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Absorbing Boundary Conditions for Variable Potential Schrödinger Equations via Titchmarsh-Weyl Theory

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Abstract. We propose a novel approach to simulate the solution of the time-dependent Schrödinger equation with a general variable potential. The key idea is to approximate the Titchmarsh-Weyl m-function (exact Dirichlet-to-Neumann operator) by a rational function with respect to an appropriate spectral parameter. By using this method, we overcome the usual high-frequency restriction associated with absorbing boundary conditions in general variable potential problems. The resulting fast computational algorithm for absorbing boundary conditions ensures accuracy over the entire frequency range.

AMS subject classifications: 65M99, 81-08

Key words: Absorbing boundary conditions, variable potential, Schrödinger equation, Titchmarsh-Weyl m-function, unbounded domain.

1 Introduction

In this paper we consider the linear Schrödinger problem of the form

$$\begin{aligned} \mathrm{i}u_t+\partial_x^2 u &= V(x)u, \quad (x,t)\in\mathbb{R}\times(0,T], \\ u(x,0) &= u_0(x), \quad x\in\mathbb{R}, \end{aligned} \tag{1.1}$$

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 (1.1) has a unique solution $u\in C(\mathbb{R}^+,L^2(\mathbb{R}))$, cf. [43], e.g.:

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Theorem 1.1. *Let $u_0 \in L^2(\mathbb{R})$ and real-valued potential $V \in L^\infty(\mathbb{R})$. Then the problem* (1.1) *has a unique solution $u \in C(\mathbb{R}^+, L^2(\mathbb{R}))$. Moreover, the "energy" is preserved, i.e.*

$$\|u(.,t)\|_{L^2(\mathbb{R})} = \|u_0\|_{L^2(\mathbb{R})}, \quad \forall t \geq 0. \tag{1.2}$$

The Schrödinger problem (1.1) is defined on an unbounded domain $x \in \mathbb{R}$. To numerically simulate its solution, it is common practice to truncate the domain to a bounded one, for example, $\Omega_{\text{int},T} = \Omega_{\text{int}} \times (0,T]$. *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 articles [8, 10, 35]. Recent applications of this methodology are Schrödinger equations on branched structures [52], nonlocal nonlinear Schrödinger equations [1], underwater acoustics [44], or implementations using a quantum computer [40].

An ABC is called *exact* if the solution of the 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 (1.1), but it can only be formulated analytically for some special potentials, such as constant potential [22], linear potential [23], quadratic potential [27], symmetric periodic potential [25], isotropic free particle potential, Morse potential, harmonic potential, and Bargeman potential, cf. e.g. [45]. In the more general case, i.e., for general variable potential problems one is led to design approximate analytical ABCs for a given frequency regime with respect to some a priori criterion. Methods in this category include the pseudo-differential calculus method [6,7,9], the perfectly matched layer (PML) method [55], and the operator splitting method [53]. To the authors' knowledge, all of them are essentially based on the *high frequency approximations*. For low-frequency problems, the ABCs would be less accurate by these methods.

This paper proposes a new approach to the design of ABCs for the Schrödinger problem. Inspired by the work of Alpert, Greengard, and Hagstrom [3] on the fast evaluation of nonreflecting boundary kernels for time-domain wave propagation, we approximate the *Titchmarsh-Weyl m-function* (equivalently, the 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 the asymptotic behavior of the m-function. Since our approximation is performed in the whole frequency regime, the proposed ABCs are expected to be more versatile and accurate, especially in the low-frequency regime, thus overcoming the typical high-frequency restriction. Note that the Titchmarsh-Weyl m-function is nothing else but the so-called *total symbol* in microdifferential calculus, which is treated by an asymptotic expansion to obtain a hierarchy of ABCs, cf. [6, 7, 9]. Note also that Titchmarsh-Weyl theory is used in the analysis of initial value problems for Schrödinger equations operator-valued potentials [30] or strongly singular potentials [37]. It is also used in practical applications