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Journal of Computational Physics 219 (2006) 879–898

JOURNAL OF COMPUTATIONAL PHYSICS

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The stability and convergence of an explicit difference scheme for the Schrödinger equation on an infinite domain by using artificial boundary conditions

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Received 19 December 2005; received in revised form 5 July 2006; accepted 6 July 2006
Available online 17 August 2006

Abstract

This article is concerned with the numerical solution to the time-dependent Schrödinger equation on an infinite domain. Two exact artificial boundary conditions are introduced to reduce the original problem into an initial boundary value problem with a finite computational domain. The artificial boundary conditions involve the 1/2 order fractional derivative in t. Then, a fully discrete explicit three-level difference scheme is derived. The truncation errors are analyzed in detail. The stability and convergence with the convergence order of $O(h^{3/2}+\tau h^{-1/2})$ are proved under the condition $\tau/h^2<1/2$ by the energy method. A numerical example is given to demonstrate the accuracy and efficiency of the proposed method. Two open problems are brought forward at the end of the article.

MSC: 65M12; 65M06; 65M15; 65M20

Keywords: Schrödinger equation; Finite difference; Convergence; Solvability; Stability; Infinite domain; Artificial boundary condition; Fractional derivative boundary condition

1. Introduction

The time-dependent Schrödinger equation is the basic of quantum mechanics [8,16]. This model equation also arises in many other practical domains of physical and technological interest, e.g. optics, seismology and plasma physics. There are a lot of studies on the numerical solution of initial and initial-boundary problems for solving the linear or nonlinear Schrödinger equation, see e.g. [9–14,22,23,28,31,32,40,43].

When we wish to solve numerically a differential equation defined on an infinite domain, it is necessary to consider a finite sub-domain and to use artificial boundary conditions in such a way that the solutions in the

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doi:10.1016/j.jcp.2006.07.001

finite sub-domain approximate the original solution. If the approximation is exact, the transfer is called exact and the corresponding artificial boundary condition is called exact or transparent. For instance, different transparent boundary conditions (TBCs) for the wave equation are derived in [15,18,19,35,36,41,42].

In this article, we study the problem of the numerical approximation of a dispersive wave $\psi(x,t)$, solution to the Schrödinger equation in an unbounded domain. More concretely, we consider the following linear equation:

$$\mathrm{i}\frac{\partial\psi}{\partial t} = -\frac{1}{2}\frac{\partial^2\psi}{\partial x^2} + V(x,t)\psi, \quad x \in R, \quad t > 0, \tag{1.1}$$

$$\psi(x,0) = \phi(x), \quad x \in R, \tag{1.2}$$

$$\lim_{|x|\to\infty} \psi(x,t) = 0, \quad t > 0, \tag{1.3}$$

where the electrostatic potential function $V(x,t)$ is assumed to be given with $\mathrm{Im}(V(x,t)) \leqslant 0$, and for the sake of conciseness, we assume that ϕ is a compactly supported datum. The solution to (1.1)–(1.3) is defined on the whole domain $\Omega = \{(x,t)|x \in R, t > 0\}$. However, from a practical point of view, the infinite domain of propagation has to next use a well-adapted discretization scheme for Eqs. (1.1)–(1.3). To this end, let us split the initial domain Ω into three regions. We designate by $\Omega_i = \{(x,t)|x_l \leqslant x \leqslant x_r, t > 0\}$ the interior domain where one wishes to compute an approximate solution, and the two other complementary regions can be defined by $\Omega_l = \{(x,t)|x < x_l, t > 0\}$ and $\Omega_r = \{(x,t)|x > x_r, t > 0\}$. To simplify the problem, we suppose that $\mathrm{supp}(\phi) \subset [x_l, x_r]$ and

$$V(x,t) = V_- \equiv \text{const}, \quad \text{for } x \leqslant x_l, \quad V(x,t) = V_+ \equiv \text{const}, \quad \text{for } x \geqslant x_r,$$

with $\mathrm{Im}(V_-) = \mathrm{Im}(V_+) = 0$.

The transparent boundary conditions (TBCs) for Schrödinger equation were independently derived by several authors from various application fields [2,7,21,29]; Inhomogeneous extensions are analyzed in [1,4]. They are non-local in t and read

$$\frac{\partial\psi(x_l,t)}{\partial x} = \sqrt{\frac{2}{\pi}}\mathrm{e}^{-(\frac{\pi}{4}+V_-t)i}\frac{\mathrm{d}}{\mathrm{d}t}\int_0^t \frac{\psi(x_l,s)\mathrm{e}^{\mathrm{i}V_-s}}{\sqrt{t-s}}\,\mathrm{d}s \tag{1.4}$$

for the left boundary at $x = x_l$, and

$$\frac{\partial\psi(x_r,t)}{\partial x} = -\sqrt{\frac{2}{\pi}}\mathrm{e}^{-(\frac{\pi}{4}+V_+t)\mathrm{i}}\frac{\mathrm{d}}{\mathrm{d}t}\int_0^t \frac{\psi(x_r,s)\mathrm{e}^{\mathrm{i}V_+s}}{\sqrt{t-s}}\,\mathrm{d}s \tag{1.5}$$

for the right boundary at $x = x_r$. Using the notations of the Riemann–Liouville fractional derivative, the boundary conditions (1.4) and (1.5) can be written as

$$\frac{\partial\psi(x_l,t)}{\partial x} = \sqrt{2}\mathrm{e}^{-(\frac{\pi}{4}+V_-t)\mathrm{i}}\frac{\mathrm{d}^{1/2}[\psi(x_l,t)\mathrm{e}^{\mathrm{i}V_-t}]}{\mathrm{d}t^{1/2}},$$

$$\frac{\partial\psi(x_r,t)}{\partial x} = -\sqrt{2}\mathrm{e}^{-(\frac{\pi}{4}+V_+t)\mathrm{i}}\frac{\mathrm{d}^{1/2}[\psi(x_r,t)\mathrm{e}^{\mathrm{i}V_+t}]}{\mathrm{d}t^{1/2}}.$$

There are also an equivalent form to (1.4) and (1.5) as follows

$$\psi(x_l,t) = \sqrt{\frac{2}{\pi}}\mathrm{e}^{-(\frac{\pi}{4}+V_-t)\mathrm{i}}\int_0^t \frac{\frac{\partial}{\partial x}[\psi(x_l,s)\mathrm{e}^{\mathrm{i}V_-s}]}{\sqrt{t-s}}\,\mathrm{d}s \tag{1.6}$$

for the left boundary at $x = x_l$, and

$$\psi(x_r,t) = -\sqrt{\frac{2}{\pi}}\mathrm{e}^{-(\frac{\pi}{4}+V_+t)i}\int_0^t \frac{\frac{\partial}{\partial x}[\psi(x_r,s)\mathrm{e}^{\mathrm{i}V_+s}]}{\sqrt{t-s}}\,\mathrm{d}s \tag{1.7}$$