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Two-Grid Finite Element Method with Crank-Nicolson Fully Discrete Scheme for the Time-Dependent Schrödinger Equation

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Abstract. In this paper, we study the Crank-Nicolson Galerkin finite element method and construct a two-grid algorithm for the general two-dimensional time-dependent Schrödinger equation. Firstly, we analyze the superconvergence error estimate of the finite element solution in H^1 norm by use of the elliptic projection operator. Secondly, we propose a fully discrete two-grid finite element algorithm with Crank-Nicolson scheme in time. With this method, the solution of the Schrödinger equation on a fine grid is reduced to the solution of original problem on a much coarser grid together with the solution of two Poisson equations on the fine grid. Finally, we also derive error estimates of the two-grid finite element solution with the exact solution in H^1 norm. It is shown that the solution of two-grid algorithm can achieve asymptotically optimal accuracy as long as mesh sizes satisfy $H = \mathcal{O}(h^{\frac{1}{2}})$.

AMS subject classifications: 65M15, 65M55, 65M60

Key words: Schrödinger equations, two-grid algorithms, Crank-Nicolson scheme, finite element method.

1. Introduction

The Schrödinger equation is a fundamental equation in quantum mechanics which can describe many physical phenomena in plasma physics, optics and water waves. In this paper, we consider the following initial boundary value problem of the two-dimensional time-dependent Schrödinger equation:

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

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where $\Omega \subset R^2$ is a convex polygonal domain with smooth boundary $\partial\Omega$, functions $f(\mathbf{x},t)$ and unknown function $u(\mathbf{x},t)$ are complex-valued, Δ is the usual Laplace operator, $u_0(\mathbf{x})$ is a smooth given complex-valued function, the potential function $V(\mathbf{x},t)$ is real-valued and non-negative for all $(\mathbf{x},t) \in \Omega \times [0,T]$, functions $V(\mathbf{x},t)$, $V_t(\mathbf{x},t)$ and $V_{tt}(\mathbf{x},t)$ are bounded for all $(\mathbf{x},t) \in \Omega \times [0,T]$, and i is the complex unit with $i = \sqrt{-1}$.

Numerical methods for the Schrödinger equation have been studied extensively, such as spectral method [1–4], finite element method [5–18], local discontinuous Galerkin method [19–21], finite difference method [22–24], and others [25, 26]. Huang et al. [2] applied the time-splitting Fourier pseudospectral method on the generalized sparse grids to solve the space-fractional Schrödinger equation. Akrivis et al. [5] approximated the solutions of a nonlinear Schrödinger equations by two Crank-Nicolson fully discrete finite element schemes. Shi and Wang [12] studied a linearized Crank-Nicolson Galerkin finite element method with bilinear element for nonlinear Schrödinger equation. Wang and Chen [16] analyzed the superconvergence result for a two-dimensional time-dependent linear Schrödinger equation with the finite element method. Xu and Shu [21] developed a local discontinuous Galerkin method to solve the generalized nonlinear Schrödinger equation and the coupled nonlinear Schrödinger equation. Bao and Cai [22] establish uniform error estimates of finite difference methods for the nonlinear Schrödinger equation (NLS) perturbed by the wave operator (NLSW) with a perturbation strength described by a dimensionless parameter ε ($\varepsilon \in (0,1]$).

Two-grid method is proposed by Xu [27–29] as a discretization method for nonsymmetric, indefinite and nonlinear partial differential equations. Huang et al. [30,31] proposed the multi-level iterative method for solving finite element equations of nonlinear elliptic problems. Chen et al. [33–35] applied this method to reaction-diffusion equations and miscible displacement problem. Bi et al. [36] considered two-grid finite element methods for nonlinear elliptic problems. Hou et al. [37] investigated a two grid discretization scheme for semilinear parabolic integro-differential equations by expanded mixed finite element methods. Zhou et al. [38, 39] proposed two-grid algorithms for solving Cahn-Hilliard equation and Maxwell eigenvalue problem. Xu and Zhou [40, 41] extended two-grid method to other problems. Especially, two-grid method was used for solving the Schrödinger equations [42–48]. Jin et al. [42] firstly proposed a two-grid finite element method for solving coupled partial differential equations, e.g., the Schrödinger-type equation. With this method, the solution of the coupled equations on a fine grid is reduced to the solution of coupled equations on a much coarser grid together with the solution of two Poisson equations on the same fine grid. Chien et al. [43] studied efficient two-grid discretization schemes with two-loop continuation algorithms for computing wave functions of two-coupled nonlinear Schrödinger equations defined on the unit square and the unit disk. Jin et al. [48] constructed semi-discrete two-grid finite element schemes which were proved to be convergent with an optimal convergence order, and constructed full-discrete two-grid finite element schemes with applying the Crank-Nicolson scheme for the time discretization which were verified only by a numerical example.