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High Order Scheme for Schrödinger Equation with Discontinuous Potential I: Immersed Interface Method

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Abstract. The immersed interface method is modified to compute Schrödinger equation with discontinuous potential. By building the jump conditions of the solution into the finite difference approximation near the interface, this method can give at least second order convergence rate for the numerical solution on uniform cartesian grids. The accuracy of this algorithm is tested via several numerical examples.

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Key words: Schrödinger equation, discontinuous potential, immersed interface method, finite difference method.

1. Introduction

Consider Schrödinger equation in different forms

$$\text{Stationary}: \quad -\frac{1}{2}\varepsilon^2\triangle\varphi + V\varphi = E\varphi, \tag{1.1}$$

$$\text{Eigenvalue}: \quad -\frac{1}{2}\varepsilon^2\triangle\phi + V\phi = E\phi, \tag{1.2}$$

$$\text{Dynamic}: \quad i\varepsilon\psi_t + \frac{1}{2}\varepsilon^2\triangle\psi = V\psi, \tag{1.3}$$

where ε is the re-scaled Plank constant, $\boldsymbol{x} \in \Omega \subset \mathbb{R}^d$ denotes the computational domain, and $V = V(\boldsymbol{x})$ is the potential. We can use different types of boundary conditions, e.g., transparent boundary condition, periodic boundary condition and reflection boundary condition. In the stationary problem, the energy E is specified. In the eigenvalue problem, the energy E is eigenvalue. In the dynamic problem, we need to specify the initial condition as

$$\psi(0,\boldsymbol{x}) = A_0(\boldsymbol{x})e^{\frac{iS_0(\boldsymbol{x})}{\varepsilon}}. \tag{1.4}$$

Our goal is to compute the wave functions $\varphi(\boldsymbol{x})$, $\phi(\boldsymbol{x})$ and $\psi(t,\boldsymbol{x})$ on a uniform Cartesian grid up to second order accuracy, even if the discontinuities curves of potential $V(\boldsymbol{x})$ are not aligned with the grid.

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Schrödinger equation with discontinuous potential can be used to model motion of electrons in quantum zones, e.g., quantum barrier, quantum well, quantum dot and p-n junctions [11, 30, 37]. The quantum zone is an active region of electronic structure, which connects to two highly conduct large reservoirs. The whole structure is a basic and fundamental semiconductor device in modern industry, e.g., memory chip, microprocessor and integrated circuit [9, 10, 31].

There have been numerous studies on direct numerical methods of Schrödinger equation, including the finite difference method [28,29,38], the discontinuous Galerkin method [26, 27, 40], spectral type methods [7, 8, 13], the WKB scheme [3, 4, 36] and other related technics [1, 2, 5, 17, 34]. However, none of these methods could satisfy all the following requirements for solving Schrödinger equation with discontinuous potential: (i) at least second order convergence, (ii) robust processing in interface conditions, (iii) easy generalization to high dimensions, (iv) taking the advantages of the Cartesian grid.

The immersed interface method, originally developed for elliptic equations with discontinuous coefficients and singular sources [12, 18, 20–24], can maintain at least second order accuracy on a uniform grid even when the discontinuities curves of potential are not aligned with the grid. The idea is to modify the standard finite difference approximation at grid points near the interface to keep jump conditions of solutions' derivatives. Such method has succeed in many applications, e.g., the heat equation [6, 25], the acoustic wave equation [33, 41], stokes flow and Navier-Stokes equations [15, 16, 19].

In this paper, we develop an immersed interface method to solve Schrödinger equation with discontinuous potential. The solutions are shown to have at least second order convergence in both one and two dimensions. A more interesting question is how to extend such idea for the dynamic Schrödinger equation with discontinuous potential in the semi-classical regime [14]. Based on the results here, we will propose two new methods in a consecutive paper [39].

The paper is organized as follows. In Section 2, we show how the immersed interface method is applied to Schrödinger equation with discontinuous potential. The method in higher space dimensions is given in Section 3. In Section 4, we present numerical examples to test the accuracy of the method. We make some conclusive remarks in Section 5.

2. One dimensional Schrödinger equation

We begin by considering the one dimensional stationary Schrödinger equation

$$-\frac{1}{2}\varepsilon^2\varphi_{xx}+V\varphi=E\varphi, \tag{2.1}$$

on the computational domain $[a,b]$. The potential $V(x)$ is split into a smooth part $V_s(x)\in C^\infty([a,b])$ and a discontinuous part $V_d(x)$

$$V(x)=V_s(x)+V_d(x). \tag{2.2}$$