Advances in Applied Mathematics and Mechanics
Adv. Appl. Math. Mech., Vol. **5**, No. 2, pp. 180-193

DOI: 10.4208/aamm.12-m1206
April 2013

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

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Received 18 January 2012; Accepted (in revised version) 28 August 2012

Available online 22 February 2013

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:

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

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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, verified by a numerical example, work well and are more efficient than the standard finite element method.

The rest of the paper is organized as follows: in Section 2, we propose the semi-discrete finite element method for the Schrödinger equation and then analyse the semi-discrete finite element approximation. In Section 3, we construct semi-discrete two-grid finite element schemes and full-discrete two-grid finite element schemes and estimate the error of the semi-discrete schemes. In Section 4, we demonstrate a numerical example to verify the effectiveness of the full-discrete schemes.

2 The semi-discrete finite element approximation

Let $Q_T=\Omega\times[0,T]$. For any complex-valued function $w(\mathbf{x})$ and $v(\mathbf{x})$, let (w,v) denote the inner product

$$(w,v)=\int_\Omega w\bar{v}d\mathbf{x},$$

and $\|w\|$ denote the corresponding norm

$$\|w\|=\sqrt{(w,w)},$$

where $\bar{v}$ denotes the complex conjugate of v. We introduce the complex-valued function spaces

$$\begin{aligned}&H^1(Q_T)=\{w(\mathbf{x},t)|w,w_t,w_{x_1},w_{x_2}\in L^2(Q_T)\},\\&S=\{w(\mathbf{x},t)|w\in H^1(Q_T),\ \ w|_{\partial\Omega}=0\},\end{aligned}$$

and the standard Sobolev space $H^m(\Omega)$ with a norm given by

$$\|\phi\|_m=\Big(\sum_{|\alpha|\le m}\|D^\alpha\phi\|^2\Big)^{\frac{1}{2}}$$

for any $\phi\in H^m(\Omega)$. Then $u(\mathbf{x},t)$, the weak solution of problem (1.1a)-(1.1c) is defined as follows: find $u(\mathbf{x},t)\in S$ such that for any $v\in S$ and nearly all $t\in(0,T]$

$$i(u_t,v)=a(u,v)+(f,v),\quad u(\mathbf{x},0)=u_0(\mathbf{x}),\quad \mathbf{x}\in\bar{\Omega},\tag{2.1}$$

where $a(u,v)=(\nabla u,\nabla v)/2+(Vu,v)$.

Let T_h be a quasi-uniform quadrilateral or trilateral partition of Ω with meshsize $h>0$, $S_h\subset S$ be the corresponding piecewise linear finite element space, $\tau=T/N$ be the time step size, N be a positive integer and $t_n=n\tau$ $(n=0,1,\cdots,N)$ be the time discrete point. For any function $w(\mathbf{x},t)$, $v(\mathbf{x},t)$ and function series $\{w^n(\mathbf{x})\}_{n=0}^N$, we introduce the notations:

$$
\begin{aligned}
&w_n = w(\mathbf{x},t_n), && \hat{w}_n = \frac{1}{2}(w_n + w_{n-1}),\\
&\hat{w}^n = \frac{1}{2}(w^n + w^{n-1}), && d_t w^n = \frac{1}{\tau}(w^n - w^{n-1}),\\
&a_n(w,v) = \frac{1}{2}(\nabla w, \nabla v) + (\hat{V}_n w, v).
\end{aligned}
$$

Notice that $a(w,v)$ is bounded and coercive on $S\times S$, so for any fixed $t\in[0,T]$ and given $w\in S$, we can define its elliptic projection $P_h w\in S_h$ such that

$$a(P_h w, v_h) = a(w, v_h), \quad \forall v_h \in S_h. \tag{2.2}$$

Now, we can define the semi-discrete finite element solution $u_h(\mathbf{x},t)$ of problem (1.1a)-(1.1c) as follows: find $u_h\in S_h$ such that for any $v_h\in S_h$ and nearly all $t\in(0,T]$

$$i((u_h)_t, v_h) = a(u_h, v_h) + (f, v_h), \tag{2.3a}$$
$$u_h(\mathbf{x},0) = P_h u_0 \tag{2.3b}$$

or

$$u_h(\mathbf{x},0) = u_{0,I}, \tag{2.3c}$$

where $u_{0,I}\in S_h$ is the interpolating function of u_0. Also, we can define the full-discrete finite element solution series $\{u_h^n(\mathbf{x})\}_{n=0}^N$ of problem (1.1a)-(1.1c) as follows: find $\{u_h^n(\mathbf{x})\}_{n=0}^N \subset S_h$ such that

$$i(d_t u_h^n, v_h) = a_n(\hat{u}_h^n, v_h) + (\hat{f}_n, v_h), \quad \forall v_h \in S_h, \quad n = 1,2,\cdots,N, \tag{2.4a}$$
$$u_h^0 = P_h u_0 \tag{2.4b}$$

or

$$u_h^0 = u_{0,I}. \tag{2.4c}$$

For simplicity, let the notation "$\lesssim$" be equivalent to "$\le C$" for some positive constant C. We introduce the following lemmas:

Lemma 2.1. *If for any $t\in[0,T]$, $w(\mathbf{x},t)$, $w_t(\mathbf{x},t)\in H^2(\Omega)$, then $P_h w(\mathbf{x},t)$ has the estimates:*

$$\|w - P_h w\|_s \lesssim h^{2-s}\|w\|_2, \qquad s = 0,1, \tag{2.5a}$$
$$\|(w - P_h w)_t\|_s \lesssim h^{2-s}(\|w\|_2 + \|w_t\|_2), \qquad s = 0,1. \tag{2.5b}$$

Proof. Similar to the proof of Lemma 3 in [6]. □

Lemma 2.2. *If for any $t\in[0,T]$, $w(\mathbf{x},t),w_t(\mathbf{x},t),w_{tt}(\mathbf{x},t)\in H^2(\Omega)$, then*

$$\|(w-P_hw)_{tt}\|_s \lesssim h^{2-s}(\|w\|_2+\|w_t\|_2+\|w_{tt}\|_2),\quad s=0,1. \tag{2.6}$$

Proof. Let

$$\rho=w-P_hw,\qquad \rho_{tt}=E_{11}+E_{22},$$

where

$$E_{11}=w_{tt}-P_hw_{tt},\qquad E_{22}=P_hw_{tt}-\frac{\partial^2}{\partial t^2}P_hw.$$

For any $t\in[0,T]$ and $\chi\in S_h$, from (2.2), we get

$$\begin{aligned} a(E_{22},\chi)=&a(\rho_{tt}-E_{11},\chi)=a(\rho_{tt},\chi)\\ =&\frac{d^2}{dt^2}a(\rho,\chi)-(V_{tt}\rho,\chi)-2(V_t\rho_t,\chi)\\ =&-(V_{tt}\rho,\chi)-2(V_t\rho_t,\chi). \end{aligned}$$

Taking $\chi=E_{22}$, we have

$$\|E_{22}\|_1^2\lesssim a(E_{22},E_{22})\lesssim(\|\rho\|+\|\rho_t\|)\|E_{22}\|,$$

which implies that

$$\|E_{22}\|_1\lesssim\|\rho\|+\|\rho_t\|.$$

From (2.5a) and (2.5b), we get

$$\|E_{22}\|_1\lesssim h^2(\|w\|_2+\|w_t\|_2). \tag{2.7}$$

Therefore, (2.6) follows from (2.5a) and (2.7). ☐

Lemma 2.3. *If for any $t\in[0,T]$, $u,u_t,u_{tt}\in H^2(\Omega)$, then u_h, the finite element solution defined in* (2.3a) *and* (2.3b) *has the estimates:*

$$\|P_hu-u_h\|\lesssim h^2, \tag{2.8a}$$
$$\|(P_hu-u_h)_t\|\lesssim h^2. \tag{2.8b}$$

Also, if $u_0\in H^2(\Omega)$, then u_h, the finite element solution defined in (2.3a) *and* (2.3c) *has the estimate:*

$$\|P_hu-u_h\|\lesssim h^2. \tag{2.9}$$

Proof. From (2.1) and (2.3a), we can get

$$i((u-u_h)_t,v_h)=a(u-u_h,v_h),\quad \forall v_h\in S_h. \tag{2.10}$$

Let

$$u-u_h=\rho+\theta$$

with

$$\rho = u - P_h u, \qquad \theta = P_h u - u_h,$$

then

$$i(\rho_t + \theta_t, v_h) = a(\rho + \theta, v_h).$$

From (2.2), it is easy to obtain

$$i(\theta_t, v_h) - a(\theta, v_h) = -i(\rho_t, v_h). \tag{2.11}$$

Taking $v_h = \theta$ in (2.11) and noticing that

$$\frac{d}{dt}\|\theta\|^2 = (\theta_t, \theta) + (\theta, \theta_t) = 2Re\{(\theta_t, \theta)\},$$

we have

$$\begin{aligned}\frac{1}{2}\frac{d}{dt}\|\theta\|^2 &= Re\{(\theta_t, \theta)\} = Im\{a(\theta, \theta)\} - Re\{(\rho_t, \theta)\} \\ &= -Re\{(\rho_t, \theta)\} \lesssim \|\rho_t\| \cdot \|\theta\|,\end{aligned}$$

which implies that

$$\frac{d}{dt}\|\theta\| \lesssim \|\rho_t\|. \tag{2.12}$$

By integral and (2.12), we see that

$$\|\theta(\cdot,t)\| - \|\theta(\cdot,0)\| \lesssim h^2 \int_0^T (\|u\|_2 + \|u_t\|_2) dt. \tag{2.13}$$

If $u_h(\mathbf{x},0)$ satisfies (2.3b), then

$$\theta(\cdot,0) = 0. \tag{2.14}$$

If $u_h(\mathbf{x},0)$ satisfies (2.3c), then

$$\|\theta(\cdot,0)\| \le \|u_0 - P_h u\| + \|u_0 - u_{0,I}\| \lesssim h^2 \|u_0\|_2. \tag{2.15}$$

Therefore, (2.8a) and (2.9) follow from (2.13), (2.14) and (2.15). Next we show the validity of (2.8b).

Taking $v_h = \theta_t(\cdot,0)$ in (2.11) with $t = 0$ and using (2.14), we have

$$\|\theta_t(\cdot,0)\| \lesssim \|\rho_t(\cdot,0)\|. \tag{2.16}$$

In addition, by the partial derivative of (2.11) with $v_h = \theta_t$, we get

$$i(\theta_{tt}, \theta_t) - a(\theta_t, \theta_t) - (V_t \theta, \theta_t) = -i(\rho_{tt}, \theta_t).$$

Noticing that

$$\frac{d}{dt}\|\theta_t\|^2 = 2Re\{(\theta_{tt},\theta_t)\},$$

we obtain

$$\begin{aligned}\frac{d}{dt}\|\theta_t\|^2 &= 2Im\{a(\theta_t,\theta_t)+(V_t\theta,\theta_t)\} - 2Re\{(\rho_{tt},\theta_t)\}\\ &= 2Im\{(V_t\theta,\theta_t)\} - 2Re\{(\rho_{tt},\theta_t)\}\\ &\lesssim \|\theta\|\|\theta_t\| + \|\rho_{tt}\|\|\theta_t\|,\end{aligned}$$

thus

$$\frac{d}{dt}\|\theta_t\| \lesssim \|\theta\| + \|\rho_{tt}\|.$$

From (2.13) and (2.6), it is easy to obtain

$$\frac{d}{dt}\|\theta_t\| \lesssim h^2,$$

thus

$$\|\theta_t(\cdot,t)\| \lesssim \|\theta_t(\cdot,0)\| + h^2. \tag{2.17}$$

Therefore, (2.8b) follows from (2.17), (2.16) and (2.5b). □

Lemma 2.4. *If for any $t\in[0,T]$, $u,u_t\in H^4(\Omega)$, $u_{tt}\in H^3(\Omega)$, then u_h, the bilinear finite element solution defined in* (2.3a) *and* (2.3c) *has the estimates:*

$$\|u_I - u_h\| \lesssim h^2, \tag{2.18a}$$

$$\|(u_I - u_h)_t\| \lesssim h^2, \tag{2.18b}$$

where u_I is the corresponding interpolating function of u.

Proof. Let

$$u - u_h = (u-u_I)+\eta,$$

with $\eta = u_I - u_h$, then from (2.10), we get

$$\begin{aligned}i(\eta_t,v_h) =& \frac{1}{2}(\nabla\eta,\nabla v_h)+(V\eta,v_h) - i((u-u_I)_t,v_h)\\ &+\frac{1}{2}(\nabla(u-u_I),\nabla v_h)+(V(u-u_I),v_h).\end{aligned} \tag{2.19}$$

Taking $v_h=\eta$ in (2.19), then

$$\begin{aligned}i(\eta_t,\eta) =& \frac{1}{2}(\nabla\eta,\nabla\eta)+(V\eta,\eta) - i((u-u_I)_t,\eta)\\ &+\frac{1}{2}(\nabla(u-u_I),\nabla\eta)+(V(u-u_I),\eta).\end{aligned}$$

Noticing that

$$\frac{1}{2}\frac{d}{dt}\|\eta\|^2 = Re\{(\eta_t,\eta)\},$$

we obtain

$$\frac{1}{2}\frac{d}{dt}\|\eta\|^2 = -Re\{((u-u_I)_t,\eta)\} + Im\Big\{\frac{1}{2}(\nabla(u-u_I),\nabla\eta) + (V(u-u_I),\eta)\Big\}.$$

Now, we introduce the following estimates given in [23].

$$|((u-u_I)_t,v)| \lesssim ch^2\|u_t\|_3\|v\|, \qquad \forall v\in S_h, \tag{2.20a}$$

$$|(\nabla(u-u_I),\nabla v)| \lesssim ch^2\|u\|_4\|v\|, \qquad \forall v\in S_h. \tag{2.20b}$$

Then from the above inequalities, we can get

$$\frac{d}{dt}\|\eta\| \lesssim h^2(\|u_t\|_3 + \|u\|_4),$$

which implies that

$$\|\eta\| \lesssim \|\eta(\cdot,0)\| + h^2\int_0^T (\|u_t\|_3 + \|u\|_4)dt.$$

Noticing that $\eta(\cdot,0)=0$, therefore, (2.18a) holds. Next we show the validity of (2.18b).

Taking $v_h=\eta_t(\cdot,0)$ in (2.19) with $t=0$, then from (2.20a) and (2.20b), we get

$$\|\eta_t(\cdot,0)\|^2 \lesssim h^2(\|u_t(\cdot,0)\|_3 + \|u(\cdot,0)\|_4)\|\eta_t(\cdot,0)\|,$$

thus

$$\|\eta_t(\cdot,0)\| \lesssim h^2. \tag{2.21}$$

In addition, by the partial derivative of (2.19) with $v_h=\eta_t$, we can obtain

$$\begin{aligned} i(\eta_{tt},\eta_t) =& \frac{1}{2}(\nabla\eta_t,\nabla\eta_t) + (V_t\eta,\eta_t) + (V\eta_t,\eta_t) - i((u-u_I)_{tt},\eta_t) \\ &+ \frac{1}{2}(\nabla((u-u_I)_t),\nabla\eta_t) + (V_t(u-u_I),\eta_t) + (V(u-u_I)_t,\eta_t). \end{aligned}$$

Noticing that $d\|\eta_t\|^2/dt = 2Re\{(\eta_{tt},\eta_t)\}$, we have

$$\begin{aligned} \frac{1}{2}\frac{d}{dt}\|\eta_t\|^2 =& Im\{(V_t\eta,\eta_t)\} - Re\{((u-u_I)_{tt},\eta_t)\} + \frac{1}{2}Im\{(\nabla((u-u_I)_t),\eta_t)\} \\ &+ Im\{(V_t(u-u_I),\eta_t) + (V(u-u_I)_t,\eta_t)\}. \end{aligned}$$

From (2.18a), (2.20a) and (2.20b), we get

$$\frac{d}{dt}\|\eta_t\| \lesssim h^2. \tag{2.22}$$

Therefore, (2.18b) follows from (2.21) and (2.22). $\square$

Theorem 2.1. *If for any $t\in[0,T]$, $u,u_t\in H^2(\Omega)$, then u_h, the finite element solution defined in* (2.3a) *and* (2.3b) *has the estimate:*

$$\|u-u_h\|_s \lesssim h^{2-s}, \quad s=0,1. \tag{2.23}$$

Proof. Noticing that

$$\|u-u_h\|_s \lesssim \|u-P_hu\|_s+\|P_hu-u_h\|_s,$$

therefore, (2.23) follows from (2.5a), (2.8a) and the well-known inverse inequality. □

Similar to the Theorem 2.1, we have the following theorem:

Theorem 2.2. *If for any $t\in[0,T]$, $u,u_t\in H^4(\Omega)$, $u_{tt}\in H^3(\Omega)$, then u_h, the bilinear finite element solution defined in* (2.3a) *and* (2.3c) *has the estimate:*

$$\|u-u_h\|_s \lesssim h^{2-s}, \quad s=0,1. \tag{2.24}$$

Proof. Noticing that

$$\|u-u_h\|_s \lesssim \|u-u_I\|_s+\|u_I-u_h\|_s,$$

therefore, (2.24) follows from (2.18a), (2.20b) and the well-known inverse inequality. □

3 The two-grid finite element schemes

In order to reduce the computational cost, following Jin et al. [15], we construct the following two-grid finite element schemes for problem (1.1a)-(1.1c). The basic ingredient in our approach is another finite element space S_H $(\subset S_h\subset S)$ defined on a coarser quasi-uniform quadrilateral or trilateral partition of Ω with mesh size $H>h>0$.

By the different initial value (2.3b) and (2.3c), we first construct and analyse the following semi-discrete two-grid finite element algorithms:

Algorithm 3.1: Semi-discrete two-grid finite element scheme with projection initial value

---

Step 1: Find $u_H\in S_H$ such that

$$\begin{cases} i((u_H)_t,v_H)=\frac{1}{2}(\nabla u_H,\nabla v_H)+(Vu_H,v_H)+(f,v_H), & \forall v_H\in S_H, \quad t>0,\\ u_H(\mathbf{x},0)=P_Hu_0(\mathbf{x})\in S_H. \end{cases}$$

Step 2: Find $u_h^s\in S_h$ such that

$$\begin{cases} \frac{1}{2}(\nabla u_h^s,\nabla v_h)=i((u_H)_t,v_h)-(Vu_H,v_h)-(f,v_h), & \forall v_h\in S_h, \quad t>0,\\ u_h^s(\mathbf{x},0)=P_hu_0(\mathbf{x})\in S_h. \end{cases} \tag{3.1}$$

Algorithm 3.2: Semi-discrete two-grid finite element scheme with interpolating initial value

---

Step 1: Find $u_H \in S_H$ such that

$$\begin{cases} i((u_H)_t, v_H) = \frac{1}{2}(\nabla u_H, \nabla v_H) + (V u_H, v_H) + (f, v_H), \quad \forall v_H \in S_H, \quad t > 0, \\ u_H(\mathbf{x}, 0) = u_{0,I}(\mathbf{x}) \in S_H. \end{cases}$$

Step 2: Find $u_h^s \in S_h$ such that

$$\begin{cases} \frac{1}{2}(\nabla u_h^s, \nabla v_h) = i((u_H)_t, v_h) - (V u_H, v_h) - (f, v_h), \quad \forall v_h \in S_h, \quad t > 0, \\ u_h^s(\mathbf{x}, 0) = u_{0,I}(\mathbf{x}) \in S_h. \end{cases}$$

Theorem 3.1. *If for any $t \in [0,T]$, $u, u_t, u_{tt} \in H^2(\Omega)$, then u_h^s, the two-grid solution defined in Algorithm* 3.1 *has the estimates:*

$$\|u_h - u_h^s\|_1 \lesssim H^2, \tag{3.2a}$$

$$\|u - u_h^s\|_1 \lesssim h + H^2, \tag{3.2b}$$

where u_h is the finite element solution defined in (2.3a) *and* (2.3b).

Proof. From (2.3a) and (3.1), we get

$$\frac{1}{2}(\nabla(u_h - u_h^s), \nabla v_h) = i((u_h - u_H)_t, v_h) - (V(u_h - u_H), v_h), \quad \forall v_h \in S_h,$$

which, by taking $v_h = u_h - u_h^s$, gives

$$|u_h - u_h^s|_1^2 \lesssim (\|(u_h - u_H)_t\| + \|u_h - u_H\|)\|u_h - u_h^s\|.$$

From Friechriechs inequality $\|u_h - u_h^s\|_{1,\Omega} \lesssim |u_h - u_h^s|_{1,\Omega}$, we obtain

$$\|u_h - u_h^s\|_1 \lesssim \|(u_h - u_H)_t\| + \|u_h - u_H\|. \tag{3.3}$$

In addition, from (2.5b) and (2.8b), we see that

$$\|(u - u_h)_t\| \lesssim \|(u - P_h u)_t\| + \|(P_h u - u_h)_t\| \lesssim h^2,$$

which implies that

$$\|(u - u_H)_t\| \lesssim H^2. \tag{3.4}$$

So, (3.2a) follows from (2.23), (3.3), (3.4). And (3.2b) follows from (2.23), (3.2a). □

Theorem 3.2. *If for any $t \in [0,T]$, $u, u_t \in H^4(\Omega)$, $u_{tt} \in H^3(\Omega)$, then u_h^s, the two-grid bilinear finite element solution defined in Algorithm* 3.2 *has the estimates:*

$$\|u_h - u_h^s\|_1 \lesssim H^2, \tag{3.5a}$$

$$\|u - u_h^s\|_1 \lesssim h + H^2, \tag{3.5b}$$

where u_h is the bilinear finite element solution defined in (2.3a) *and* (2.3c).

Proof. Following the idea in proof of Theorem 3.1, inequality (3.3) also holds in this case.

In addition, from (2.18b) and (2.20a), we have

$$\|(u-u_h)_t\| \le \|(u-u_I)_t\| + \|(u_I-u_h)_t\| \lesssim h^2, \tag{3.6}$$

which implies that

$$\|(u-u_H)_t\| \lesssim H^2. \tag{3.7}$$

Therefore, (3.5a) follows from (2.24), (3.3), (3.6) and (3.7). And (3.5b) follows from (2.24) and (3.5a). ☐

Finally, by applying the Crank-Nicolson scheme for the time discretization, we propose the full-discrete two-grid finite element algorithms as follows:

Algorithm 3.3: Full-discrete two-grid finite element scheme with projection initial value

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Step 1: Find $\{u_H^n\}_{n=0}^N \subset S_H$ such that

$$\begin{cases} i(d_t u_H^n, v_H) = \frac{1}{2}(\nabla \hat{u}_H^n, \nabla v_H) + (\hat{V}_n \hat{u}_H^n, v_H) + (\hat{f}_n, v_H), \quad \forall v_H \in S_H, \ \ t>0, \ \ n=1,2,\cdots,N, \\ u_H^0 = P_H u_0 \in S_H. \end{cases}$$

Step 2: Find $\{u_h^{*n}\}_{n=0}^N \subset S_h$ such that

$$\begin{cases} \frac{1}{2}(\nabla \hat{u}_h^{*n}, \nabla v_h) = i(d_t u_H^n, v_h) - (\hat{V}_n \hat{u}_H^n, v_h) - (\hat{f}_n, v_h), \quad \forall v_h \in S_h, \ \ t>0, \ \ n=1,2,\cdots,N, \\ u_h^{*0} = P_h u_0 \in S_h. \end{cases}$$

Algorithm 3.4: Full-discrete two-grid finite element scheme with interpolating initial value

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Step 1: Find $\{u_H^n\}_{n=0}^N \subset S_H$ such that

$$\begin{cases} i(d_t u_H^n, v_H) = \frac{1}{2}(\nabla \hat{u}_H^n, \nabla v_H) + (\hat{V}_n \hat{u}_H^n, v_H) + (\hat{f}_n, v_H), \quad \forall v_H \in S_H, \ \ t>0, \ \ n=1,2,\cdots,N, \\ u_H^0 = u_{0,I} \in S_H. \end{cases}$$

Step 2: Find $\{u_h^{*n}\}_{n=0}^N \subset S_h$ such that

$$\begin{cases} \dfrac{1}{2}(\nabla \hat{u}_h^{*n}, \nabla v_h) = i(d_t u_H^n, v_h) - (\hat{V}_n \hat{u}_H^n, v_h) - (\hat{f}_n, v_h), \quad \forall v_h \in S_h, \ \ t>0, \ \ n=1,2,\cdots,N, \\ u_h^{*0} = u_{0,I} \in S_h. \end{cases}$$

We note that the linear system in Step 2 both in Algorithms 3.3 and 3.4 is a decoupled system which involves only two separate Poisson equations and only on the coarser space a coupled system needs to be solved in Step 1. As a result, the computational complexity of solving problem (1.1a)-(1.1c) is comparable to solving two decoupled Poisson equations on the same fine grid.

4 Numerical example

In this section, we carry out a numerical example to demonstrate the efficiency of Algorithms 3.3 and 3.4.

For problem (1.1a)-(1.1c), let $V(\mathbf{x},t)=1$, $\Omega=[0,1]\times[0,1]$, $T=20$ second and f be so chosen that

$$u=e^{3t}(1-x_1)(1-x_2)\sin(x_1x_2)+i(1-x_1)x_2t\sin(x_1(1-x_2))$$

is the exact solution.

Ω is uniformly divided into families T_H and T_h of quadrilaterals and $S_H,S_h\subset S$ are bilinear finite element spaces defined on T_H, T_h, respectively. For the full-discrete two-grid methods, we solve the original problem by the conjugate gradient method on the coarse grid and solve the modified fine grid equation by multigrid method on the fine grid. For $h=H^2$, $\tau=H$, $N=T/\tau$ and $H=1/4$, $1/8$, $1/16$, $\{u_h^{*n}\}_{n=0}^N$ are computed by Algorithm 3.3 and Algorithm 3.4 respectively and $\{u_h^n\}_{n=0}^N$, the full-discrete standard finite element solution, are computed by (2.4a). From the numerical results at $t=20$s listed in Tables 1 and 2, we can see that

$$\frac{\|u-u_h^N\|_1}{\|u\|_1}\approx\mathcal{O}(h) \quad \text{and} \quad \frac{\|u-u_h^{*N}\|_1}{\|u\|_1}\approx\mathcal{O}(H^2)(\approx\mathcal{O}(h)),$$

and the two-grid finite element method is more efficient than the standard finite element method on running CPU time.

If the domain Ω is uniformly divided into families T_H and T_h of triangulation meshes, we can get the same conclusions from the Tables 3 and 4.

Table 1: Numerical results of the Algorithm 3.3 on quadrilateral meshes.

mesh	$\frac{\|u-u_h^N\|_1}{\|u\|_1}$	ratio	cpu time (s)	$\frac{\|u-u_h^{*N}\|_1}{\|u\|_1}$	ratio	cpu time (s)
$h=1/16$	6.18E-2		2.35	6.87E-2		1.62
$h=1/64$	1.54E-2	4.01	145.66	1.71E-2	4.02	44.98
$h=1/256$	3.84E-3	4.01	44133.76	4.27E-3	4.01	1535.90

Table 2: Numerical results of the Algorithm 3.4 on quadrilateral meshes.

mesh	$\frac{\|u-u_h^N\|_1}{\|u\|_1}$	ratio	cpu time (s)	$\frac{\|u-u_h^{*N}\|_1}{\|u\|_1}$	ratio	cpu time (s)
$h=1/16$	6.18E-2		2.36	6.87E-2		1.62
$h=1/64$	1.54E-2	4.01	145.19	1.71E-2	4.02	45.15
$h=1/256$	3.84E-3	4.01	48682.56	4.27E-3	4.01	1543.77

Table 3: Numerical results of the Algorithm 3.3 on triangulation meshes.

mesh	$\frac{\|u-u_h^N\|_1}{\|u\|_1}$	ratio	cpu time (s)	$\frac{\|u-u_h^{*N}\|_1}{\|u\|_1}$	ratio	cpu time (s)
$h=1/16$	9.93E-2		5.26	1.11E-1		3.97
$h=1/64$	2.48E-2	4.00	281.76	2.81E-2	3.95	100.63
$h=1/256$	6.18E-3	4.01	43478.90	7.04E-3	3.99	3593.79

Table 4: Numerical results of the Algorithm 3.4 on triangulation meshes.

mesh	$\frac{\|u-u_h^N\|_1}{\|u\|_1}$	ratio	cpu time (s)	$\frac{\|u-u_h^{*N}\|_1}{\|u\|_1}$	ratio	cpu time (s)
$h=1/16$	9.93E-2		2.32	1.11E-1		3.45
$h=1/64$	2.48E-2	4.00	142.89	2.81E-2	3.95	100.74
$h=1/256$	6.18E-3	4.01	44949.76	7.04E-3	3.99	3642.19

5 Conclusions

In this paper, we presented the semi-discrete two-grid finite element schemes and full-discrete two-grid finite element schemes for the time-dependent Schrödinger equation. We also provided the error analysis of the semi-discrete schemes and a numerical example of the full-discrete schemes. Numerical example showed that our two-grid schemes work well, give very good numerical results and partly verify the convergence results.

Acknowledgments

This work is supported by National Science Foundation of China (10971059), Young Scientists Foundation of the National Science Foundation of China (11101136), Hunan Provincial National Science Foundation of China (09JJ3007), Hunan Provincial Education Department Scientific Research Foundation of China (11C0411).

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