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An Exact Absorbing Boundary Condition for the Schrödinger Equation With Sinusoidal Potentials at Infinity

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Abstract. In this paper we study numerical issues related to the Schrödinger equation with sinusoidal potentials at infinity. An exact absorbing boundary condition in a form of Dirichlet-to-Neumann mapping is derived. This boundary condition is based on an analytical expression of the logarithmic derivative of the Floquet solution to Mathieu's equation, which is completely new to the author's knowledge. The implementation of this exact boundary condition is discussed, and a fast evaluation method is used to reduce the computation burden arising from the involved half-order derivative operator. Some numerical tests are given to show the performance of the proposed absorbing boundary conditions.

AMS subject classifications: 65M99, 81-08

Key words: Absorbing boundary condition, sinusoidal potential, Schrödinger equation, unbounded domain.

1 Introduction

Wave propagation is usually modeled by partial differential equations on unbounded domains. For a practical numerical treatment, however, the equations need to be confined to a bounded computational domain in a neighborhood of the region of physical interest. This can be achieved by introducing artificial boundaries, which then necessitates imposing boundary conditions. The ideal boundary conditions should not only present well-posed problems, but also mimic the perfect absorption of waves traveling out of the computational domain through the artificial boundaries. Right in this context, these boundary conditions are usually called absorbing (or transparent, non-reflecting in the same spirit) in the literature.

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Absorbing boundary condition for the Schrödinger equation and related problems has been a hot research topic for many years. From one-dimensional [2, 3, 6, 7, 10, 12, 15, 19–22, 24, 26] to high-dimensional [5, 8, 11, 13, 18, 23, 28], from linear to nonlinear [4, 14, 25, 27, 29], many developments have been made on the designing and implementing of various absorbing boundary conditions. In this paper we will consider the Schrödinger equation of the form

$$iu_t + u_{xx} = V(x)u, \quad x \in \mathbf{R}, \tag{1.1}$$

$$u(x,0) = u_0(x), \quad x \in \mathbf{R}, \tag{1.2}$$

$$u(x,t) \to 0, \quad x \to \pm\infty. \tag{1.3}$$

The initial function u_0 is assumed to be compactly supported in an interval $[x_L, x_R]$, with $x_L < x_R$, and the real potential function V is supposed to be sinusoidal on $(-\infty, x_L]$ and $[x_R, +\infty)$. More precisely, we assume

$$V(x) = V_L + 2q_L \cos\frac{2\pi(x_L - x)}{S_L}, \quad \forall x \in (-\infty, x_L],$$

$$V(x) = V_R + 2q_R \cos\frac{2\pi(x - x_R)}{S_R}, \quad \forall x \in [x_R, +\infty),$$

where S_L and S_R are the periods, V_L and V_R are the average potentials, and the non-negative numbers q_L and q_R relate to the amplitudes of sinusoidal part of the potential function V on $(-\infty, x_L]$ and $[x_R, +\infty)$, respectively.

The Schrödinger equation with periodic potentials has wide applications in quantum mechanics and solid physics. For example, it can be used to model electrons immersed in optical lattices, or simulate quantum dots embedded in crystals. The problem (1.1)-(1.3) is linear, and the tool of Laplace transform is thus applicable. Formally an exact relation can be built at each boundary point. This relation expresses a convolution, with its kernel defined by the inverse Laplace transform of the logarithmic derivative of the Floquet solution to Mathieu's equation. However, if the property of this kernel is not fully explored, this formal exact relation has little practical use. Recently, Galicher [16] considered the same problem but with a general periodic potential. Formally he set up at each artificial boundary point an exact Dirichlet-to-Dirichlet mapping, which is nonlocal in both time and space.

The organization of the rest is as follows. In Section 2, we conjecture an elegant analytical expression of the logarithmic derivative of the Floquet solution. Based on this expression, an exact absorbing boundary condition in a form of Dirichlet-to-Neumann mapping is presented in Section 3. The related numerical issues are discussed in Section 4. A fast evaluation method is employed to reduce the computation burden arising from the convolution operations. Some numerical tests are given in Section 5 to demonstrate the performance of our absorbing boundary condition. The results show that highly accurate numerical solutions can be computed. We conclude this paper in Section 6.