A Review of Artificial Boundary Conditions for the Schrödinger Equation

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In this review we discuss techniques to solve numerically the time–dependent linear Schrödinger equation on unbounded domains. We present some recent approaches and describe alternative ideas pointing out the relations between these works.

1 Introduction

The equation under consideration is the 1D Schrödinger equation given on the unbounded domain $\Omega = \{(x,t) \in \mathbb{R} \times \mathbb{R}^+\}$:

$$\begin{aligned} &i\partial_t u = -\partial_x^2 u + V(x,t)u, \quad x \in \mathbb{R},\, t > 0, \\ &u(x,0) = u^I(x), \qquad \lim_{|x|\to\infty} u(x,t) = 0, \end{aligned} \tag{1}$$

where V denotes a given real potential. We assume that the initial data is compactly supported, i.e. $\mathrm{supp}(u^I) \subset [x_l, x_r]$. Furthermore, we assume that V is constant outside an interval $[x_l, x_r]$, i.e. $V(x) = V_l$ for $x < x_l$, $V(x) = V_r$ for $x > x_r$.

Equation (1) is one of the basic equations of quantum mechanics and it arises in many areas of physical and technological interest, e.g. in quantum semiconductors, in electromagnetic wave propagation, and in seismic migration. The Schrödinger equation is the lowest order one-way approximation (*paraxial wave equation*) to the Helmholtz equation and is called *Fresnel equation* in optics , or *standard parabolic equation* in underwater acoustics.

If one wants to solve such a whole space evolution problem numerically, one has to restrict the computational (interior) domain $\Omega_{int} = \{(x,t) \in]x_l, x_r[\times \mathbb{R}^+\}$ by introducing artificial boundary conditions or absorbing layers. Artificial boundary conditions are constructed with the objective to approximate the exact solution of the whole–space problem, restricted to Ω_{int}. Such BCs are called *absorbing boundary conditions* (ABCs) if they yield a well–posed initial boundary value problem (IBVP), where some 'energy functional' is absorbed at the boundary. If this approximate solution actually coincides on Ω_{int} with the exact solution of the whole–space problem, one refers to these BCs as *transparent boundary conditions* (TBCs). While TBCs for the Schrödinger equation are nonlocal in time (and space for multi-dimensional cases), it is often desirable to construct ABCs that are *local* in space and/or time to allow for an efficient numerical implementation.

2 Transparent boundary conditions for the Schrödinger equation

Here we sketch the different ways of deriving transparent boundary conditions (TBCs). We start with the classical derivation of the *analytic* TBC for the IBVP (1). Secondly, we shall mimic this procedure for the time–discrete Schrödinger equation to derive temporally discrete TBCs. Note that the Schrödinger equation discretized in time is also the starting point for TBCs based on the *perfectly matched layer method* and the *pole condition*. Finally, we shall consider *fully discrete TBCs*.

2.1 Analytic TBCs

Analytic TBCs for the Schrödinger equation (1) were independently derived by several authors from various application fields They are non–local in t and connect $\partial_x v(x_{l,r}, t)$ with $v(x_{l,r}, t)$. As a Dirichlet-to-Neumann (DtN) map they read

$$\partial_{\mathbf{n}} v(x,t) = -\frac{e^{-\frac{\pi}{4}i}}{\sqrt{\pi}}\, e^{-iV_{l,r}t} \frac{d}{dt} \int_0^t \frac{v(x,\tau) e^{iV_{l,r}\tau}}{\sqrt{t-\tau}}\, d\tau \quad \text{at } x = x_l, x_r, \tag{2}$$

where $\mathbf{n}$ denotes the outwardly unit normal vector at $x_l,\, x_r$.

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These TBCs may be derived by the following *general procedure*. First, split original problem into coupled equations, interior and exterior problems. Secondly, apply a Laplace transformation in time t and solve the resulting ordinary differential equations in x. Allow only 'outgoing' waves by selecting the decaying solution as $x \to \pm\infty$. Finally, match Dirichlet and Neumann values at $x = x_l$, $x = x_r$. and apply the inverse Laplace transformation to obtain the TBCs (2) .

2.2 Temporally discrete TBCs

We consider the problem (1) discretized uniformly in time with the step size Δt by the *trapezoidal rule*

$$\begin{aligned} i\frac{u^{n+1}-u^n}{\Delta t} &= -\partial_x^2\frac{u^{n+1}+u^n}{2} + \frac{V^{n+1}(x)u^{n+1}+V^n(x)u^n}{2}, \quad x\in\mathbb{R}, \forall n\in\mathbb{N}_0,\\ u^0 &= u^I(x) \quad \text{given for } x\in\mathbb{R}, \qquad \lim_{|x|\to\infty} u^n(x) = 0, \quad \forall n\in\mathbb{N}_0, \end{aligned} \tag{3}$$

Instead of a Laplace transformation w.r.t. t to (1), we apply a $\mathcal{Z}$-transformation $\mathcal{Z}(u^n) = \hat{u}(z) := \sum_{n=0}^{\infty} u^n z^{-n}$, $z\in\mathbb{C}$ and obtain by the above described procedure:

$$\begin{aligned} i\frac{v^{n+1}-v^n}{\Delta t} &= -\partial_x^2\frac{v^{n+1}+v^n}{2} + \frac{V^{n+1}(x)v^{n+1}+V^n(x)v^n}{2}, \quad x\in\Omega, \forall n\in\mathbb{N}_0,\\ v^0(x) &= u^I(x), \quad x\in\Omega,\\ \partial_{\mathbf{n}} v^{n+1} &= \sum_{k=0}^{n+1}\psi_k^{(l,r)} v^{n+1-k}, \quad \text{at } x = x_l, x_r, \end{aligned} \tag{4}$$

where the weights $\psi_n^{(l,r)}$ are given (in case of a vanishing potential) by

$$\psi_k = -e^{-\frac{i\pi}{4}}\frac{\sqrt{2}}{\sqrt{\Delta t}}(-1)^k\tilde{\psi}_k, \quad k\in\mathbb{N}_0, \quad (\tilde{\psi}_0,\tilde{\psi}_1,\tilde{\psi}_2,\tilde{\psi}_3,\tilde{\psi}_4,\tilde{\psi}_5,\dots) = \left(1,1,\frac{1}{2},\frac{1}{2},\frac{1\cdot 3}{2\cdot 4},\frac{1\cdot 3}{2\cdot 4},\dots\right). \tag{5}$$

2.3 Fully discrete TBCs

Fully discrete TBCs are obtained if we discretize (3) additionally in space, e.g. using the uniform grid $x_j = x_l + j\Delta x$, $j\in\mathbb{Z}$:

$$\begin{aligned} i\frac{u_j^{n+1}-u_j^n}{\Delta t} &= -D_x^2\frac{u_j^{n+1}+u_j^n}{2} + \frac{V_j^{n+1}u_j^{n+1}+V_j^n u_j^n}{2}, \quad j\in\mathbb{Z},\ n\in\mathbb{N}_0,\\ \lim_{|j|\to\infty} u_j^n &= 0, \quad n\in\mathbb{N}_0,\\ u_j^0 &= u^I(j\Delta x), \quad j\in\mathbb{Z}, \end{aligned} \tag{6}$$

where D_x^2 denotes the standard second order difference quotient. The right artificial boundary is located at $x_J = x_l + J\Delta x = x_r$ and the left boundary at $x_0 = x_l$. The right discrete TBC is obtained analogously and reads (written as DtN map):

$$u_J^n - u_{J-1}^n = -\sum_{k=1}^{n} s_{n-k}u_J^k + u_{J-1}^{n-1}, \quad n\in\mathbb{N}, \tag{7}$$

with the explicitly calculated convolution weights:

$$\begin{aligned} s_n &= (-iR+\sigma)\,\delta_n^0 + (1+iR+\sigma)\,\delta_n^1 + \gamma\, e^{-in\varphi}\frac{P_n(\mu)-P_{n-2}(\mu)}{2n-1}, \quad \varphi = \arctan\frac{2R(\sigma+1)}{R^2-2\sigma-\sigma^2},\\ \sigma &= \Delta x^2 V_r, \quad \gamma = i\sqrt[4]{(R^2+\sigma^2)\,(R^2+(\sigma+2)^2)}\,e^{i\varphi/2}, \quad \mu = \frac{R^2+2\sigma+\sigma^2}{\sqrt{(R^2+\sigma^2)\,(R^2+(\sigma+2)^2)}}. \end{aligned} \tag{8}$$

P_n denotes the Legendre polynomials ($P_{-1}\equiv P_{-2}\equiv 0$), δ_n^k is the Kronecker symbol and $R = \Delta x^2/\Delta t$ is the mesh ratio.

3 Further Reading

For a much more detailed description of the previous derivations and a concise discussion of the situation for multidimensional and nonlinear (cubic) Schrödinger equations, efficient approximations and numerical examples we refer the reader to [1]. Moreover, there exists supplementary MATLAB software with a graphical user interface to compare the different approaches.

References

[1] X. Antoine, A. Arnold, C. Besse, M. Ehrhardt, and A. Schädle, Preprint No. 18–2007 of the Institute of Mathematics, TU Berlin, May 2007. (submitted to: Applied Numerical Mathematics) see: `http://www.tbc-review.de.vu`