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Two-Grid Finite-Element Method for the Two-Dimensional Time-Dependent Schrödinger Equation

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Abstract. In this paper, we construct semi-discrete two-grid finite element schemes and full-discrete two-grid finite element schemes for the two-dimensional time-dependent Schrödinger equation. The semi-discrete schemes are proved to be convergent with an optimal convergence order and the full-discrete schemes, verified by a numerical example, work well and are more efficient than the standard finite element method.

AMS subject classifications: 65N30, 65N55

Key words: Schrödinger equation, two-grid method, finite element method.

1 Introduction

In physics, especially quantum mechanics, the Schrödinger equation is used to describe how the quantum state of a physical system changes in time [1]. Currently, this equation is widely applied in many areas, for example in optics [2], seismic wave propagation [3] and Bose-Einstein condensation [4]. For simplification, we consider the following initial-boundary value problem of Schrödinger equation:

$$
\begin{aligned}
&iu_t(\mathbf{x},t)=-\frac{1}{2}\triangle u(\mathbf{x},t)+V(\mathbf{x},t)u(\mathbf{x},t)+f(\mathbf{x},t), && \forall\mathbf{x}\in\Omega, \quad 0<t\leq T, && (1.1a)\\
&u(\mathbf{x},t)=0, && \text{on } \partial\Omega, \quad 0<t\leq T, && (1.1b)\\
&u(\mathbf{x},0)=u_0(\mathbf{x}), && \forall\mathbf{x}\in\bar{\Omega}, && (1.1c)
\end{aligned}
$$

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where $\Omega \in R^2$ is a convex polygonal domain, $u_0(\mathbf{x})$, $f(\mathbf{x},t)$ and unknown function $u(\mathbf{x},t)$ are complex-valued functions, the potential function $V(\mathbf{x},t)$ is a non-negative function and $V(\mathbf{x},t)$, $V_t(\mathbf{x},t)$, $V_{tt}(\mathbf{x},t)$ are bounded for $\mathbf{x} \in \Omega$, $0 \le t \le T$. For any complex-valued function w, we denote its real part by w_1, the imaginary part by w_2. Then problem (1.1a)-(1.1b) is equivalent to the following coupled equations:

$$
\begin{aligned}
&u_{1t}(\mathbf{x},t) = -\frac{1}{2}\triangle u_2(\mathbf{x},t) + V(\mathbf{x},t)u_2(\mathbf{x},t) + f_2(\mathbf{x},t), && \forall \mathbf{x} \in \Omega, && 0 < t \le T,\\
&u_{2t}(\mathbf{x},t) = \frac{1}{2}\triangle u_1(\mathbf{x},t) - V(\mathbf{x},t)u_1(\mathbf{x},t) - f_1(\mathbf{x},t), && \forall \mathbf{x} \in \Omega, && 0 < t \le T,\\
&u_j(\mathbf{x},t) = 0, \quad j = 1,2, && \forall \mathbf{x} \text{ on } \partial\Omega, && 0 < t \le T.
\end{aligned}
$$

Numerically solving the time-dependent Schrödinger equation has been studied in many literature, e.g., in [5–7], where the approaches were designed for solving the original problem directly. However, as we know, the Schrödinger equation is actually a coupled system of partial differential equations, so it may be costly to solve the original problem directly. In this paper, we apply the two-grid discretization method to numerically solve the time-dependent Schrödinger equation.

The idea of the two-grid discretization method was originally proposed by Xu in [8–10] for discretizing nonsymmetric and indefinite partial differential equations and then was used for linearization for nonlinear problems [9–11], for localization and parallelization for solving a large class of partial differential equations [12–14], for decoupling the coupled system of partial differential equations [15]. The application areas of this method include nonlinear elasticity problems [16], Navier-Stokes problems [17], stationary MHD equations [18], reaction diffusion equations [19] and so on. As to solving the coupled system of partial differential equations by two-grid method, the first work was done by Jin et al. [15] in 2006. They extended the idea of two-grid finite element method to solving the steady-state Schrödinger equation by first discretizing the original problem on the coarse grid and then discretizing a decoupled system on the fine grid, so that the computational complexity of solving the Schrödinger equation is comparable to solving two decoupled Poisson equations on the same fine grid. Also, the convergence was analyzed. Later, Chien et al. [20] proposed 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, where the centered difference approximations, the six-node triangular elements and the Adini elements were employed for the spatial discretization, but did not give error estimates for the discrete solutions. Recently, Wu [21, 22] developed two-grid mixed finite element schemes for solving both steady state and unsteady state nonlinear Schrödinger equations, where the schemes were based on a mixed finite-element method and their error estimates were not given. In this paper, basing on a finite-element discretization, we extend the idea proposed in [15] to the case of the time-dependent Schrödinger equation (1.1a)-(1.1c) and construct the semi-discrete two-grid schemes and the full-discrete two-grid schemes. The semi-discrete schemes are proved to be convergent with a optimal convergence order and the full-discrete schemes,