COMMUNICATIONS IN COMPUTATIONAL PHYSICS
Vol. **4**, No. 4, pp. 729-796

Commun. Comput. Phys.
October 2008

Review Article

A Review of Transparent and Artificial Boundary Conditions Techniques for Linear and Nonlinear Schrödinger Equations

Xavier Antoine[1], Anton Arnold[2], Christophe Besse[3], Matthias Ehrhardt[4,*] and Achim Schädle[5]

[1] *Institut Elie Cartan Nancy (IECN), Université Henri Poincaré Nancy 1, UMR 7502, INRIA Corida, Nancy-Université, France.*
[2] *Institut für Analysis und Scientific Computing, Technische Universität Wien, Wiedner Hauptstr. 8, 1040 Wien, Austria.*
[3] *Project-Team SIMPAF INRIA Lille Nord Europe Research Centre, Laboratoire Paul Painlevé U.M.R CNRS 8524*
Université des Sciences et Technologies de Lille, France.
[4] *Weierstrass Institute for Applied Analysis and Stochastics, Mohrenstr. 39, 10117 Berlin, Germany.*
[5] *Zuse-Institut Berlin, Takustrasse 7, 14195 Berlin, Germany.*

Received 28 February 2008; Accepted (in revised version) 3 April 2008

Available online 16 May 2008

Abstract. In this review article we discuss different techniques to solve numerically the time-dependent Schrödinger equation on unbounded domains. We present in detail the most recent approaches and describe briefly alternative ideas pointing out the relations between these works. We conclude with several numerical examples from different application areas to compare the presented techniques. We mainly focus on the one-dimensional problem but also touch upon the situation in two space dimensions and the cubic nonlinear case.

AMS subject classifications: 65M12, 35Q40, 45K05

PACS: 02.70.Bf, 31.15.Fx

Key words: Schrödinger equation, transparent boundary conditions, discrete convolution, unbounded domain, finite difference schemes, finite elements.

*Corresponding author. *Email addresses:* `Xavier.Antoine@iecn.u-nancy.fr` (X. Antoine), `anton.arnold@tuwien.ac.at` (A. Arnold), `Christophe.Besse@math.univ-lille1.fr` (C. Besse), `ehrhardt@wias-berlin.de` (M. Ehrhardt), `schaedle@zib.de` (A. Schädle)

Contents

1 Introduction

The equation under consideration is the 1D Schrödinger equation

$$\begin{aligned} &i\partial_t u = -\partial_x^2 u + V(x,t)u, \quad x \in \mathcal{R}, \ t>0, \\ &\lim_{|x|\to\infty} u(x,t) = 0, \\ &u(x,0) = u^I(x), \end{aligned} \tag{1.1}$$

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 $x > x_r$ (t-dependent exterior potentials will be discussed in Remark 2.5).

Eq. (1.1) 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 [28], in electromagnetic wave propagation [87], and in seismic migration [33]. The Schrödinger equation is also the lowest order one-way approximation (*paraxial wave equation*) to the Helmholtz equation and is called *Fresnel equation* in optics [112], or *standard parabolic equation* in underwater acoustics [129]. We will return to these applications in the numerical examples of Section 6.

The solution to (1.1) is defined on the unbounded domain $\Omega = \{(x,t) \in \mathcal{R} \times \mathcal{R}^+\}$. If one wants to solve such a whole space evolution problem numerically, one has to restrict the computational (interior) domain $\Omega_{int} = \{(x,t) \in]x_l, x_r[\times \mathcal{R}^+\}$ by introducing artificial boundary conditions or absorbing layers [81, 105]. Note that the method of "exterior complex scaling" [95] belongs also to this last mentioned class. Alternative methods are infinite element methods (IEM) [45].

We remark that in some cases the original whole space problem can be transformed into a differential equation on a finite domain. However, this *coordinate transform technique* is restricted to special cases and yields quite complicated differential equations. This