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Analysis of High-Order Absorbing Boundary Conditions for the Schrödinger Equation

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Abstract. The paper is concerned with the numerical solution of Schrödinger equations on an unbounded spatial domain. High-order absorbing boundary conditions for one-dimensional domain are derived, and the stability of the reduced initial boundary value problem in the computational interval is proved by energy estimate. Then a second order finite difference scheme is proposed, and the convergence of the scheme is established as well. Finally, numerical examples are reported to confirm our error estimates of the numerical methods.

AMS subject classifications: 65M12, 65M06, 65M15

Key words: Schrödinger equation, finite difference method, high-order absorbing boundary condition, convergence.

1 Introduction

Schrödinger equation is one of the basic equations of quantum mechanics, and can be found in many areas of physical and technological interest, e.g., optics, seismology and plasma physics. In this paper, the numerical approximation of Schrödinger equation of the following form is considered:

$$i\partial_t \psi(x,t) = -\partial_x^2 \psi(x,t) + V(x,t)\psi, \qquad x \in \mathbb{R}, \quad 0 < t \le T, \tag{1.1a}$$

$$\lim_{|x|\to\infty} \psi(x,t) = 0, \qquad t \ge 0, \tag{1.1b}$$

$$\psi(x,0) = \psi_0(x), \qquad x \in \mathbb{R}, \tag{1.1c}$$

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where $V(x,t)$ is the potential function and $V(x,t)\in L^\infty$ with real (or negative complex) part. It is assumed that the initial data is compactly supported on a finite (interior) domain $\Omega_i=\{x|x_l<x<x_r\}$, $V(x,t)$ is constant on the complementary region $\Omega_c=\mathbb{R}/\Omega_i$. If the initial value is not compactly supported, one refers to [13] and references therein to see how to treat it. A great numerical challenge lies on the unboundedness of the definition domain of the model equation (1.1a)-(1.1c), since the traditional methods (finite difference method and finite element method et al.) can not be used directly. In practical numerical simulations, people are concerned about the evolution of the solution in a finite domain of physical interest, rather than the whole space. Thus the equations need to be reduced to a problem on bounded (computational) domain in a neighborhood of the region of physical interest. An often used method is to limit the interest region by an artificial boundary, impose the ideal absorbing boundary conditions (ABCs), and then solve a reduced initial boundary value problem on a bounded domain. This procedure is usually called artificial boundary methods [3, 12, 15, 20–22, 24, 25, 28, 38, 40]. Artificial boundary conditions consist of two categories: nonlocal and local. The nonlocal ABCs in time (and in space for multimensional cases) are well-posed, but are expensive. It is often desirable to design local ABCs which are both computationally efficient and easy to implement. However, the proposed ABCs often result in a degradation of accuracy and stability. Other solutions to address the unboundedness issue are the perfectly matched layer method [8,45], infinite element or boundary element method [41] and so on.

Many efforts have been continuously devoted to the study of using artificial boundary methods for Schrödinger equations [1,6,9–11,14,23,26,30,36,37,46] and the references therein. For recent development, we shall refer to a review paper [3]. When the simulation is for a long time or high accuracy is needed, high-order ABCs are necessary for efficiently minimizing the unphysical reflection. The high-order method has been widely used in wave equations [7,16–19], based on which, in this paper we construct a family of high-order ABCs for Schrödinger equation. To differ from ABCs obtained by Di Menza, Szeftel and Antoine etc [2,10,11,36,37] and use the idea of Kuska [30], a physical parameter k_0 is introduced to adjust the performance of high-order ABCs, which is related to the velocity of wave impinged on the artificial boundary. The boundary condition can efficiently absorb the "fast" or "slow" waves by choosing suitable values k_0. In [2] (with $k_0=1$), the authors proposed high-order ABCs for Schrödinger equation with an exterior repulsive potential, which is a more difficult case. The aims of this paper are to establish the theoretical aspects of the reduced problem and design a corresponding finite difference scheme. The focuses of the presentation are on the stability of the initial boundary value problem with high-order ABCs on finite (computational) domain, and then on the difference scheme. We prove the solvability and convergence of the difference scheme and obtain the optimal convergence rate at the order of $\mathcal{O}(h^2+\tau^2)$ with mesh size h and time step τ (see Theorem 4). One is also recommended to refer to the strategy of proving the well-posedness of the corresponding initial boundary problem in [36]. The theoretical results in this paper have formed a basis to study the stability of ABCs for the nonlinear Schrödinger equation in the future [42,43].