V(x), \qquad x \in \mathbb{R}, \tag{3}$$

with a real–valued, locally integrable potential $V \in L^1_{\mathrm{loc}}(\mathbb{R})$. Let $x_0 \in \mathbb{R}$ denote an arbitrarily chosen point which is called *reference point*. In the sequel, we investigate how solutions depend on this parameter $x_0$.

To do so, we consider $\theta(x; x_0, \lambda)$ and $\phi(x; x_0, \lambda)$ being the *fundamental solutions* to the Schrödinger eigenvalue problem

$$-u_{xx} + V(x)u = \lambda u, \qquad x \in \mathbb{R}, \quad \lambda \in \mathbb{C}, \tag{4}$$

supplied with the following initial conditions at the reference point $x_0$:

$$\theta(x_0; x_0, \lambda) = 1, \qquad \theta_x(x_0; x_0, \lambda) = 0 \tag{5a}$$

$$\phi(x_0; x_0, \lambda) = 0, \qquad \phi_x(x_0; x_0, \lambda) = 1. \tag{5b}$$

It can be shown that under these assumptions, $\theta(x; x_0, \lambda)$ and $\phi(x; x_0, \lambda)$ exist on the whole real axis, and they are entire functions of $\lambda$ and real for $\lambda \in \mathbb{R}$. Now as a basic fact of the TW theory, equation (4) possess at least one solution $\psi_\pm$, called *Weyl's solution* with

$$\psi_\pm(x_0; x_0, \lambda) = 1, \tag{6a}$$

and

$$\psi_\pm(x; x_0, \lambda) \in L^2(\mathbb{R}^{x_0}_\pm) \tag{6b}$$

for any $\lambda \in \mathbb{C}_+$. Here, $\mathbb{R}^{x_0}_\pm$ stands for the interval $[x_0, \pm\infty)$ and $\mathbb{C}_+$ denotes the upper half complex plane, i.e. $\mathbb{C}_+ = \{z \in \mathbb{C} \,|\, \mathrm{Im}\ z > 0\}$. A potential $V(x)$ is said to be in the *limit-point case* at $\pm\infty$ if and only if there exists only one Weyl's solution in the corresponding $L^2$ space. The reader would realize immediately that assuming $V(x)$ in the limit-point case is necessary for the well-posedness of the Schrödinger problem (1) in a more general setting. At positive infinity point, a standard sufficient condition for the limit-point case is from [32]:

**Theorem 2 ([32, Theorem X.8]).** *Let $V(x)$ be a continuous real-valued function on $(x_0, \infty)$ and suppose that there exists a positive differentiable function $M(x)$ so that*

*(i)* $V(x) \geq -M(x)$ *if* $x > x_0$*;*

*(ii)* $\int_{x_1}^{\infty} \big(M(x)\big)^{-1/2}\, dx = \infty$ *for any* $x_1 > x_0$*;*

*(iii)* $M'(x)/\big(M(x)\big)^{3/2}$ *is bounded near* $\infty$*.*

*Then $V(x)$ is in the limit point case at $\infty$.*

An analogous result can be given at negative infinity point.

According to this theorem, a potential $V(x)$ is in the limit-point case provided that $V(x) \geq -kx^2$ for some constant $k$ and for all large enough $x$. This implies that the restriction to the potential for the limit point case is very weak: it only excludes some especially strange potential, which might not be physically relevant at all. Roughly speaking, the limit point case does not admit potentials that tend too fast (faster than quadratically) to $-\infty$ for $x \to \pm\infty$.

Due to the boundary conditions (6a) we can write

$$\psi_{\pm}(x; x_0, \lambda) = \theta(x; x_0, \lambda) + m_{\pm}(x_0, \lambda)\, \phi(x; x_0, \lambda), \tag{7}$$

with some uniquely determined coefficient, the *Titchmarsh-Weyl m-function* $m_{\pm}(x_0, \lambda)$. This function plays a fundamental role in the spectral theory of the Schrödinger operator (3) on the half–line $\mathbb{R}_{\pm}^{x_0}$.

We will now summarize some of the most important properties about the Titchmarsh-Weyl m-function. First,

$$m_{\pm}(x_0, \lambda) \text{ is analytic with respect to } \lambda \text{ on } \mathbb{C}\backslash\mathbb{R} \text{ and } m_{\pm} : \mathbb{C}_+ \to \mathbb{C}_+ \tag{8}$$

and is thus called a *Herglotz function* (or Nevanlinna or Pick function), cf. [23, Lemma 2.3]. It is an easy matter to show that this Herglotz property is directly linked to the positive-type of the DtN-map in the sense of memory equations, cf. [17] for the corresponding constant exterior potential case. Hence, it is an essential ingredient of the stability w.r.t. the $L^2$-norm.

Moreover, we have the *symmetry property*

$$\overline{m_{\pm}(x_0, \lambda)} = m_{\pm}(x_0, \bar{\lambda}) \tag{9}$$

and the local singularities of $m$ are real and and most of them are first order, i.e.

$$\lim_{\epsilon\to 0+} (-i\epsilon)\, m_\pm(x_0, \lambda + i\epsilon) \geq 0, \quad \lambda \in \mathbb{R}, \tag{10}$$

cf. [23, Theorem A.2].

Another important property is given by the Borg–Marchenko theorem [12, 29] stating that the Titchmarsh-Weyl m-function $m_\pm(x_0, \lambda)$ determines uniquely the potential $V(x)$ on $x > x_0$ (or $x < x_0$, respectively). Besides, since $\psi_\pm(x; x_0, \lambda)$ changes with a simple multiplication when changing the reference point $x_0$, one has

$$m_\pm(x, \lambda) = \frac{\partial_x \psi_\pm(x; x_0, \lambda)}{\psi_\pm(x; x_0, \lambda)}. \tag{11}$$

It is thus easy to verify that the $m$-function satisfies the following *Riccati* equation:

$$\partial_x m_\pm(x, \lambda) = -m_\pm^2(x, \lambda) + V(x) - \lambda. \tag{12}$$

## 3. The exact ABC by Titchmarsh-Weyl theory

We apply the Laplace transform

$$\hat{u}(x, s) = \mathcal{L}(u(x, t))(s) = \int_0^{+\infty} u(x, t)\, e^{-st}\, dt, \quad \text{Re } s > 0, \tag{13}$$

to the Schrödinger equation (1) on the right exterior domain $\Omega_+ = \{x \in \mathbb{R} |\, x > x_+\}$ and on the left exterior domain $\Omega_- = \{x \in \mathbb{R} |\, x < x_-\}$. In the frequency domain, the Schrödinger equation is a second order homogeneous ODE

$$-\hat{u}_{xx} + V(x)\hat{u} = \lambda \hat{u}, \quad x \in \Omega_\pm, \tag{14}$$

with $\lambda = is \in \mathbb{C}_+$. The exact absorbing boundary condition of the DtN form in the frequency domain is thus

$$\hat{u}_x(x_\pm, \lambda) = m_\pm(x_\pm, \lambda)\hat{u}(x_\pm, \lambda).$$

Only in some special cases, the m-function has a closed analytical form [13, 22]. For example, in the case of a constant potential $V \equiv V_0$ one gets

$$m_+(x_+, \lambda) = -\sqrt[+]{-\lambda + V_0}. \tag{15}$$

If the potential represents a *harmonic oscillator*, i.e. $V(x) = x^2$ on the interval $[0, \infty)$, one obtains a meromorphic m-function given by the ratio of two gamma functions:

$$m_+(0,\lambda) = -\frac{2\Gamma(\frac{3}{4} - \frac{1}{4}\lambda)}{\Gamma(\frac{1}{4} - \frac{1}{4}\lambda)}. \tag{16}$$

Finally, for the *Bargmann potential*

$$V(x) = -8\beta^2 \frac{\beta - \gamma}{\beta + \gamma} \frac{e^{-2\beta x}}{(1 + \frac{\beta-\gamma}{\beta+\gamma} e^{-2\beta x})^2}, \quad \beta > 0, \quad \gamma \geq 0, \tag{17}$$

one obtains the m-function

$$m_+(0,\lambda) = -\sqrt[+]{-\lambda} - \frac{\gamma^2 - \beta^2}{\sqrt[+]{-\lambda} + \gamma}. \tag{18}$$

However, in the general case numerical methods have to be considered. This issue has been investigated in many papers, e.g. [13, 36, 25, 27]. In this paper we simply compute the $m$-function by evolving the Riccati equation (12) with fourth-order classical Runge-Kutta scheme and setting an initial data $m_\pm(x_{\pm,\lambda}, \lambda) = \mp \sqrt[+]{-\lambda}$ at sufficiently far away point $x_{\pm,\lambda} = \pm 200$. This treatment is reasonable since the potentials in our numerical tests actually decay to zero for $x \to \infty$.

## 4. The frequency–domain method

The solution of the time-dependent Schrödinger equation could then be computed with the following frequency-domain method:

Step 1. Fix $\sigma > 0$. For each $s = \sigma + i\mu$ with $\mu \in \mathbb{R}$, solve the Laplace-transformed Schrödinger equation in the bounded interval $[x_-, x_+]$:

$$\begin{aligned} -\hat{u}_{xx} + V(x)\hat{u} &= is\,\hat{u} - iu_0(x), \quad x \in [x_-, x_+], \\ \hat{u}_x(x_-) &= m_-(x_-, is)\,\hat{u}(x_-), \\ \hat{u}_x(x_+) &= m_-(x_+, is)\,\hat{u}(x_+). \end{aligned}$$

Step 2. Perform the inverse Laplace transformation

$$\begin{aligned} u(x,t) &= \mathcal{L}^{-1}(\hat{u}(s,t))(x) \\ &= \frac{1}{2\pi i} \int_{\sigma - i\infty}^{\sigma + i\infty} e^{st} \hat{u}(s,t)\, ds = \frac{e^{\sigma t}}{2\pi} \int_{-\infty}^{\infty} e^{ift} u(x, \sigma + if)\, df, \end{aligned} \tag{19}$$

to derive the wave function $u(x,t)$ for any $t \in (0,T]$.

In the numerical implementation, some parameters need to be tuned. The function $\hat{u}$ is more smooth for larger *damping factor* $\sigma$, but the evolution time span is then limited since an exponential term gets involved in the inverse Laplace transformation. As a common practice, we set $\sigma = 1/T$ where $T$ is a prescribed evolution time. The integrating domain is unbounded in (19), and has to be truncated. We introduce a cut-off frequency $f_c$ and confine the integration to the interval $[-f_c, f_c]$. Besides, to get rid of high frequency oscillations in the inversely-transformed function we should introduce another filtering function $\chi$, which remains 1 at a large enough frequency band with zero frequency being its center, and vanishes smoothly when close to the ending points of $[-f_c, f_c]$. A good candidate (empirically) is

$$\chi = \exp\left(-(1.2f/f_c)^{20}\right).$$

After these treatments, we then derive an approximate inverse transformation as

$$\frac{e^{\sigma t}}{2\pi}\int_{-\infty}^{\infty} e^{ift}u(x,\sigma+if)\,df \approx \frac{e^{\sigma t}}{2\pi}\int_{-f_c}^{f_c} \chi(f)\,e^{ift}u(x,\sigma+if)\,df. \tag{20}$$

The right hand side is computed with a suitable quadrature scheme.

## 5. The time-domain method

From Section 2 it follows that the exact ABC we seek for is now explicitly known, at least from the numerical point of view. But this is not the whole story for simulating the solution of the time-dependent Schrödinger equation. The difficulty does not lie in the computation of m-function itself, but its inverse Laplace transformation. Of course, a numerical inverse transformation is possible, but this would be too much costly.

Hence, we design in this section an approximate ABC based on the rational approximation of the m-function. The kernel functions are of exponential type with respect to the half-order time derivative operator, thus the fast evaluation technique proposed in [38] (cf. Appendix) is applicable. For a couple of alternative fast evaluation methods we refer the reader to [7] and the references therein. The rational approximation will be realized by solving a least squares problem, an analogous technique as used in [2] for a fast evaluation of the boundary kernel functions of the hyperbolic wave equation.

In the time domain, the truncated Schrödinger problem reads

$$\begin{aligned} iu_t + \partial_x^2 u &= V(x)u, \quad (x,t) \in [x_-, x_+] \times (0,T], \\ u(x,0) &= u_0(x), \quad x \in [x_-, x_+], \\ u_x(x_\pm, t) &= \mathcal{L}^{-1}\big(m_\pm(x_\pm, is)\,\hat{u}(x_\pm, s)\big)(t), \quad t \in (0,T]. \end{aligned} \tag{21}$$

To simplify the notation, we will focus on the right boundary at $x = x_+$. Let us recall the DtN map in the frequency domain reads

$$\hat{u}_x(x_+, s) = m_+(x_+, is)\,\hat{u}(x_+, s).$$

Returning to the time domain we have to consider the convolution

$$u_x(x_+, t) = \mathrm{K}(t) * u(x_+, t), \quad \text{with} \quad \mathrm{K}(t) = \mathcal{L}^{-1}\big(m_+(x_+, is)\big)(t).$$

Here we encounter two major difficulties. First, it is generally *hard to compute* $\mathrm{K}(t)$ and second the involved convolution leads naturally to a *nonlocal-in-time DtN map*.

To get an idea, let us first consider two specific simple examples. In the case of the free Schrödinger ($V \equiv 0$), cf. (15), we have

$$m_+(is) = -\sqrt[+]{-is} \quad \text{and thus} \quad \mathcal{L}^{-1}\big(m_+(is)\big) = -e^{-i\pi/4}\,\partial_t^{\frac{1}{2}}, \tag{22}$$

with the half-order time derivative defined as

$$\partial_t^{\frac{1}{2}} v(t) = \frac{1}{\sqrt{\pi}} \frac{\mathrm{d}}{\mathrm{dt}} \int_0^t v(\tau)(t-\tau)^{-1/2}\, d\tau, \tag{23}$$

which can be efficiently evaluated with some existing methods, e.g. [9, 26, 38]. Secondly we consider the Bargmann potential (17), and in this case the m-function reads

$$m_+(0, is) = -\sqrt[+]{-is} - \frac{\gamma^2 - \beta^2}{\sqrt{-is} + \gamma},$$

thus we have

$$\mathcal{L}^{-1}\big(m_+(0, is)\big) = -e^{-i\pi/4}\,\partial_t^{\frac{1}{2}} - (\gamma^2 - \beta^2)(e^{-i\pi/4}\,\partial_t^{\frac{1}{2}} + \gamma)^{-1}.$$

This operator can then be efficiently evaluated by introducing an unknown function and using the fast methods for $\partial_t^{\frac{1}{2}}$.

Inspired by these two examples it naturally leads us to think about the possibility of approximating the $m$-function with a rational function with respect to a new spectral parameter $k = \sqrt[+]{-is}$ (NOT $s$), i.e.,

$$m_+(x_+, is) \approx \tilde{m}_+(x_+, is) = -\sqrt[+]{-is} + \sum_{n=1}^{d} \frac{\alpha_n}{\sqrt[+]{-is} + \beta_n}. \tag{24}$$

If this is done, we can then replace the exact $m$-function with the approximate alternative $\tilde{m}$, which leads to the approximate kernel function

$$\mathcal{L}^{-1}\big(\tilde{m}_+(x_+, is)\big) = -e^{-i\pi/4}\,\partial_t^{\frac{1}{2}} + \sum_{n=1}^{d} \alpha_n (e^{-i\pi/4}\,\partial_t^{\frac{1}{2}} + \beta_n)^{-1}.$$

The analogous idea for the Bargmann potential (17) can then be used to handle this kernel function.

The answer for the possibility is affirmative considering the *asymptotic expansion* has been given in [16] as

$$m_+(x_+, \lambda) = -\sqrt[+]{-\lambda} + \mathrm{o}(1/\sqrt{r}), \quad r \to \infty, \tag{25}$$

where $\lambda = \mu r$, $r \in \mathbb{R}$ and the convergence is uniform for $\mu$ in any compact subset of $\mathbb{C}_+$, cf. [33, Theorem C.4].

Now putting

$$\mathrm{g}_+(\lambda) = m_+(x_+, \lambda) + \sqrt[+]{-\lambda}, \tag{26}$$

in view of (25) we know that $\mathrm{g}_+(\lambda)$ is analytic in $\mathbb{C}_+$ with respect to $\lambda$ and it tends to zero for $\lambda \to \infty$. We then use the method of Alpert, Greengard and Hagstrom [2] to approximate $\mathrm{g}_+(\lambda)$ with a rational function with respect to $\sqrt[+]{-\lambda}$ (NOT $\lambda$). In terms of (25) we consider the following *nonlinear least square problem*

$$\epsilon = \min_{P,Q} \int_{-\infty+i\sigma}^{\infty+i\sigma} \left| \frac{P(\sqrt[+]{-\lambda})}{Q(\sqrt[+]{-\lambda})} - \mathrm{g}_+(\lambda) \right|^2 |d\sqrt[+]{-\lambda}|, \tag{27}$$

where $P$, $Q$ are polynomials with $\deg(P) + 1 = \deg(Q) = d$, and $d$ is determined by making $\epsilon \le \epsilon_0$, where $\epsilon_0$ is a prescribed tolerance number. This nonlinear problem (27) is then solved with the technique of linearization and orthogonalization [2]. Finally, by expressing $P/Q$ with a sum of poles we arrive at

$$m_+(x_+, \lambda) \approx \tilde{m}_+(x_+, \lambda) = -\sqrt[+]{-\lambda} + \sum_{n=1}^{d} \frac{\alpha_n}{\sqrt[+]{-\lambda} + \beta_n}. \tag{28}$$

Note that the coefficients $\alpha_n$ and $\beta_n$ should appear as conjugate pairs, due to the symmetry property (9). Unfortunately, it is not clear if the rational approximation $\tilde{m}_+(x_+, \lambda)$ in (28) has still the important Herglotz–property of the m-function. Moreover, the Herglotz–property cannot be checked by some conditions on the poles due to the leading square root in (28).

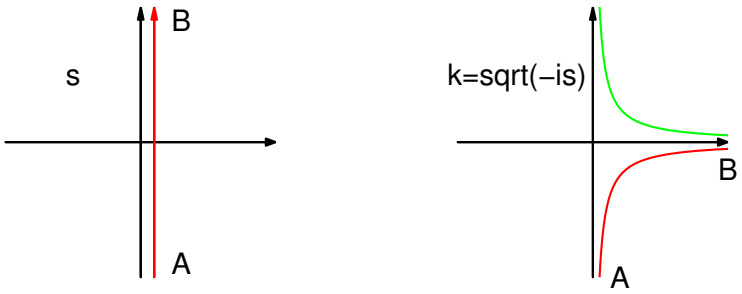


Figure 1: $s$-plane and $k$-plane.

Employing the same idea to the $m$-function $m_-(x_-, \lambda)$ and we get the approximate boundary condition in the frequency domain

$$\hat{u}_x(x_\pm, s) = \left( \mp \sqrt[\pm]{-is} + \sum_{n=1}^{d_\pm} \frac{\alpha_{n,\pm}}{\sqrt[\pm]{-is} + \beta_{n,\pm}} \right) \hat{u}(x_\pm, s). \tag{29}$$

If we introduce new unknowns $\hat{w}_{n,\pm}$ as

$$\hat{w}_{n,\pm} = \frac{\hat{u}(x_\pm, s)}{\sqrt[\pm]{-is} + \beta_{n,\pm}}, \tag{30}$$

then we can rewrite (29) as

$$\hat{u}_x(x_\pm, s) \pm \sqrt[\pm]{-is}\, \hat{u} = \sum_{n=1}^{d_\pm} \alpha_{n,\pm} \hat{w}_{n,\pm}, \tag{31a}$$

$$\sqrt[\pm]{-is}\, \hat{w}_{n,\pm} + \beta_{n,\pm} \hat{w}_{n,\pm} = \hat{u}(x_\pm, s), \qquad n = 1, \ldots, d_\pm. \tag{31b}$$

In the time domain, the approximate boundary condition reads

$$u_x(x_\pm, t) \pm e^{-i\pi/4}\, \partial_t^{\frac{1}{2}} u(x_\pm, t) = \sum_{n=1}^{d_\pm} \alpha_{n,\pm} w_{n,\pm}(t), \tag{32a}$$

$$e^{-i\pi/4}\, \partial_t^{\frac{1}{2}} w_{n,\pm}(t) + \beta_{n,\pm} w_{n,\pm}(t) = u(x_\pm, t), \qquad n = 1, \ldots, d_\pm. \tag{32b}$$

The final approximate truncated time-domain problem is formulated as

$$\begin{aligned} iu_t + \partial_x^2 u &= V(x)u, \quad (x,t) \in \Omega_{\text{int}} \times (0,T], \\ u(x,0) &= u_0(x), \quad x \in \Omega_{\text{int}}, \\ u_x(x_\pm,t) \pm e^{-i\pi/4}\, \partial_t^{\frac{1}{2}} u(x_\pm,t) &= \sum_{n=1}^{d_\pm} \alpha_{n,\pm} w_{n,\pm}(t), \\ e^{-i\pi/4}\, \partial_t^{\frac{1}{2}} w_{n,\pm}(t) + \beta_{n,\pm} w_{n,\pm}(t) &= u(x_\pm,t), \qquad n = 1,\dots,d_\pm. \end{aligned} \tag{33}$$

## 6. Numerical results

In this section we present some numerical results to test the accuracy of the proposed methods. In every example the standard Crank-Nicolson scheme for the time–discretization is employed. The fast evaluation of the half–order time derivative operator (23) is performed with the method of Zheng [38]. The computational domain is chosen to be $\Omega_{\text{int}} = [x_-, x_+] = [-5, 5]$ and the initial data is a Gaussian beam: $u_0(x) = e^{-x^2+4ix}$. We use a $8^{th}$-order FEM method with 1024 elements for the spatial discretization and a uniform time step of size $\Delta t = 10^{-4}$.

### *6.1. The Free Schrödinger Equation*

The exact solution for the free Schrödinger equation ($V(x) \equiv 0$) reads

$$u_{\text{exa}}(x,t) = \sqrt{\frac{i}{-4t+i}} \exp\left(\frac{-ix^2 - 4x + 16t}{-4t+i}\right).$$

We set the cut–off frequency $f_c$ in (20) to be $f_c = 256$ and used a filtering function $\chi(f) = \exp\left(-(1.2f/f_c)^{20}\right)$. The following Table 1 shows the relative $L^2$–errors to the exact solution at certain time points when using 8097 quadrature points with Simpson's rule. By using this simple example we can

| Time points | 0.5 | 0.6 | 0.7 | 0.8 | 0.9 |
|---|---|---|---|---|---|
| Relative $L^2$ errors | 2.26e-7 | 3.46e-8 | 7.60e-9 | 5.60e-9 | 6.25e-9 |

Table 1: Relative $L^2$–error at certain time steps for the free Schrödinger equation.

see that the frequency method with truncating and filtering works pretty well: the magnitude of the relative $L^2$–errors is at most on the order of $10^{-7}$.

*6.2. The Coulomb–like Potential*

In the second example we test the time–domain method using a Coulomb–like potential

$$V(x) = \frac{1}{\sqrt{1+x^2}}. \tag{34}$$

We fixed $\sigma$ for Step 1 to be $\sigma = 1$ and set the tolerance number for nonlinear least square problem (27) as $\epsilon_0 = 10^{-8}$. Here, we obtain 4 poles. In Figure 2 the time evolution is shown in a colored contour plot. One can see how the initial beam spreads out with time increasing. Figure 3 shows how the

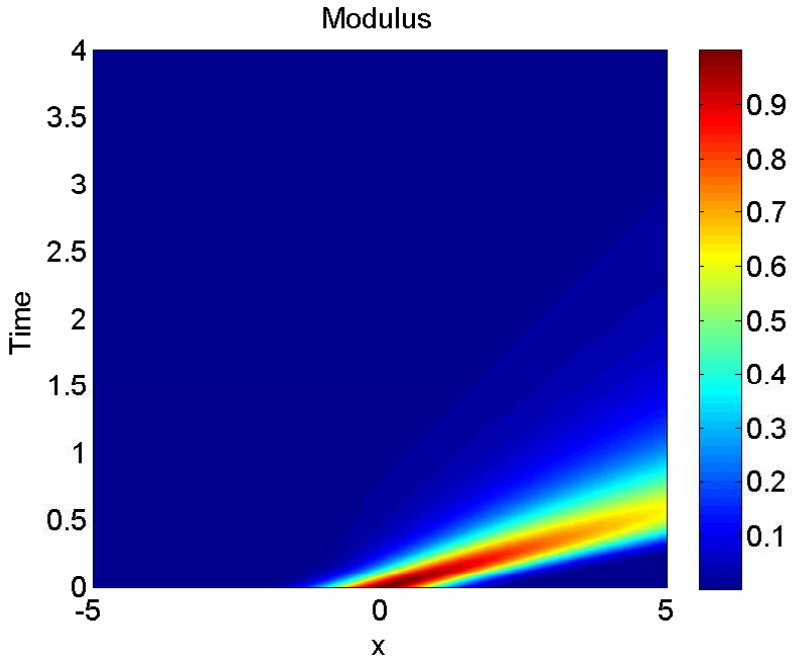


Figure 2: Time evolution of solution with Coulomb potential (34).

relative $L^2$–error evolves in time. In this example with a varying external potential the magnitude of the relative $L^2$–errors stays below $10^{-5}$.

*6.3. The Gaussian Barrier*

Next we change the potential to a Gaussian barrier

$$V(x) = 30e^{-36(x-8)^2} \tag{35}$$

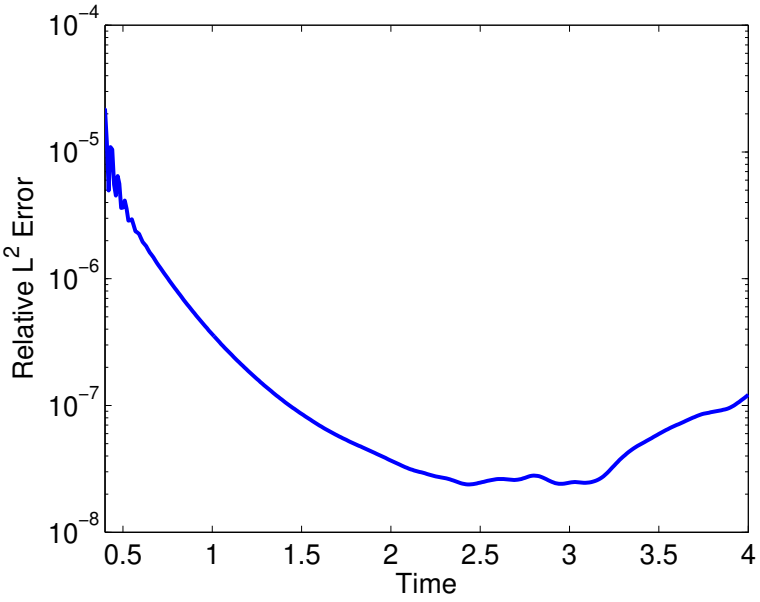


Figure 3: Time evolution of the relative $L^2$–error.

with the height of 30, located in the exterior domain $x > 5$ and centered at $x = 8$. We set $\sigma = 1$ and $\epsilon_0 = 10^{-4}$, and get 21 poles with the nonlinear least squares algorithm. In Figure 4 the temporal evolution of the solution is shown. One clearly observes how the initial beam propagates, spreads out and is (partially) reflected by the Gaussian barrier (35). The time evolution of the corresponding relative $L^2$–error is presented in Figure 5. The relative $L^2$–errors remain below $5 \times 10^{-4}$.

Unfortunately the nonlinear least squares algorithm used in this paper failed to bring a rational approximation within an error tolerance much smaller than $\epsilon_0$. More efficient algorithm is still on demand, and this issue is now under investigation.

## Conclusion and Outlook

In this work we presented a new approach for simulating the solution to the Schrödinger equation with a general space–dependent potential in unbounded domain. Both frequency-domain and time-domain methods were developed.

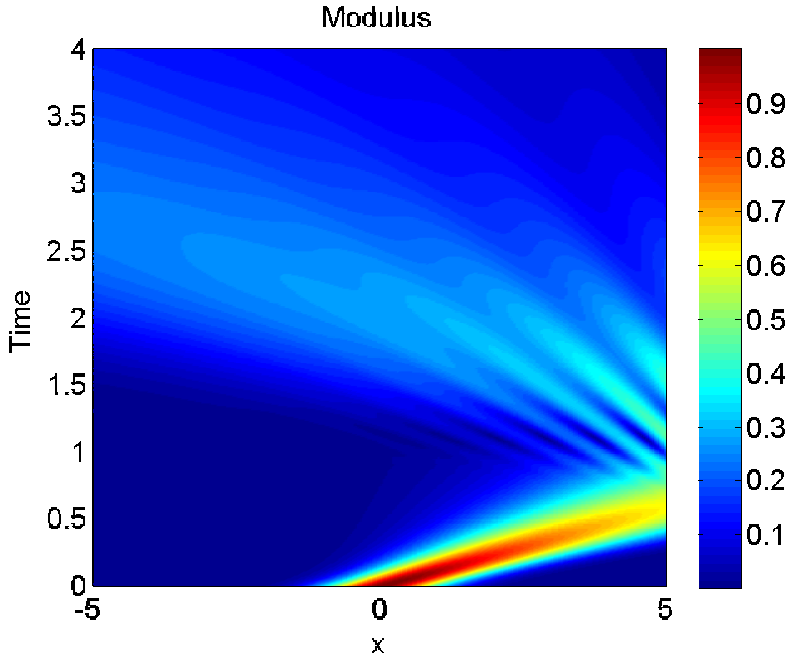


Figure 4: Time evolution of solution with Gaussian barrier (35).

Future work will consist of implementing a more sophisticated algorithm for computing the $m$-function. Instead of solving the Riccati equation (12) we will consider computing the Weyl circles [13, 27] or the recent boundary control approach [10]. Moreover, we will seek for a more stable algorithm for its rational approximation. It will also be clarified how this rational approximation can be made to conserve the essential Herglotz–property of the analytic m-function. This study will enable us for a rigorous stability analysis of this new approach. Finally, as a future goal, we want to extend our approach to the multi–dimensional Schrödinger problem, hereby following the idea of Amrein and Pearson [3].

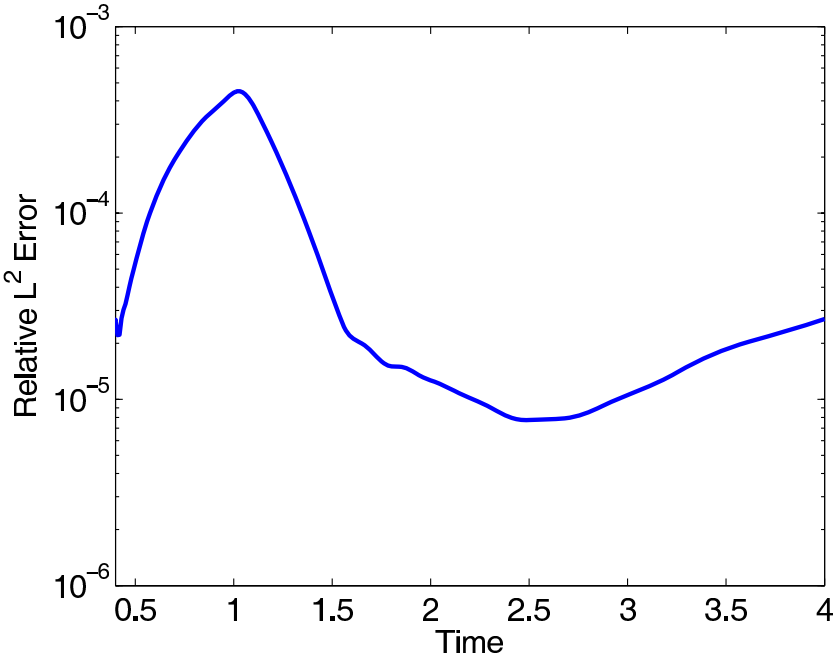


Figure 5: Time evolution of the relative $L^2$–error.

## Appendix: Fast Evaluation Method

Here we present a short description of the method in [38] for evaluating the half–order time derivative $\partial_t^{\frac{1}{2}}$. For any smooth function $v = v(t)$ with $v(0) = v'(0) = 0$, it is known that the semi-discrete half-order derivative

$$D_t^{\frac{1}{2}} v(t_n) \stackrel{def}{=} \sqrt{\frac{2}{\Delta t}} \sum_{m=0}^{n} \alpha_m v(t_{n-m}) \tag{36}$$

with

$$\alpha_m = \begin{cases} \beta_k = \dfrac{(2k)!}{2^{2k}(k!)^2} & , \ m = 2k, \\ -\beta_k & , \ m = 2k+1 \end{cases} \tag{37}$$

gives a second-order approximation of $\partial_t^{\frac{1}{2}} v(t_n)$ (see [4, 38]). Suppose there exists a sum of decaying exponentials satisfying

$$\tilde{\beta}_k = \sum_{j=1}^{L} w_j e^{-s_j k}, \ s_j > 0, \ |\beta_k - \tilde{\beta}_k| \leq \epsilon, \ k = 0, 1, \cdots, \left[\frac{N}{2}\right]. \tag{38}$$

Here $N$ denotes the total number of time steps. If $\epsilon$ is small enough, it is reasonable to approximate (36) with

$$\tilde{D}_t^{\frac{1}{2}} v(t_n) \stackrel{def}{=} \sqrt{\frac{2}{\Delta t}}(v(t_n) - v(t_{n-1})) + \sqrt{\frac{2}{\Delta t}} \sum_{m=2}^{n} \tilde{\alpha}_m v(t_{n-m}), \tag{39}$$

where

$$\tilde{\alpha}_m = \begin{cases} \tilde{\beta}_k & , \ m = 2k, \\ -\tilde{\beta}_k & , \ m = 2k+1. \end{cases} \tag{40}$$

Set $v_k = v(t_k)$, $\mathbf{v} = (v_0, v_1, \cdots)$, and define

$$\mathcal{F}_{odd}(w, s; \mathbf{v}, k) \stackrel{def}{=} \sum_{m=1}^{k} w e^{-sm} v_{2k+1-2m}$$

and

$$\mathcal{F}_{even}(w, s; \mathbf{v}, k) \stackrel{def}{=} \sum_{m=1}^{k} w e^{-sm} v_{2k-2m}.$$

Thus $\mathcal{F}_{odd}(w, s; \mathbf{v}, 0) = \mathcal{F}_{even}(w, s; \mathbf{v}, 0) = 0$. In addition, we have the following recursions

$$\begin{aligned} \mathcal{F}_{odd}(w, s; \mathbf{v}, k) &= e^{-s} \left[ w v_{2k-1} + \mathcal{F}_{odd}(w, s; \mathbf{v}, k-1) \right], \\ \mathcal{F}_{even}(w, s; \mathbf{v}, k) &= e^{-s} \left[ w v_{2k-2} + \mathcal{F}_{even}(w, s; \mathbf{v}, k-1) \right]. \end{aligned}$$

The summation (39) is then computed within $O(L)$ operations as

$$\sum_{m=2}^{n} \tilde{\alpha}_m v_{n-m} = \begin{cases} \sum_{j=1}^{L} \mathcal{F}_{even}(w_j, s_j; \mathbf{v}, k) - \sum_{j=1}^{L} \mathcal{F}_{odd}(w_j, s_j; \mathbf{v}, k-1) & , n = 2k, \\ \sum_{j=1}^{L} \mathcal{F}_{odd}(w_j, s_j; \mathbf{v}, k) - \sum_{j=1}^{L} \mathcal{F}_{even}(w_j, s_j; \mathbf{v}, k) & , n = 2k+1. \end{cases}$$

In [38] for $N = 1,000,000$, the authors found a sum of 81 decaying exponentials which approximates $\beta_k$ with an error less than $5.0 \times 10^{-11}$.

## References


[1] T. Aktosun, *Mathematical Studies in Nonlinear Wave Propagation*, Contemporary Mathematics **379**, American Mathematical Society, Providence, RI, 2005.

[2] B. Alpert, L. Greengard and T. Hagstrom, *Rapid evaluation of nonreflecting boundary kernels for time-domain wave propagation*, SIAM J. Numer. Anal. **37** (2000), 1138–1164.

[3] W.O. Amrein and D.B. Pearson, *M operators: a generalisation of Weyl–Titchmarsh theory*, J. Comput. Appl. Math. **171** (2004), 1–26.

[4] X. Antoine and C. Besse, Unconditionally stable discretization schemes of non-reflecting boundary conditions for the one-dimensional Schrödinger equation, J. Comput. Phys. **181** (2003), 157–175.

[5] X. Antoine, C. Besse and V. Mouysset, *Numerical Schemes for the simulation of the two–dimensional Schrödinger equation using non–reflecting boundary conditions*, Math. Comp. **73** (2004), 1779–1799.

[6] X. Antoine, C. Besse and S. Descombes, *Artificial boundary conditions for one-dimensional cubic nonlinear Schrödinger equations*, SIAM J. Numer. Anal. **43** (2006), 2272–2293.

[7] X. Antoine, A. Arnold, C. Besse, M. Ehrhardt and A. Schädle, *A Review of Transparent and Artificial Boundary Conditions Techniques for Linear and Nonlinear Schrödinger Equations*, Commun. Comput. Phys. **4** (2008), 729–796. (open–access article)

[8] X. Antoine, C. Besse and J. Szeftel, *Towards accurate artificial boundary conditions for nonlinear PDEs through examples*, CUBO A Mathematical Journal **11** (2009), 29–48.

[9] A. Arnold, M. Ehrhardt and I. Sofronov, *Discrete transparent boundary conditions for the Schrödinger equation: fast calculation, approximation, and stability*, Comm. Math. Sci. **1** (2003), 501–556.

[10] S. Avdonin, V. Mikhaylov and A. Rybkin, *The boundary control approach to the Titchmarsh-Weyl m-function*, Comm. Math. Phys. **275** (2007), 791–803.

[11] C. Bennewitz and W.N. Everitt, *Some remarks on the Titchmarsh–Weyl m-coefficient.* Proc. Pleijel Conference, Uppsala, Sweden, 1979, pp. 49–108.

[12] G. Borg, *Uniqueness theorems in the spectral theory of* $y''+(\lambda-q(x))y = 0$, Proc. 11th Scandinavian Congress of Mathematicians, Johan Grundt Tanums Forlag, Oslo, 1952, pp. 276–287.

[13] B.M. Brown, V.G. Kirby and J.D. Pryce, *A numerical method for the determination of the Titchmarsh–Weyl m-coefficient*, Proc. R. Soc. Lond. A **435** (1991), 535–549.

[14] Y. Chiba and S. Ohnishi, *Resonance-state calculation applying the Weyl–Titchmarsh theory: Application for the quantum-confined Stark effects on excitons in a* $GaAs$–$Al_xGa_{1-x}As$ *quantum well*, Phys. Rev. B **41** (1990), 6065–6068

[15] E.A. Coddington and N. Levinson, *Theory of Ordinary Differential Equations*, McGraw–Hill, New York, 1955.

[16] A.A. Danielyan and B.M. Levitan, *On the asymptotic behavior of the Weyl-Titchmarsh m-function*, Math. USSR Izvestiya **36** (1991), 487–496.

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

[18] M. Ehrhardt and R.E. Mickens, *Solutions to the discrete Airy equation: Application to parabolic equation calculations*, J. Comput. Appl. Math. **172** (2004), 183–206.

[19] M. Ehrhardt, *Discrete transparent boundary conditions for Schrödinger–type equations for non–compactly supported initial data*, Appl. Numer. Math. **58** (2008), 660–673.

[20] M. Ehrhardt and C. Zheng, *Exact artificial boundary conditions for problems with periodic structures*, J. Comput. Phys. **227** (2008), 6877–6894.

[21] M. Ehrhardt, H. Han and C. Zheng, *Numerical simulation of waves in periodic structures*, Commun. Comput. Phys. **5** (2009), 849–870.

[22] F. Gesztesy and B. Simon, *A new approach to inverse spectral theory, II. General real potentials and the connection to the spectral measure*, Ann. Math. **152** (2000), 593–643.

[23] F. Gesztesy and M. Zinchenko, *On spectral theory for Schrödinger operators with strongly singular potentials*, Math. Nachr. **279** (2006), 1041–1082.

[24] G.N. Gibson, G. Dunne and K.J. Bergquist, *Tunneling Ionization Rates from Arbitrary Potential Wells*, Phys. Rev. Lett. **81** (1998), 2663–2666.

[25] N. Gordon, J.P. Killingbeck and M.R.M. Witwit, *Numerical Determination of the Titchmarsh-Weyl m-coefficient*, Comput. Math. & Math. Phys. **40**, (2000), 108–117.

[26] S. Jiang and L. Greengard, *Fast evaluation of nonreflecting boundary conditions for the Schrödinger equation in one dimension*, Comp. Math. Appl. **47** (2004), 955–966.

[27] V.G. Kirby, *A numerical method for determining the Titchmarsh–Weyl m-coefficient and its application to certain integro-differential inequalities*, Ph.D. Thesis, University of Wales, College of Cardiff, UK, 1990.

[28] Y. Li and J.E Zhang, *Option pricing with Weyl-Titchmarsh theory*, Quant. Finance **4** (2004), 457–464.

[29] V.A. Marchenko, *Certain problems in the theory of second-order differential operators*, Doklady Akad. Nauk SSSR **72** (1950), 457–460. (Russian).

[30] A. Pazy, *Semigroups of Linear Operators and Applications to Partial Differential Equations*, Springer, New York 1983.

[31] A.D. Polyanin, *Handbook of Linear Partial Differential Equations for Engineers and Scientists*, Chapman & Hall/CRC, 2002.

[32] M. Reed and B. Simon, *Methods of modern mathematical physics II: Fourier analysis, self-adjointness*, Academic Press, San Diego 1975.

[33] R. Sims, *Reflectionless Sturm–Liouville equations*, J. Comput. Appl. Math. **208** (2007), 207–225.

[34] E.C. Titchmarsh, *Eigenfunction Expansions Associated with Second-Order Differential Equations*, Oxford University Press, London, 1946, Volumes 1 and 2.

[35] H. Weyl, *Über gewöhnliche Differentialgleichungen mit Singularitäten und die zugehörigen Entwicklungen willkürlicher Funktionen*, Math. Ann. **68** (1910), 220–269.

[36] M.R.M. Witwit, N. Gordon and J.P. Killingbeck, *Numerical computation and analysis of the Titchmarsh-Weyl m(l) function for some simple potentials*, J. Comput. Appl. Math. **106** (1999), 131–143.

[37] J. Zhang, Z. Xu and X. Wu, *Unified approach to split absorbing boundary conditions for nonlinear Schrödinger equations*, Phys. Rev. E **78** (2008), 026709.

[38] C. Zheng, *Approximation, stability and fast evaluation of exact artificial boundary condition for the one-dimensional heat equation*, J. Comput. Math. **25** (2007), 730–745.

[39] C. Zheng, *A perfectly matched layer approach to the nonlinear Schrödinger wave equations*, J. Comput. Phys. **227** (2007), 537–556.