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Two-Grid Crank-Nicolson Finite Volume Element Method for the Time-Dependent Schrödinger Equation

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Abstract. In this paper, we construct a Crank-Nicolson finite volume element scheme and a two-grid decoupling algorithm for solving the time-dependent Schrödinger equation. Combining the idea of two-grid discretization, the decoupling algorithm involves solving a small coupling system on a coarse grid space and a decoupling system with two independent Poisson problems on a fine grid space, which can ensure the accuracy while the size of coarse grid is much coarser than that of fine grid. We further provide the optimal error estimate of these two schemes rigorously by using elliptic projection operator. Finally, numerical simulations are provided to verify the correctness of the theoretical analysis.

AMS subject classifications: 65N12, 65M60

Key words: Finite volume element method, two-grid method, Crank-Nicolson scheme, error estimates, Schrödinger equation.

1 Introduction

The time-dependent Schrödinger equation is one of the most important equations of mathematical physics. This model has been widely used in many fields, such as plasma physics, nonlinear optics, seismology, bimolecular dynamics and protein chemistry. In this article, we consider the initial boundary value problem of two-dimensional time-dependent linear Schrödinger equation as follows:

$$\begin{cases} iu_t = -\Delta u(x,t) + V(x)u(x,t) + f(x,t) & \text{in } \Omega\times(0,T], \\ u(x,t) = 0 & \text{on } \partial\Omega\times(0,T], \\ u(x,0) = u_0(x) & \text{in } \bar{\Omega}, \end{cases} \tag{1.1}$$

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where $x=(x_1,x_2)^T$, $\Omega\subset R^2$ is a bounded convex polygonal domain with smooth boundary $\partial\Omega$, the function $f(x,t)$ and unknown function $u(x,t)$ are complex-valued, $u_0(x)$ is a smooth known complex-valued function, the trapping potential function $V(x)$ is real-valued and non-negative bounded for all $x\in\Omega$, and $i=\sqrt{-1}$ is the complex unit.

At present, many scholars have studied the numerical solutions of the Schrödinger equation. For example, Akrivis et al. [1] used the standard Galerkin method in space and two implicit Crank-Nicholson schemes in time to approximate the solution of nonlinear Schrödinger equation. Jin et al. [2] studied the convergence of a finite element scheme for the two-dimensional time-dependent Schrödinger equation in a long strip. Antonopoulou et al. [3] investigated the generalized Schrödinger equation with mixed boundary conditions in a two-dimensional noncylindrical domain. Wang, Tian et al. [4,5] studied the superconvergence property of time-dependent nonlinear Schrödinger equations. It is well known that the finite volume element (FVE) method is not only simple in structure, but also can maintain the local conservation of physical quantities. Two-grid method was first proposed by professor Xu [6, 7]. The theoretical framework and basic tools of FVE method and two-grid method have developed rapidly [8–26]. In [27–29], a two-grid finite element scheme was proposed for solving the nonlinear Schrödinger equation.

For the problem (1.1), Zhang et al. [30] constructed semi-discrete two grid finite element scheme and performed the corresponding convergence analysis. Afterwards, Tian [31] and Wang [32] solved this problem by backward Euler and Crank-Nicolson finite element methods respectively and obtained the optimal error estimates. By now, the Schrödinger equation is mainly studied by spectral method, finite element method and finite difference method. Considering the advantages of FVE method and two grid method, we want to apply them to investigate the Schrödinger problem.

In this paper, we use the finite volume element method and Crank-Nicolson scheme in space and time respectively to solve the linear Schrödinger equation. Furthermore, the corresponding error estimates are analyzed by using elliptic projection operator. At the same time, we propose a two-grid finite volume element decoupling algorithm for the Schrödinger equation and derive the corresponding error estimate. With this decoupling algorithm, the solution of the original coupling problem is simplified to the solution of the same problem on a much coarser grid together with the solutions of two Poisson problems on the fine grid. It is worth noting that the two-grid algorithm can still maintain good approximation accuracy under the coarse grid which is much coarser than the fine grid.

The rest of this paper is organized as follows. In Section 2, we recall some notations and present finite volume element scheme for the time-dependent Schrödinger equation (1.1). Section 3 is devoted to provide the error estimates of FVE method by an elliptic projection operator. The two-grid FVE decoupling algorithm for the Schrödinger equation is developed in Section 4 and the optimal error estimates in the H^1 norm are also derived. Finally, two numerical examples are presented in Section 5 to validate the established theoretical findings.