Applied Mathematics and Mechanics (English Edition)

https://doi.org/10.1007/s10483-018-2369-9

Superconvergence analysis of bi-k-degree rectangular elements for two-dimensional time-dependent Schrödinger equation[∗]

Jianyun WANG¹, Yanping CHEN^{2,†}

1. School of Science, Hunan University of Technology, Zhuzhou 412007, Hunan Province, China; 2. School of Mathematical Sciences, South China Normal University,

Guangzhou 510631, China

(Received Dec. 13, 2017 / Revised Apr. 20, 2018)

Abstract Superconvergence has been studied for long, and many different numerical methods have been analyzed. This paper is concerned with the problem of superconvergence for a two-dimensional time-dependent linear Schrödinger equation with the finite element method. The error estimate and superconvergence property with order $O(h^{k+1})$ in the $H¹$ norm are given by using the elliptic projection operator in the semi-discrete scheme. The global superconvergence is derived by the interpolation post-processing technique. The superconvergence result with order $O(h^{k+1} + \tau^2)$ in the \hat{H}^1 norm can be obtained in the Crank-Nicolson fully discrete scheme.

Key words superconvergence, elliptic projection, Schrödinger equation, interpolation post-processing

Chinese Library Classification O241.82 2010 Mathematics Subject Classification 65M12, 65M15, 65M60

1 Introduction

We shall consider a linear Schrödinger equation as follows. Let $\Omega \subset \mathbb{R}^2$ be a bounded rectangular-type domain with a smooth boundary $\partial\Omega$. We find a complex-valued function $u(x, t)$ defined on $\Omega \times [0, T]$ and satisfying

$$
\begin{cases}\ni u_t(\boldsymbol{x},t) = -\frac{1}{2}\Delta u(\boldsymbol{x},t) + V(\boldsymbol{x})u(\boldsymbol{x},t) + f(\boldsymbol{x},t) & \text{in} \quad \Omega \times [0,T], \\
u(\boldsymbol{x},t) = 0 & \text{on} \quad \partial\Omega \times [0,T], \\
u(\boldsymbol{x},0) = u_0(\boldsymbol{x}) & \text{in} \quad \Omega,\n\end{cases}
$$
\n(1)

where $u_0(x)$ is a given initial complex-valued function, and the trapping potential function $V(\boldsymbol{x})$ is non-negative bounded and real-valued.

The Schrödinger equation is an important equation in quantum mechanics. There are many numerical methods to solve the Schrödinger equation in the literature, such as the spectral

[∗] Citation: WANG, J. Y. and CHEN, Y. P. Superconvergence analysis of bi-k-degree rectangular elements for two-dimensional time-dependent Schrödinger equation. Applied Mathematics and Mechanics (English Edition), 39(9), 1353–1372 (2018) https://doi.org/10.1007/s10483-018-2369-9

[†] Corresponding author, E-mail: yanpingchen@scnu.edu.cn

Project supported by the National Natural Science Foundation of China (No. 11671157) c Shanghai University and Springer-Verlag GmbH Germany, part of Springer Nature 2018

method^[1–2], the finite difference method^[3–5], the finite element method^[6–12], the discontinuous Galerkin method^[13–15], and the local discontinuous Galerkin method^[16–18]. Bao et al.^[1] studied the performance of time-splitting spectral approximations for the general nonlinear Schrödinger equation in the semiclassical regimes. Han et al.^[5] introduced an artificial boundary condition to reduce the one-dimensional time-dependent Schrödinger equation into an initialboundary value problem in a finite computational domain. Antonopoulou et al.^[7] considered an initial and boundary-value problem for a general Schrödinger-type equation posed on a two space-dimensional noncylindrical domain with mixed boundary conditions. Karakashian and $Makridakis^[14]$ analyzed the convergence of the discontinuous Galerkin method for the nonlinear Schrödinger equation. Guo and $Xu^{[16]}$ presented a fully discrete scheme by discretizing the space with the local discontinuous Galerkin method and the time with the Crank-Nicholson scheme to simulate the multi-dimensional Schrödinger equation with wave operator.

Superconvergence has been studied for long. Many different numerical methods have been analyzed. It is a powerful tool to improve the approximation accuracy and efficiency. There are numerous studies by many famous scholars^[19–22]. At present, superconvergence results were obtained widely for elliptic, parabolic, Maxwell's equations, and optimal control problems^[23–31]. However, there were not many superconvergence results for the Schrödinger equation^[32–36]. In 1998, Lin and Liu^[32] studied a time-dependent linear Schrödinger equation and analyzed the superconvergence error results. In 2014, Shi et al.^[33] considered a nonlinear Schrödinger equation by the finite element method in the triangular anisotropic meshes and proved the superconvergence result in the semi-discrete scheme. Later, Wang et al.^[35] conducted the superconvergence analysis for a time-dependent Schrödinger equation by using the interpolation operator and obtained the error result in the H^1 norm with $O(h^{p+1})$ in the semi-discrete scheme and $O(h^{p+1} + \tau^{\frac{3}{2}})$ in the Crank-Nicolson scheme, respectively. Recently, Zhou et al.^[36] studied the superconvergence properties of the local discontinuous Galerkin method for the one-dimensional linear Schrödinger equation.

In this paper, we study a general complex linear Schrödinger equation (1) and extend the previous work[35]. We analyze the error estimate using the elliptic projection operator. We obtain the error result with $O(h^{k+1})$ in the L^2 norm and the H^1 norm in the semi-discrete finite element scheme. The global superconvergence result is presented by use of the interpolation post-processing technique. Next, we analyze the error estimate in the L^2 norm with order $O(h^{k+1} + \tau^2)$ in the Crank-Nicolson fully discrete scheme. We extend the idea^[37] and certify that the time-difference of error $\eta^n = U^n - P_h u^n$ has a high order error in the L^2 norm, that is, $\|\eta^n - \eta^{n-1}\| \leq C\tau(h^{k+1} + \tau^2)$, where U^n is the fully discrete solution of Crank-Nicolson scheme. At last, we obtain the superconvergence result in the H^1 norm with $O(h^{k+1} + \tau^2)$ on this basis.

The paper is organized as follows. The notations and the projection operator are given in Section 2. In Section 3, we present a finite element semi-discrete scheme with bi-k-degree rectangular elements. Furthermore, we obtain error results with $O(h^{k+1})$ in the L^2 norm and the $H¹$ norm by use of the elliptic projection operator, respectively. In Section 4, we prove the global superconvergence result with $O(h^{k+1})$. In Section 5, we obtain the superconvergence result in the H^1 norm with $O(h^{k+1} + \tau^2)$ in the Crank-Nicolson fully discrete scheme. In Section 6, numerical examples are given to partly verify the theoretical results.

2 Notation and preliminaries

For an integer $m \geqslant 0$ and $1 \leqslant p \leqslant \infty$, we shall use $W^{m,p}$ to denote the standard Sobolev space of complex-valued measurable functions defined on Ω with the norm $\|\phi\|_n^p$ obolev space of complex-valued measurable functions defined on Ω with the norm $\|\phi\|_{m,p}^p = \sum \|D^{\alpha}\phi\|_{L^p(Q)}^p$. When $p = 2$, we shall also use the symbol H^m for $W^{m,2}$, $\|\cdot\|_m$ instead of $|\alpha|\leqslant m$ $\|D^{\alpha}\phi\|_{L^p(\Omega)}^p$. When $p=2$, we shall also use the symbol H^m for $W^{m,2}$, $\|\cdot\|_m$ instead of

 $\|\cdot\|_{m,2}$, and $\|\cdot\|$ instead of $\|\cdot\|_{0,2}$.

For complex-valued functions $\omega(x)$ and $\nu(x)$, we define the inner product (ω, ν) with

$$
(\omega,\nu)=\int_\Omega \omega(\boldsymbol{x})\overline{\nu}(\boldsymbol{x})\mathrm{d}\boldsymbol{x},
$$

where $\overline{\nu}$ denotes the complex conjugate of function ν .

Then, we can define the weak solution $u(x, t)$ of problem (1): find a function $u(x, t) \in H_0^1(\Omega)$ such that

$$
\begin{cases}\n\mathbf{i}(u_t, v) = a(u, v) + (f, v), & \forall v \in H_0^1(\Omega), \quad 0 \leq t \leq T, \\
u(\mathbf{x}, 0) = u_0(\mathbf{x}), & \forall \mathbf{x} \in \Omega,\n\end{cases}
$$
\n(2)

where $a(u, v) = \frac{1}{2}(\nabla u, \nabla v) + (Vu, v)$.

Let Γ_h be a quasi-uniform rectangular partition of Ω with the mesh size $h > 0$, and let e be an arbitrary element of Γ_h . We can define the finite element space of order k as

$$
V^{h,k} = \{ v \in C(\Omega) : v|_e \in Q_p, \ \forall e \in \Gamma_h \},\
$$

where

$$
Q_p = \text{span}\{x^i y^j, \ \ 0 \leqslant i, j \leqslant k\}.
$$

In addition,

$$
V_0^{h,k} = V^{h,k} \cap H_0^1(\Omega).
$$

Let $V_0^{h,k} \subset H_0^1(\Omega)$ be the corresponding finite element space of order k. In general given $w(\boldsymbol{x},t) \in H_0^1(\Omega)$, the elliptic projection $P_h w(\boldsymbol{x},t) \in V_0^{h,k}$ can be defined by

$$
a(P_h w, v_h) = a(w, v_h), \quad \forall v_h \in V_0^{h,k}.
$$
\n
$$
(3)
$$

.

Let $\tau = T/N$ be the time step of the interval $[0, T]$, time nodes $t_j = j\tau$ $(j = 0, 1, \dots, N)$, $t_{j+\frac{1}{2}} = (t_{j+1} + t_j)/2$, and time elements $I_j = [t_j, t_{j+1}]$ $(j = 0, 1, \dots, N-1)$, and set

$$
\phi(\cdot, t_j) = \phi^j,
$$

$$
\|\phi\|_{L^2(0,T;\Omega)} = \left(\int_0^T \|\phi(\cdot,t)\|_{\Omega}^2 dt\right)^{\frac{1}{2}}
$$

3 Superconvergence analysis for semi-discrete approximation problem

The semi-discrete finite element solution $u_h(x, t)$ of problem (1) can be defined: find $u_h(x, t)$ $\in V_0^{h,k}$ satisfying

$$
\begin{cases}\n\mathbf{i}(u_{ht}, v_h) = a(u_h, v_h) + (f, v_h), & \forall v_h \in V_0^{h,k}, \quad 0 \leq t \leq T, \\
u_h(\mathbf{x}, 0) = P_h u_0(\mathbf{x}), & \forall \mathbf{x} \in \Omega,\n\end{cases} \tag{4}
$$

where $P_h u_0(\boldsymbol{x}) \in V_0^{h,k}$ is the elliptic projection of $u_0(\boldsymbol{x})$.

Lemma $1^{[34]}$ If for any $t \in [0, T]$, the functions $u(x, t), u_t(x, t), u_{tt}(x, t) \in H^{k+1}(\Omega)$, then $P_h u(\boldsymbol{x},t) \in V_0^{h,k}$ has the following results:

$$
||u - P_h u||_q \leq C h^{k-q+1} ||u||_{k+1}, \quad q = 0, 1,
$$
\n⁽⁵⁾

$$
||(u - P_h u)_t||_q \leq Ch^{k-q+1}||u_t||_{k+1}, \quad q = 0, 1,
$$
\n(6)

$$
||(u - P_h u)_{tt}||_q \leq C h^{k-q+1} ||u_{tt}||_{k+1}, \quad q = 0, 1.
$$
 (7)

Lemma 2^[20] Let u be the solution to the problem (2), and let $u_I \in V_0^{h,k}$ be the interpolation of u. If $u \in H^{k+2}(\Omega)$, then

$$
|(\nabla(u - u_I), \nabla v)| \le C h^{k+1} ||u||_{k+2} ||v||_1, \quad \forall v \in V_0^{h,k}.
$$
 (8)

Theorem 1 If u and u_h are the solutions to the problems (2) and (4), respectively, and $u, u_t, u_{tt} \in H^{k+1}(\Omega)$, there hold

$$
||u_h - P_h u|| \leq C h^{k+1},\tag{9}
$$

$$
||(u_h - P_h u)_t|| \leq C h^{k+1}.
$$
\n
$$
(10)
$$

Proof It follows from (2) and (4) that

$$
i((u - u_h)_t, v_h) = a(u - u_h, v_h), \quad \forall v_h \in V_0^{h,k}.
$$
\n(11)

Let $u - u_h = \rho - \xi$ with

$$
\rho = u - P_h u, \quad \xi = u_h - P_h u. \tag{12}
$$

Then, from (11) and (12) , we have

$$
i(\rho_t, v_h) - i(\xi_t, v_h) = a(\rho, v_h) - a(\xi, v_h).
$$
\n(13)

From (3), we can obtain

$$
a(\rho, v_h) = 0.\t\t(14)
$$

Substituting (14) into (13) yields

$$
i(\xi_t, v_h) = i(\rho_t, v_h) + a(\xi, v_h).
$$
\n(15)

Taking $v_h = \xi$ in (15), we have

$$
i(\xi_t, \xi) = i(\rho_t, \xi) + a(\xi, \xi).
$$
\n(16)

Noticing

$$
\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}||\xi||^2 = \mathrm{Re}\{(\xi_t, \xi)\}
$$

and comparing the imaginary parts of (16), we get

$$
\frac{1}{2} \frac{d}{dt} ||\xi||^2 = \text{Re}\{(\rho_t, \xi)\} + \text{Im}\{a(\xi, \xi)\}\
$$

= Re\{(\rho_t, \xi)\}
 $\leq C ||\rho_t|| ||\xi||.$ (17)

Combining (6) with (17) yields

$$
\frac{d}{dt} \|\xi\| \le C h^{k+1} \|u_t\|_{k+1}.
$$
\n(18)

Integrating from 0 to t in (18), we have

$$
\|\xi\| \le \|\xi(\cdot, 0)\| + Ch^{k+1} \int_0^t \|u_t\|_{k+1} ds.
$$
\n(19)

It follows from (4) that

$$
\|\xi(\cdot,0)\| = 0.\tag{20}
$$

From (19) and (20) , we obtain

$$
\|\xi\| \leq C h^{k+1} \int_0^t \|u_t\|_{k+1} \, \mathrm{d} s.
$$

Therefore, (9) holds. Next, we prove (10). Taking $v_h = \xi_t(\cdot, 0)$ in (15) with $t = 0$ and combining (20), we have

$$
i(\xi_t(\cdot,0),\xi_t(\cdot,0)) = i(\rho_t(\cdot,0),\xi_t(\cdot,0)).
$$

Thus,

$$
\|\xi_t(\cdot,0)\|^2 \le \|\rho_t(\cdot,0)\| \|\xi_t(\cdot,0)\|,
$$

that is,

$$
\|\xi_t(\cdot,0)\| \le \|\rho_t(\cdot,0)\|.\tag{21}
$$

Combining (6) with (21) gives

$$
\|\xi_t(\cdot,0)\| \le C h^{k+1} \|u_t(\cdot,0)\|_{k+1}.
$$
\n(22)

Differentiating (15) with respect to t and taking $v_h = \xi_t$, we can obtain

$$
i(\xi_{tt}, \xi_t) = i(\rho_{tt}, \xi_t) + a(\xi_t, \xi_t). \tag{23}
$$

Noticing

$$
\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}||\xi_t||^2 = \mathrm{Re}\{(\xi_{tt}, \xi_t)\}
$$

and comparing the imaginary parts of (23) yield

$$
\frac{1}{2} \frac{d}{dt} ||\xi_t||^2 = \text{Re}\{(\rho_{tt}, \xi_t)\} + \text{Im}\{a(\xi_t, \xi_t)\} \\
= \text{Re}\{(\rho_{tt}, \xi_t)\} \\
\leq C ||\rho_{tt}|| ||\xi_t||. \tag{24}
$$

From (22) and (25) , we get

$$
\frac{d}{dt} \|\xi_t\| \le C h^{k+1} \|u_{tt}\|_{k+1}.
$$
\n(25)

Integrating from 0 to t in (25) , we can obtain

$$
\|\xi_t\| \le \|\xi_t(\cdot, 0)\| + Ch^{k+1} \int_0^t \|u_{tt}\|_{k+1} ds.
$$
 (26)

It follows from (22) and (26) that

$$
\|\xi_t\| \leq C h^{k+1} \Big(\|u_t(\cdot,0)\|_{k+1} + \int_0^t \|u_{tt}\|_{k+1} ds \Big),
$$

which completes the proof of (10).

Theorem 2 Let u and u_h be the solutions to the problems (2) and (4), respectively, and $u, u_t, u_{tt} \in H^{k+1}(\Omega)$. Then, we have

$$
||u_h - P_h u||_1 \le C h^{k+1}.
$$
\n(27)

Proof Taking $v_h = \xi_t$ in (15), we can get

$$
i(\xi_t, \xi_t) = i(\rho_t, \xi_t) + a(\xi, \xi_t),
$$

that is,

$$
i(\xi_t, \xi_t) = i(\rho_t, \xi_t) + \frac{1}{2}(\nabla \xi, \nabla \xi_t) + (V\xi, \xi_t).
$$
 (28)

Noticing

$$
\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t} \|\nabla \xi\|^2 = \mathrm{Re}\{(\nabla \xi, \nabla \xi_t)\}
$$

and comparing the real parts of (28) give

$$
\frac{1}{2} \frac{d}{dt} \|\nabla \xi\|^2 = \text{Im}\{(\rho_t, \xi_t) + (\xi_t, \xi_t)\} - \text{Re}\{(V\xi, \xi_t)\}\
$$

$$
= \text{Im}\{(\rho_t, \xi_t)\} - \text{Re}\{(V\xi, \xi_t)\}\
$$

$$
\leq C(\|\rho_t\| + \|\xi\|) \|\xi_t\|.
$$
(29)

From (6) , (9) , (10) , and (29) , we can obtain

$$
\frac{\mathrm{d}}{\mathrm{d}t} \|\nabla \xi\|^2 \leqslant Ch^{2k+2}.\tag{30}
$$

Integrating from 0 to t in (30) yields

$$
\|\nabla \xi\|^2 \le \|\nabla \xi(\cdot, 0)\|^2 + Ch^{2k+2}.\tag{31}
$$

Notice

$$
\|\nabla \xi(\cdot,0)\| = 0.\tag{32}
$$

Substituting (32) into (31) yields

$$
\|\nabla \xi\| \le C h^{k+1}.\tag{33}
$$

Therefore, (27) follows from (33).

4 Global superconvergence analysis

Let \tilde{e} be a macro element which is the union of four elements $e_i \in \Gamma_h$ $(i = 1, 2, 3, 4)$, where the intersection of $\overline{e}_i \in \Gamma_h$ $(i = 1, 2, 3, 4)$ is nonempty (see Fig. 1).

\mathbb{Z}_3	l_{11}	\mathbb{Z}_8	l_{12}	\mathbb{Z}_4
$l_{8}% =-1\cdot10^{-4}$	e_3	l_9	e_4	l_{10}
Z_9	l_6	$\ensuremath{\mathnormal{Z}}_5$	l_7	Z_7
l_3	e_1	l_4	e_2	l_5
Z_1	l_1	$\ensuremath{\mathnormal{Z}}_6$	l_2	Z_2

Fig. 1 Structure of macro element \widetilde{e}

Let the interpolation operator Π_{2h}^2 satisfy $\Pi_{2h}^2 w \in Q_2(\tilde{e})$, where Q_2 is the space of biquadratic functions, and

$$
\Pi_{2h}^2 w(Z_i) = w(Z_i),\tag{34}
$$

where Z_i $(i = 1, 2, \dots, 9)$ are the nodes of Γ_h .

When $k \geq 2$, let $\Pi_{2h}^{2k} w \in Q_{2k}(\tilde{e})$ such that

$$
\Pi_{2h}^{2k}w(Z_i) = w(Z_i),\tag{35}
$$

$$
\int_{l_i} (\Pi_{2h}^{2k} w - w) v \, \mathrm{d}l = 0, \quad \forall v \in P_{k-2}(l_i),\tag{36}
$$

$$
\int_{e_i} (\Pi_{2h}^{2k} w - w) v \, dx \, dy = 0, \quad \forall v \in Q_{k-2}(e_i), \tag{37}
$$

where Z_i $(i = 1, 2, \dots, 9)$ are the nodes of Γ_h , l_i $(i = 1, 2, \dots, 12)$ are the edges of Γ_h , e_i $(i =$ 1, 2, 3, 4) are the elements of Γ_h , P_{k-2} is the set of polynomials of order $k-2$, and $Q_{k-2}(\tilde{e})$ is the polynomials of order $k - 2$ in x and y.

Lemma 3^[20,22] The interpolation operator Π_{2h}^{2k} is defined in (34)–(37) such that

$$
\Pi_{2h}^{2k}w_I = \Pi_{2h}^{2k}w, \quad \forall w \in C(\tilde{e}),\tag{38}
$$

$$
\|\Pi_{2h}^{2k}w - w\|_{l,\tilde{e}} \le C h^{r+1-l} \|w\|_{r+1,\tilde{e}}, \quad 1 \le r \le 2k, \quad l = 0, 1,
$$
\n(39)

$$
\|\Pi_{2h}^{2k}v\|_{l,\tilde{e}} \leqslant C\|v\|_{l,\tilde{e}}, \quad \forall v \in V^{h,k}, \quad l = 0, 1,
$$
\n
$$
(40)
$$

where $w_I \in V^{h,k}$ is the interpolant of w.

Lemma 4 Let u and u_h be the solutions to the problems (2) and (4) , respectively. If $u \in H^{k+2}(\Omega)$, and $u_t, u_{tt} \in H^{k+1}(\Omega)$, then

$$
||u_h - u_I||_1 \le C h^{k+1},
$$
\n(41)

where u_I is the interpolant of u .

Proof From (14) , we can obtain

$$
a(u - P_h u, u_h - u_I) = 0,
$$

that is,

$$
(\nabla(u - P_h u), \nabla(u_h - u_I)) = -(V(u - P_h u), u_h - u_I). \tag{42}
$$

It is easy to check

$$
(\nabla(u_h - u_I), \nabla(u_h - u_I)) = (\nabla(u_h - P_h u), \nabla(u_h - u_I)) - (\nabla(u - P_h u), \nabla(u_h - u_I))
$$

$$
+ (\nabla(u - u_I), \nabla(u_h - u_I)). \tag{43}
$$

Combining (42) with (43) yields

$$
|u_h - u_I|^2 = (\nabla(u_h - P_h u), \nabla(u_h - u_I)) + (V(u - P_h u), u_h - u_I) + (\nabla(u - u_I), \nabla(u_h - u_I)) \n\leq \|u_h - P_h u\|_1 \|u_h - u_I\|_1 + C \|u - P_h u\| \|u_h - u_I\| + (\nabla(u - u_I), \nabla(u_h - u_I)).
$$
\n(44)

It follows from (5) that

$$
||u - P_h u|| \leq C h^{k+1} ||u||_{k+1},
$$
\n(45)

and from (8), we have

$$
(\nabla(u - u_I), \nabla(u_h - u_I)) \le C h^{k+1} ||u||_{k+2} ||u_h - u_I||_1.
$$
\n(46)

In addition,

$$
||u_h - u_I|| \le ||u_h - u_I||_1.
$$
\n(47)

Substituting (27) and (45) – (47) into (44) , we can get

$$
|u_h - u_I|^2 \le C(h^{k+1} + h^{k+1} ||u||_{k+1} + h^{k+1} ||u||_{k+2}) ||u_h - u_I||_1.
$$
 (48)

By the Poincaré inequality, we can obtain

$$
||u_h - u_I||_1 \leq C|u_h - u_I|_1.
$$
\n(49)

Therefore, (48) and (49) show the validity of (41).

Theorem 3 Let u and u_h be the solutions to the problems (2) and (4), respectively. If $u \in H^{k+2}(\Omega)$, and $u_t, u_{tt} \in H^{k+1}(\Omega)$, then

$$
||u - \Pi_{2h}^{2k} u_h||_1 \leq C h^{k+1},
$$
\n(50)

where Π_{2h}^{2k} is the interpolation post-processing operator.

Proof It follows from (40) and (41) that

$$
\|\Pi_{2h}^{2k}u_h - \Pi_{2h}^{2k}u_I\|_1 \leqslant C\|u_h - u_I\|_1 \leqslant Ch^{k+1}.
$$
\n(51)

From (38) and (39), we have

$$
\|\Pi_{2h}^{2k}u_I - u\|_1 = \|\Pi_{2h}^{2k}u - u\|_1 \le Ch^{k+1}.
$$
\n(52)

Notice

$$
||u - \Pi_{2h}^{2k} u_h||_1 \le ||\Pi_{2h}^{2k} u_h - \Pi_{2h}^{2k} u_I||_1 + ||\Pi_{2h}^{2k} u_I - u||_1.
$$
\n(53)

Therefore, (50) follows from (51) – (53) .

5 Superconvergence analysis in fully discrete scheme

For the function series $U^n(\boldsymbol{x})$ $(n = 0, 1, \dots)$, let

$$
\partial_t U^{n+\frac{1}{2}} = \frac{1}{\tau} (U^{n+1}(\mathbf{x}) - U^n(\mathbf{x})),
$$

$$
U^{n+\frac{1}{2}} = \frac{1}{2} (U^{n+1}(\mathbf{x}) + U^n(\mathbf{x})).
$$

Then, the Crank-Nicolson fully discrete finite element solution $U^n(\boldsymbol{x}) \in V^{h,k}_0$ $(n = 0, 1, \cdots, N)$ to the problem (1) can be defined by

$$
\begin{cases}\n\mathrm{i}(\partial_t U^{n+\frac{1}{2}}, v_h) = a(U^{n+\frac{1}{2}}, v_h) + (f^{n+\frac{1}{2}}, v_h), & \forall v_h \in V_0^{h,k}, \\
U^0(\mathbf{x}) = P_h u_0(\mathbf{x}).\n\end{cases} \tag{54}
$$

Theorem 4 Let $u(x, t)$ be the solution to the problem (2) , and let the function series $U^{n}(\boldsymbol{x})$ be the solution to the problem (54). Then, we have

$$
||U^n - P_h u^n|| \le C h^{k+1} + C\tau^2.
$$
\n(55)

Proof From (2) and (54) , we can get

$$
i(u_t^{n+\frac{1}{2}} - \partial_t U^{n+\frac{1}{2}}, v_h) = a(u^{n+\frac{1}{2}} - U^{n+\frac{1}{2}}, v_h).
$$
\n(56)

Let $u - U = \rho - \eta$ with

$$
\rho = u - P_h u, \quad \eta = U - P_h u. \tag{57}
$$

Combining (56) with (57) and (14) , we have

$$
i(\partial_t \eta^{n+\frac{1}{2}}, v_h) - i(\partial_t \rho^{n+\frac{1}{2}}, v_h) - i(u_t^{n+\frac{1}{2}} - \partial_t u^{n+\frac{1}{2}}, v_h) = a(\eta^{n+\frac{1}{2}}, v_h).
$$
(58)

Taking $v_h = \eta^{n + \frac{1}{2}}$ in (58), we can obtain

$$
i(\partial_t \eta^{n+\frac{1}{2}}, \eta^{n+\frac{1}{2}}) - i(\partial_t \rho^{n+\frac{1}{2}}, \eta^{n+\frac{1}{2}}) - i(u_t^{n+\frac{1}{2}} - \partial_t u^{n+\frac{1}{2}}, \eta^{n+\frac{1}{2}}) = a(\eta^{n+\frac{1}{2}}, \eta^{n+\frac{1}{2}}). \tag{59}
$$

Notice

$$
\frac{1}{2\tau}(\|\eta^{n+1}\|^2 - \|\eta^n\|^2) = \text{Re}\{(\partial_t \eta^{n+\frac{1}{2}}, \eta^{n+\frac{1}{2}})\}.
$$

Comparing the imaginary parts of (59) yields

$$
\frac{1}{2\tau}(\|\eta^{n+1}\|^2 - \|\eta^n\|^2) = \text{Re}\{(\partial_t \rho^{n+\frac{1}{2}}, \eta^{n+\frac{1}{2}}) + (u_t^{n+\frac{1}{2}} - \partial_t u^{n+\frac{1}{2}}, \eta^{n+\frac{1}{2}})\}\
$$

\n
$$
\leq |(\partial_t \rho^{n+\frac{1}{2}}, \eta^{n+\frac{1}{2}})| + |(u_t^{n+\frac{1}{2}} - \partial_t u^{n+\frac{1}{2}}, \eta^{n+\frac{1}{2}})|
$$

\n
$$
\leq (\|\partial_t \rho^{n+\frac{1}{2}}\| + \|u_t^{n+\frac{1}{2}} - \partial_t u^{n+\frac{1}{2}}\|)\|\eta^{n+\frac{1}{2}}\|
$$

\n
$$
= \frac{1}{2}(\|\partial_t \rho^{n+\frac{1}{2}}\| + \|u_t^{n+\frac{1}{2}} - \partial_t u^{n+\frac{1}{2}}\|)\|\eta^{n+1} + \eta^n\|
$$

\n
$$
\leq \frac{1}{2}(\|\partial_t \rho^{n+\frac{1}{2}}\| + \|u_t^{n+\frac{1}{2}} - \partial_t u^{n+\frac{1}{2}}\|)(\|\eta^{n+1}\| + \|\eta^n\|).
$$

Thus,

$$
\|\eta^{n+1}\| - \|\eta^n\| \leq C\tau(\|\partial_t \rho^{n+\frac{1}{2}}\| + \|u_t^{n+\frac{1}{2}} - \partial_t u^{n+\frac{1}{2}}\|). \tag{60}
$$

It follows from (5) that

$$
\|\partial_t \rho^{n+\frac{1}{2}}\| = \|\partial_t u^{n+\frac{1}{2}} - \partial_t P_h u^{n+\frac{1}{2}}\|
$$

\n
$$
= \|\tau^{-1}(u^{n+1} - u^n) - \tau^{-1}(P_h u^{n+1} - P_h u^n)\|
$$

\n
$$
= \tau^{-1}\|(u^{n+1} - u^n) - P_h(u^{n+1} - u^n)\|
$$

\n
$$
\leq C\tau^{-1}h^{k+1}\|u^{n+1} - u^n\|_{k+1}
$$

\n
$$
= C\tau^{-1}h^{k+1}\left\|\int_{t_n}^{t_{n+1}} u_t(\cdot, t)\right\|_{k+1} dt
$$

\n
$$
\leq C\tau^{-1}h^{k+1}\int_{t_n}^{t_{n+1}} \|u_t(\cdot, t)\|_{k+1} dt.
$$
 (61)

In addition,

$$
\|u_t^{n+\frac{1}{2}} - \partial_t u^{n+\frac{1}{2}}\|
$$

\n
$$
= \frac{1}{2\tau} \Big\| \int_{t_n}^{t_{n+\frac{1}{2}}} (t - t_n)^2 u_{ttt}(\cdot, t) dt + \int_{t_{n+\frac{1}{2}}}^{t_{n+1}} (t - t_{n+1})^2 u_{ttt}(\cdot, t) dt \Big\|
$$

\n
$$
\leq \frac{1}{2\tau} \Big\| \int_{t_n}^{t_{n+\frac{1}{2}}} \left(\frac{\tau}{2}\right)^2 u_{ttt}(\cdot, t) dt + \int_{t_{n+\frac{1}{2}}}^{t_{n+1}} \left(\frac{\tau}{2}\right)^2 u_{ttt}(\cdot, t) dt \Big\|
$$

\n
$$
= \frac{\tau}{8} \Big\| \int_{t_n}^{t_{n+1}} u_{ttt}(\cdot, t) dt \Big\|
$$

\n
$$
\leq C\tau \int_{t_n}^{t_{n+1}} \|u_{ttt}(\cdot, t)\| dt.
$$

\n(62)

Substituting (61) and (62) into (60) , we have

$$
\|\eta^{n+1}\| - \|\eta^n\| \le Ch^{k+1} \int_{t_n}^{t_{n+1}} \|u_t(\cdot, t)\|_{k+1} dt
$$

+ $C\tau^2 \int_{t_n}^{t_{n+1}} \|u_{ttt}(\cdot, t)\| dt.$ (63)

Summing up for n in (63) yields

$$
\|\eta^n\| - \|\eta^0\| \le C h^{k+1} \int_0^{t_n} \|u_t(\cdot, t)\|_{k+1} dt
$$

+ $C\tau^2 \int_0^{t_n} \|u_{ttt}(\cdot, t)\| dt.$ (64)

From (54), we can see

$$
\|\eta^0\| = 0.\tag{65}
$$

Therefore, (55) follows from (64) and (65).

Lemma 5 Let $u(x,t)$ be the solution to the problem (2), and let the function series $U^n(x)$ be the solution to the problem (54). Then, the time-difference of error $\eta^n = U^n - P_h u^n$ has a high order error

$$
\|\eta^n - \eta^{n-1}\| \leq C\tau(h^{k+1} + \tau^2). \tag{66}
$$

Proof It follows from (2) that

$$
\int_0^t (i(u_t, v) - a(u, v) - (f, v)) dt = 0, \quad \forall v \in V_0^{h, k}.
$$
\n(67)

Integrating (67) in I_n by trapezoid and mid-point formulae, respectively, we can obtain

$$
i(u^{n+1} - u^n, v) - \frac{\tau}{2}a(u^{n+1} + u^n, v) = \tau(f^{n+\frac{1}{2}}, v) + r_1^n(v) + r_2^n(v),
$$
\n(68)

where

$$
r_1^n(v) = O(\tau^2) \int_{I_n} ||f_{tt}|| ||v|| \mathrm{d}t,\tag{69}
$$

$$
r_2^n(v) = O(\tau^2) \int_{I_n} (||u_{tt}||_2 + ||Vu_{tt}||) ||v|| dt.
$$
 (70)

From (54), we have

$$
i(U^{n+1} - U^n, v) - \frac{\tau}{2}a(U^{n+1} + U^n, v) = \tau(f^{n+\frac{1}{2}}, v).
$$
\n(71)

Combining (68) with (71) yields

$$
i(u^{n+1} - U^{n+1} - (u^n - U^n), v) - \frac{\tau}{2} a(u^{n+1} - U^{n+1} + u^n - U^n, v)
$$

= $r_1^n(v) + r_2^n(v).$ (72)

From (57), (14), and (72), we get

$$
i(\eta^{n+1} - \eta^n, v) - \frac{\tau}{2}a(\eta^{n+1} + \eta^n, v) = r_1^n(v) + r_2^n(v) + r_3^n(v),\tag{73}
$$

where

$$
r_3^n(v) = \mathrm{i}(\rho^{n+1} - \rho^n, v) = \mathrm{i} \int_{I_n} (\rho_t, v) \mathrm{d}t. \tag{74}
$$

Further, combining (7) and (74) gives

$$
|r_3^n(v) - r_3^{n-1}(v)| = \Big| \int_{I_n} (\rho_t, v) dt - \int_{I_{n-1}} (\rho_t, v) dt \Big|
$$

= $O(\tau) \int_{I_n + I_{n-1}} |(\rho_{tt}, v)| dt$
= $O(\tau h^{k+1}) \int_{I_n + I_{n-1}} ||u_{tt}||_{k+1} ||v|| dt.$ (75)

Substituting *n* by $n - 1$ in (73), we have

$$
i(\eta^{n} - \eta^{n-1}, v) - \frac{\tau}{2}a(\eta^{n} + \eta^{n-1}, v) = r_1^{n-1}(v) + r_2^{n-1}(v) + r_3^{n-1}(v).
$$
 (76)

Let

$$
\epsilon^{n+1} = \eta^{n+1} - \eta^n.
$$

We can see

$$
(\eta^{n+1} + \eta^n) - (\eta^n + \eta^{n-1}) = \epsilon^{n+1} + \epsilon^n.
$$
 (77)

Subtracting (76) from (73) and combining (77) yield

$$
i(\epsilon^{n+1} - \epsilon^n, v) - \frac{\tau}{2} a(\epsilon^{n+1} + \epsilon^n, v) = r_h^n(v),\tag{78}
$$

where

$$
r_h^n(v) = \sum_{i=1}^3 (r_i^n(v) - r_i^{n-1}(v)).
$$
\n(79)

From (69), (70), (75), and (79), we can obtain

$$
|r_h^n(v)| \leqslant \sum_{i=1}^3 |r_i^n(v) - r_i^{n-1}(v)|
$$

\n
$$
\leqslant C\tau(h^{k+1} + \tau^2) \int_{I_n + I_{n-1}} (||f_{ttt}|| + ||u_{ttt}||_2 + ||Vu_{ttt}|| + ||u_{ttt}||_2 + ||Vu_{ttt}|| + ||u_{ttt}||_{k+1}) ||v|| dt.
$$
 (80)

Taking $v = e^{n+1} + e^n$ in (78), we get

$$
i(\epsilon^{n+1} - \epsilon^n, \epsilon^{n+1} + \epsilon^n) - \frac{\tau}{2}a(\epsilon^{n+1} + \epsilon^n, \epsilon^{n+1} + \epsilon^n) = r_h^n(\epsilon^{n+1} + \epsilon^n). \tag{81}
$$

Comparing the imaginary parts of (81), we have

$$
\|\epsilon^n\|^2 - \|\epsilon^{n-1}\|^2 = \text{Re}\{(\epsilon^{n+1} - \epsilon^n, \epsilon^{n+1} + \epsilon^n)\}
$$

=
$$
\text{Im}\{r_h^n(\epsilon^{n+1} + \epsilon^n)\}
$$

\$\leqslant |r_h^n(\epsilon^{n+1} + \epsilon^n)]. \tag{82}

Combining (80) with (82) gives

$$
\|\epsilon^n\|^2 - \|\epsilon^{n-1}\|^2 \leq C\tau(h^{k+1} + \tau^2) \int_{I_n + I_{n-1}} (\|f_{ttt}\| + \|u_{ttt}\|_2 + \|Vu_{ttt}\| + \|u_{ttt}\|_k + 1)\|\epsilon^{n+1} + \epsilon^n\|dt.
$$
\n(83)

Without loss of generality, we assume that there is an integer $1 \leq K \leq N$ such that

$$
\|\epsilon^K\| = \max_{1 \leq n \leq N} \|\epsilon^n\|.\tag{84}
$$

Summing up for n from 2 to K in (83) and combining (84) , we have

$$
\|\epsilon^{K}\|^{2} \leq \|\epsilon^{1}\|^{2} + C\tau(h^{k+1} + \tau^{2}) \int_{I} (\|f_{ttt}\| + \|u_{ttt}\|_{2} + \|Vu_{ttt}\| + \|u_{ttt}\| + \|u_{ttt}\|_{k+1})dt \|\epsilon^{K}\|.
$$
\n(85)

Taking $n = 1$ in (64) and combining (65) yield

$$
\|\epsilon^1\| = \|\eta^1\| \le C\tau(h^{k+1} + \tau^2). \tag{86}
$$

Substituting (86) into (85) and using Young's inequality, we can get

$$
\|\epsilon^K\| \leqslant C\tau(h^{k+1} + \tau^2). \tag{87}
$$

Therefore, (66) follows from (84) and (87).

Theorem 5 Let $u(x, t)$ be the solution to the problem (2), and let the function series $U^n(x)$ be the solution to the problem (54). Then, we have

$$
||U^{n} - P_{h}u^{n}||_{1} \leq C h^{k+1} + C\tau^{2}.
$$
\n(88)

Proof Taking $v_h = \partial_t \eta^{n + \frac{1}{2}}$ in (58), we have

$$
i(\partial_t \eta^{n+\frac{1}{2}}, \partial_t \eta^{n+\frac{1}{2}}) - i(\partial_t \rho^{n+\frac{1}{2}}, \partial_t \eta^{n+\frac{1}{2}}) - i(u_t^{n+\frac{1}{2}} - \partial_t u^{n+\frac{1}{2}}, \partial_t \eta^{n+\frac{1}{2}})
$$

= $\frac{1}{2}(\nabla \eta^{n+\frac{1}{2}}, \nabla \partial_t \eta^{n+\frac{1}{2}}) + (V \eta^{n+\frac{1}{2}}, \partial_t \eta^{n+\frac{1}{2}}).$ (89)

Notice

$$
\frac{1}{2\tau}(\|\nabla \eta^{n+1}\|^2 - \|\nabla \eta^{n}\|^2) = \text{Re}\{(\nabla \eta^{n+\frac{1}{2}}, \nabla \partial_t \eta^{n+\frac{1}{2}})\}.
$$

Comparing the real parts of (89), we get

$$
\frac{1}{4\tau}(\|\nabla \eta^{n+1}\|^2 - \|\nabla \eta^n\|^2) = \text{Im}\{(\partial_t \rho^{n+\frac{1}{2}}, \partial_t \eta^{n+\frac{1}{2}}) + (u_t^{n+\frac{1}{2}} - \partial_t u^{n+\frac{1}{2}}, \partial_t \eta^{n+\frac{1}{2}})\} - \text{Re}\{(V\eta^{n+\frac{1}{2}}, \partial_t \eta^{n+\frac{1}{2}})\},
$$

that is,

$$
\|\nabla \eta^{n+1}\|^2 - \|\nabla \eta^n\|^2 = 4\tau \text{Im}\{(\partial_t \rho^{n+\frac{1}{2}}, \partial_t \eta^{n+\frac{1}{2}}) + (u_t^{n+\frac{1}{2}} - \partial_t u^{n+\frac{1}{2}}, \partial_t \eta^{n+\frac{1}{2}})\}
$$

- 2V(||\eta^{n+1}||^2 - \|\eta^n\|^2). (90)

Summing up for n in (90) and combining (65), we have

$$
\|\nabla \eta^{n}\|^{2} \leq C \sum_{j=0}^{n-1} \|\partial_{t}\rho^{j+\frac{1}{2}}\| \|\eta^{j+1} - \eta^{j}\|
$$

+
$$
C \sum_{j=0}^{n-1} \|u_{t}^{j+\frac{1}{2}} - \partial_{t}u^{j+\frac{1}{2}}\| \|\eta^{j+1} - \eta^{j}\| + C\|\eta^{n}\|^{2}.
$$
 (91)

Substituting (61) , (66) , (62) , and (55) into (91) , we can obtain

$$
\|\nabla \eta^n\|^2 \leqslant (Ch^{k+1} + C\tau^2)^2,
$$

that is,

$$
\|\nabla \eta^n\| \leq C h^{k+1} + C\tau^2,
$$

which completes the proof.

Similar to Theorem 3, we can obtain the following result.

Theorem 6 Assume that $u(x, t)$ is the solution to the problem (2), and the function series $U^{n}(\boldsymbol{x})$ is the solution to the problem (54). Then, we have the global superconvergence estimate

$$
||u^n - \Pi_{2h}^{2k} U^n||_1 \leq C h^{k+1} + \tau^2,
$$
\n(92)

where Π_{2h}^{2k} is the interpolation post-processing operator.

6 Numerical examples

In this section, we carry out some numerical examples with $k = 1$ and $k = 2$ to demonstrate the validity of the theoretical analysis.

Example 1 We consider the following linear Schrödinger equation:

$$
\begin{cases}\ni u_t(\boldsymbol{x},t) = -\frac{1}{2}\Delta u(\boldsymbol{x},t) + u(\boldsymbol{x},t) + f(\boldsymbol{x},t) & \text{in} \quad \Omega \times [0,1], \\
u(\boldsymbol{x},t) = 0 & \text{on} \quad \partial\Omega \times [0,1], \\
u(\boldsymbol{x},0) = u_0(\boldsymbol{x}) & \text{in} \quad \Omega,\n\end{cases}
$$
\n(93)

where $\Omega = [0, 1] \times [0, 1]$, and let the function $f(x, t)$ be chosen that

$$
u(x, y, t) = e^{t}(1 + i)(1 - x)(1 - y)\sin x \sin y
$$

is the exact solution.

We have solved the Schrödinger equation on the uniformly rectangular meshes with the mesh size h by the bilinear finite element. First, we calculate the errors with fixing $\tau = 10^{-4}$ by varying h . The error results are presented in Tables $1-4$, where $Order_1$, $Order_2$, $Order_3$, and Order₄ denote the convergence orders of $||u_I - U^n||$, $||u - U^n||_1$, $||u_I - U^n||_1$, and $||u - \Pi_{2h}^2 U^n||_1$, respectively. Moreover, we have shown convergence orders by slopes in Figs. 2–5. Results in all tables show $O(h)$ in $||u - U^n||_1$, and $O(h^2)$ convergence rate clearly in $||u_I - U^n||$, $||u_I - U^n||_1$, and $||u - \Pi_{2h}^2 U^n||_1$.

Mesh						$ u_I - U^n $ Order ₁ $ u - U^n _1$ Order ₂ $ u_I - U^n _1$ Order ₃ $ u - \Pi_{2b}^2 U^n _1$ Order ₄	
	$h = 1/16$ 2.5160×10^{-5} $h = 1/32$ 6.308 5×10 ⁻⁶ $h = 1/64$ 1.578 2×10^{-6}	1.996 1.999	$1.982 \quad 1.6790 \times 10^{-2}$ $8.382\,7\times10^{-3}$ 4.1898×10^{-3}	1.008 1.6956×10^{-4} 1.888 $1.002 \quad 4.3226 \times 10^{-5}$ $1.001 \quad 1.0848 \times 10^{-5}$	1.972 1.994	$h = 1/8$ 9.9357×10 ⁻⁵ - 3.3771×10 ⁻² - 6.2778×10 ⁻⁴ - 1.7558×10 ⁻³ 4.4138×10^{-4} 1.1028×10^{-4} 2.7565×10^{-5}	\sim 1.992 2.001 2.000

Table 1 Numerical results at $t = 0.01$ obtained with $\tau = 10^{-4}$ in Example 1

Table 2 Numerical results at $t = 0.1$ obtained with $\tau = 10^{-4}$ in Example 1

Mesh						$ u_I - U^n $ Order ₁ $ u - U^n _1$ Order ₂ $ u_I - U^n _1$ Order ₃ $ u - \Pi_{2b}^2 U^n _1$ Order ₄	
	$h = 1/16$ $1.883\,2\times10^{-4}$ $h = 1/32$ 4.729 8×10^{-5}		1.976 1.8367×10^{-2} 1.993 9.1716×10^{-3}	1.007 9.4003×10^{-4} $1.002 \quad 2.3603 \times 10^{-4}$	1.961 1.994	$h = 1/8$ 7.4107×10^{-4} $ 3.6917 \times 10^{-2}$ $ 3.6604 \times 10^{-3}$ $ 4.2636 \times 10^{-3}$ $1.065\,6\times10^{-3}$ 2.6585×10^{-4}	Contract Contract 2.001 2.003
	$h = 1/64$ 1.184 0×10^{-5}	1.998	$4.584\,4\times10^{-3}$	1.001 5.9199×10^{-5}	1.995	6.6513×10^{-5}	1.999

Table 3 Numerical results at $t = 0.5$ obtained with $\tau = 10^{-4}$ in Example 1

Mesh						$ u_I - U^n $ Order ₁ $ u - U^n _1$ Order ₂ $ u_I - U^n _1$ Order ₃ $ u - \Pi_{2b}^2 U^n _1$ Order ₄	
	$h = 1/8$ 8.129 3×10 ⁻⁴ $h = 1/16$ 2.0388×10^{-4} $h = 1/32$ 5.084 3×10 ⁻⁵ $h = 1/64$ 1.271 9×10^{-5}	1.995 2.004 1.999	$-$ 5.496.6 \times 10 ⁻² $-$ 4.301.7 \times 10 ⁻³ 2.7386×10^{-2} 1.005 1.005 7×10^{-3} 1.3681×10^{-2} 1.001 6.8388×10^{-3} 1.000	2.4988×10^{-4} 6.2097×10^{-5}	$\mathcal{L}^{\mathcal{L}}(\mathcal{L}^{\mathcal{L}})$ and $\mathcal{L}^{\mathcal{L}}(\mathcal{L}^{\mathcal{L}})$ 2.097 2.009 2.009	$5.266\,5\times10^{-3}$ 1.2577×10^{-3} $3.150\,5\times10^{-4}$ 7.8531×10^{-5}	\sim 2.066 1.997 2.004

Table 4 Numerical results at $t = 1.0$ obtained with $\tau = 10^{-4}$ in Example 1

Fig. 2 Log of errors at $t = 0.01$ with $\tau = 10^{-4}$

Fig. 3 Log of errors at $t = 0.1$ with $\tau = 10^{-4}$

To test the convergence rate in terms of τ , we fix the time step $\tau = h$. The error results are shown in Tables 5 and 6. In addition, we also show the convergence orders by slopes in Figs. 6 and 7. Results show the convergence rate $O(\tau^2)$ clearly in $||u_I - U^n||$, $||u_I - U^n||$, and $||u - \Pi_{2h}^2 U^n||_1.$

Fig. 4 Log of errors at $t = 0.5$ with $\tau = 10^{-4}$

Fig. 5 Log of errors at $t = 1.0$ with $\tau = 10^{-4}$

Table 5 Numerical results at $t = 0.5$ obtained with $\tau = h$ in Example 1

Mesh	$ u_I - U^n $	Order ₁	$ u_I - U^n _1$	Order ₃	$ u - \Pi_{2b}^2 U^n _1$	Order ₄
$h = 1/16$ $h = 1/32$ $h = 1/64$ $h = 1/128$	2.3683×10^{-4} $5.549.9 \times 10^{-5}$ $1.266\,7\times10^{-5}$ $3.157\,4\times10^{-6}$	$\overline{}$ 2.093 2.131 2.004	1.2063×10^{-3} $2.903.9 \times 10^{-4}$ $6.079\,9\times10^{-5}$ 1.5300×10^{-5}	2.055 2.256 1.991	1.4383×10^{-3} 3.4131×10^{-4} 7.9066×10^{-5} $1.966\,5\times10^{-5}$	2.075 2.110 2.007

Table 6 Numerical results at $t = 1.0$ obtained with $\tau = h$ in Example 1

Fig. 6 Log of errors at $t = 0.5$ with $\tau = h$

Fig. 7 Log of errors at $t = 1.0$ with $\tau = h$

Example 2 We consider the problem (93) with $\Omega = [-1,1] \times [-1,1]$, and function $f(x,t)$ is chosen corresponding to the exact solution

 $u(x, y, t) = e^t x(1+x)(1-x)(1+y)(1-y) + ie^t x \sin(\pi x) \sin(\pi y).$

Similarly, we have solved the Schrödinger equation by the bilinear finite element. We calculate the errors with fixing $\tau = 10^{-4}$ by varying h. The error results at the time level $t_n = 0.01, 0.1, 0.5, 1.0$ are presented in Tables 7-10, respectively. Results in all tables show $O(h)$ in $||u - U^n||_1$, and $O(h^2)$ convergence rate clearly in $||u_I - U^n||$, $||u_I - U^n||_1$, and $||u - \Pi_{2h}^2 U^n||_1$.

Then, we take the time step $\tau = h$. The error results are listed in Tables 11 and 12. Results show the convergence rate $O(\tau^2)$ clearly in $||u_I - U^n||$, $||u_I - U^n||_1$, and $||u - \Pi_{2h}^2 U^n||_1$ as well, which are coincident with theoretical results.

The profiles of the exact solution and the numerical solution at $t = 1.0$ on the 64 \times 64 mesh grid are plotted in Figs. 8–11.

Mesh						$\ u_I - U^n\ $ Order ₁ $\ u - U^n\ _1$ Order ₂ $\ u_I - U^n\ _1$ Order ₃ $\ u - \Pi_{2b}^2 U^n\ _1$ Order ₄	
	$h = 1/16$ 3.4678×10 ⁻⁴ $h = 1/32$ 8.6958×10 ⁻⁵ $h = 1/64$ 2.175 6×10^{-5}	1.996	$h = 1/8$ 1.3695×10^{-3} $ 4.3513 \times 10^{-1}$ $ 8.8605 \times 10^{-3}$ $-$ $1.982 \quad 2.1675 \times 10^{-1}$ $1.082\,7{\times}10^{-1}$ 1.999 5.4123×10^{-2} 1.000 1.4353×10^{-4}	1.005 2.2779×10^{-3} 1.001 5.7318×10^{-4}	1.960 1.991 1.998	8.3676×10^{-2} 2.1245×10^{-2} $5.330\,2\times10^{-3}$ $1.333\,7\times10^{-3}$	$\overline{}$ 1.978 1.995 1.999

Table 7 Numerical results at $t = 0.01$ obtained with $\tau = 10^{-4}$ in Example 2

Table 8 Numerical results at $t = 0.1$ obtained with $\tau = 10^{-4}$ in Example 2

Mesh	$ u_I - U^n $ Order ₁						$ u - U^n _1$ Order ₂ $ u_I - U^n _1$ Order ₃ $ u - \Pi_{2h}^2 U^n _1$ Order ₄	
	$h = 1/8$ 1.2188 $\times 10^{-2}$ $h = 1/16$ 3.090 3×10^{-3} $h = 1/32$ 7.753 1×10^{-4} $h = 1/64$ 1.940 0×10^{-4}	1.995	$1.980 \quad 2.3714 \times 10^{-1}$ $1.184\,7{\times}10^{-1}$ 1.999 5.9220×10^{-2} 1.000 1.1171×10^{-3}	1.001	$- 4.7595 \times 10^{-1}$ $- 7.0779 \times 10^{-2}$ $- $ 1.005 1.7818×10^{-2} $4.465\,9\times10^{-3}$	1.990 1.996 1.999	1.1561×10^{-1} 2.9078×10^{-2} 7.2819×10^{-3} 1.8211×10^{-3}	Contract Contract 1.991 1.998 2.000

Table 9 Numerical results at $t = 0.5$ obtained with $\tau = 10^{-4}$ in Example 2

				Mesh $ u_I - U^n $ Order ₁ $ u - U^n _1$ Order ₂ $ u_I - U^n _1$ Order ₃ $ u - \Pi_{2b}^2 U^n _1$ Order ₄	
$h = 1/16$ 5.1357×10 ⁻³ $h = 1/32$ 1.2836×10^{-3} $h = 1/64$ 3.208 5×10^{-4}		1.999 3.5363×10^{-1} 1.004 2.7709×10^{-2} 2.012 4.4016×10^{-2} 2.000 1.7671×10^{-1} 1.001 6.9144×10^{-3} 2.000 8.8343×10^{-2} 1.000 1.7270×10^{-3}	2.003	$h = 1/8$ 2.0535×10^{-2} $-$ 7.0896×10^{-1} $-$ 1.1175×10^{-1} $-$ 1.7606×10^{-1} $1.100\,5\times10^{-2}$ $2.001 \quad 2.7508 \times 10^{-3}$	\sim 2.000 2.000 2.000

Table 10 Numerical results at $t = 1.0$ obtained with $\tau = 10^{-4}$ in Example 2

Mesh					$ u_I - U^n $ Order ₁ $ u - U^n _1$ Order ₂ $ u_I - U^n _1$ Order ₃ $ u - \Pi_{2b}^2 U^n _1$ Order ₄	
	$h = 1/8$ $2.195\,4 \times 10^{-2}$ $-$ 1.1672 $h = 1/16$ 6.052 0×10 ⁻³ $h = 1/32$ 1.550 9×10^{-3} $h = 1/64$ 3.900 9×10^{-4}	1.859 $5.828\,4\times10^{-1}$ 1.964 2.9132×10^{-1} $1.991 \quad 1.4565 \times 10^{-1} \quad 1.000 \quad 2.1879 \times 10^{-3} \quad 1.990$	$1.002 \quad 3.382\,4\times10^{-2}$ 1.001 8.6926×10^{-3}	1.866 1.960	$-$ 1.233 3×10 ⁻¹ $-$ 2.557 2×10 ⁻¹ $6.594\,2\times10^{-2}$ 1.6636×10^{-2} 4.1682×10^{-3}	\sim 1.955 1.987 1.997

Table 11 Numerical results $t = 0.5$ obtained with $\tau = h$ in Example 2

					Table 12 Numerical results at $t = 1.0$ obtained with $\tau = h$ in Example 2	
Mesh	$ u_I - U^n $	Order ₁	$ u_I - U^n _1$	Order ₃	$ u - \Pi_{2b}^2 U^n _1$	Order ₄
$h = 1/16$ $h = 1/32$ $h = 1/64$ $h = 1/128$	7.2718×10^{-3} 1.6874×10^{-3} 4.0062×10^{-4} 9.8441×10^{-5}	2.108 2.075 2.025	4.1379×10^{-2} 9.5410×10^{-3} 2.2545×10^{-3} 5.5237×10^{-4}	2.117 2.081 2.029	7.0050×10^{-2} 1.7083×10^{-2} 4.2027×10^{-3} 1.0449×10^{-3}	2.036 2.023 2.008

Fig. 8 Real parts of exact solution (color online)

Fig. 9 Imaginary parts of exact solution (color online)

Fig. 10 Real parts of numerical solution (color online)

Fig. 11 Imaginary parts of numerical solution (color online)

Example 3 We consider the problem (93) with $\Omega = [-1, 1] \times [-1, 1]$, and function $f(x, t)$ is chosen corresponding to the same exact solution with Example 2.

The domain Ω is uniformly divided into families Γ_h of quadrilaterals with mesh size h, and $V^{h,2}$ is the biquadratic rectangular element space defined on Γ_h . The Schrödinger equation is solved by the biquadratic rectangular element. We calculate the errors with fixing $\tau = 10^{-3}$ by varying h. The error results at time level $t_n = 0.1, 0.2, 0.5, 1.0$ are presented in Tables 13-16, respectively. Results in all tables also show $O(h^2)$ in $||u - U^n||_1$, and $O(h^3)$ convergence rate clearly in $||u - U^n||$ and $||u_I - U^n||_1$, which are consistent with our theoretical analysis. In addition, the results show $O(h^4)$ in $||u_I - U^n||$. When $k \geq 2$, there is the superclose property also in the L^2 norm between the numerical solution with the interpolant of exact solution.

		Table 13 Numerical results at $t = 0.1$ obtained with $\tau = 10^{-3}$				
Mesh		$ u-U^n $ Order $ u_I-U^n $ Order ₁ $ u-U^n _1$ Order ₂ $ u_I-U^n _1$ Order ₃				
		$h = 1/4 \quad 2.843 \, 4 \times 10^{-3} \quad \ - \quad \ 3.095 \, 1 \times 10^{-4} \quad \ - \quad \ 9.091 \, 1 \times 10^{-2} \quad \ - \quad \ 4.986 \, 0 \times 10^{-3}$				~ 100
	$h = 1/8$ 3.693 0×10 ⁻⁴	$2.945 \quad 2.0733 \times 10^{-5}$	3.900	2.3106×10^{-2} 1.976 6.7424 $\times10^{-4}$		2.887
	$h = 1/16$ 4.668 0×10^{-5}	2.984 1.2780×10^{-6}	4.020	$5.798\,6\times10^{-3}$	1.995 7.8974×10^{-5}	3.094
	$h = 1/32$ 5.8523×10^{-6} 2.996 7.2122×10^{-8}			$4.147 \quad 1.4510 \times 10^{-3} \quad 1.999 \quad 3.9969 \times 10^{-6}$		4.304

Table 14 Numerical results at $t = 0.2$ obtained with $\tau = 10^{-3}$

Mesh	$ u - U^n $ Order			$ u_I - U^n $ Order ₁ $ u - U^n _1$ Order ₂ $ u_I - U^n _1$ Order ₃			
	$h = 1/4$ 3.0812×10^{-3} $ 4.3760 \times 10^{-4}$ $ 1.0047 \times 10^{-1}$ $ 7.1099 \times 10^{-3}$						\sim $-$
	$h = 1/8$ 4.078 4×10 ⁻⁴	$2.917 \quad 2.629\,2 \times 10^{-5}$		4.057 2.5536×10^{-2}		1.976 6.899 3×10^{-4}	3.365
	$h = 1/16$ 5.1558×10^{-5}	2.984 1.6869×10^{-6}	3.962	$6.408\,4\times10^{-3}$	1.995	9.2336×10^{-5}	2.902
	$h = 1/32$ 6.466 5×10 ⁻⁶	$2.995 \quad 1.0013 \times 10^{-7}$		4.075 1.6036×10^{-3}	1.999	$7.038\,4\times10^{-6}$	3.714

Table 15 Numerical results at $t = 0.5$ obtained with $\tau = 10^{-3}$

Mesh	$ u-U^n $	Order			$ u_I - U^n $ Order ₁ $ u - U^n _1$ Order ₂ $ u_I - U^n _1$ Order ₃			
	$h = 1/4$ 4.2589×10^{-3} $ 4.3852 \times 10^{-4}$ $-$				1.3557×10^{-1} $- 5.2243 \times 10^{-3}$			$\overline{}$
	$h = 1/8$ 5.5136×10 ⁻⁴		$2.949 \quad 2.9882 \times 10^{-5}$		3.875 3.4468×10^{-2}	1.976	7.9431×10^{-4}	2.718
	$h = 1/16$ 6.9627×10 ⁻⁵		$2.985 \quad 1.9090 \times 10^{-6}$	3.968	8.6503×10^{-3}	1.994	1.0669×10^{-4}	2.896
	$h = 1/32$ 8.727 0×10^{-6}		$2.996 \quad 1.239\,4 \times 10^{-7}$	3.945	2.1646×10^{-3}	1.999	1.4431×10^{-5}	2.886

Table 16 Numerical results at $t = 1.0$ obtained with $\tau = 10^{-3}$

7 Conclusions

In this paper, we consider a two-dimensional time-dependent linear Schrödinger equation with the finite element method. We present the finite element semi-discrete scheme and the Crank-Nicolson fully discrete scheme in the rectangular Lagrange type finite element space of order k. We also obtain the superconvergence result in the $H¹$ norm by use of the elliptic projection in the semi-discrete scheme and the fully discrete scheme, respectively. Some numerical examples with the order $k = 1$ and $k = 2$ are provided to partly verify our theoretical results. In the future, we shall try to study the problem of superconvergence in the L^2 norm for the two-dimensional time-dependent Schrödinger equation and the superconvergence in the $H¹$ norm for the three-dimensional Schrödinger equation with the finite element method.

Acknowledgements We would like to thank anonymous referees for their insightful comments that improved this paper.

References

- [1] BAO, W. Z., JIN, S., and MARKOWICH, P. A. Numerical study of time-splitting spectral discretizations of nonlinear Schrödinger equations in the semiclassical regimes. SIAM Journal on Scientific Computing, 25(1), 27–64 (2003)
- [2] FEIT, M. D., FLECK, J. A., and STEIGER, A. Solution of the Schrödinger equation by a spectral method. Journal of Computational Physics, 47, 412–433 (1982)
- [3] AKRIVIS, G. D. Finite difference discretization of the cubic Schrödinger equation. IMA Journal of Numerical Analysis, 13(1), 115–124 (1993)
- [4] BAO, W. Z. and CAI, Y. Y. Uniform error estimates of finite difference methods for the nonlinear Schrödinger equation with wave operator. $SIAM$ Journal on Numerical Analysis, $50(2)$, 492–521 (2012)
- [5] HAN, H. D., JIN, J. C., and WU, X. N. A finite-difference method for the one-dimensional time-dependent Schrödinger equation on unbounded domain. Computers and Mathematics with Applications, 50(8), 1345–1362 (2005)
- [6] AKRIVIS, G. D., DOUGALIS, V. A., and KARAKASHIAN, O. A. On fully discrete Galerkin methods of second-order temporal accuracy for the nonlinear Schrödinger equation. Numerische Mathematik, 59(1), 31–53 (1991)
- [7] ANTONOPOULOU, D. C., KARALI, G. D., PLEXOUSAKIS, M., and ZOURARIS, G. E. Crank-Nicolson finite element discretizations for a two-dimensional linear Schrödinger-type equation posed in a noncylindrical domain. Mathematics of Computation, 84(294), 1571–1598 (2015)
- [8] JIN, J. C. and WU, X. N. Convergence of a finite element scheme for the two-dimensional timedependent Schrödinger equation in a long strip. Journal of Computational and Applied Mathematics, $234(3)$, 777-793 (2010)
- [9] KYZA, I. A posteriori error analysis for the Crank-Nicolson method for linear Schrödinger equations. ESAIM Mathematical Modelling and Numerical Analysis, 45(4), 761–778 (2011)
- [10] LEE, H. Y. Fully discrete methods for the nonlinear Schrödinger equation. Computers and Mathematics with Applications, $28(6)$, $9-24$ (1994)
- [11] TANG, Q., CHEN, C. M., and LIU, L. H. Space-time finite element method for Schrödinger equation and its conservation. Applied Mathematics and Mechanics (English Edition), $27(3)$, 335– 340 (2006) https://doi.org/10.1007/s10483-006-0308-z
- [12] WANG, J. Y. and HUANG Y. Q. Fully discrete Galerkin finite element method for the cubic nonlinear Schrödinger equation. Numerical Mathematics: Theory, Methods and Applications, $10(3)$, 670–687 (2017)
- [13] ANTONOPOULOU, D. C. and PLEXOUSAKIS, M. Discontinuous Galerkin methods for the linear Schrödinger equation in non-cylindrical domains. Numerische Mathematik, 115(4), 585–608 (2010)
- [14] KARAKASHIAN, O. A. and MAKRIDAKIS C. A space-time finite element method for the nonlinear Schrödinger equation: the discontinuous Galerkin method. Mathematics of Computation, 67(222), 479–499 (1998)
- [15] LU, W. Y., HUANG, Y. Q., and LIU, H. L. Mass preserving discontinuous Galerkin methods for Schrödinger equations. Journal of Computational Physics, 282, 210-226 (2015)
- [16] GUO, L. and XU, Y. Energy conserving local discontinuous Galerkin methods for the nonlinear Schrödinger equation with wave operator. Journal of Scientific Computing, $65(2)$, 622–647 (2015)
- [17] WANG, W. and SHU, C. W. The WKB local discontinuous Galerkin method for the simulation of Schrödinger equation in a resonant tunneling diode. Journal of Scientific Computing, $40(1-3)$, 360–374 (2009)
- [18] XU, Y. and SHU, C. W. Local discontinuous Galerkin methods for nonlinear Schrödinger equations. Journal of Computational Physics, 205, 72–97 (2005)
- [19] CHEN, C. M. and HUANG Y. Q. High Accuracy Theory of Finite Element Methods (in Chinese), Hunan Science Press, Changsha, 235–248 (1995)
- [20] LIN, Q. and YAN, N. N. Construction and Analysis of High Efficient Finite Elements (in Chinese), Hebei University Press, Baoding, 175–185 (1996)
- [21] WAHLBIN, L. B. Superconvergence in Galerkin Finite Element Methods, Springer, Berlin, 48–64 (1995)
- [22] YAN, N. N. Superconvergence Analysis and a Posteriori Error Estimation in Finite Element Methods, Science Press, Beijing, 35–156 (2008)
- [23] ARNOLD, D. N., DOUGLAS, J., Jr., and THOMÉE, V. Superconvergence of a finite element approximation to the solution of a Sobolev equation in a single space variable. Mathematics of Computation, 36(153), 53–63 (1981)
- [24] CHEN, C. M. and HU, S. F. The highest order superconvergence for bi-k degree rectangular elements at nodes: a proof of 2k-conjecture. Mathematics of Computation, 82(283), 1337–1355 (2013)
- [25] CHEN, Y. P. Superconvergence of mixed finite element methods for optimal control problems. Mathematics of Computation, 77(263), 1269–1291 (2008)
- [26] CHEN, Y. P., HUANG, Y. Q., LIU, W. B., and YAN, N. N. Error estimates and superconvergence of mixed finite element methods for convex optimal control problems. Journal of Scientific Computing, 42(3), 382–403 (2010)
- [27] HUANG, Y. Q., LI, J. C., WU, C., and YANG, W. Superconvergence analysis for linear tetrahedral edge elements. Journal of Scientific Computing, $62(1)$, 122-145 (2015)
- [28] HUANG, Y. Q., YANG, W., and YI, N. Y. A posteriori error estimate based on the explicit polynomial recovery. Natural Science Journal of Xiangtan University, 33(3), 1–12 (2011)
- [29] LIN, Q. and ZHOU, J. M. Superconvergence in high-order Galerkin finite element methods. Computer Methods in Applied Mechanics and Engineering, 196(37), 3779–3784 (2007)
- [30] SHI, D. Y. and PEI, L. F. Superconvergence of nonconforming finite element penalty scheme for Stokes problem using L^2 projection method. Applied Mathematics and Mechanics (English Edition), 34(7), 861–874 (2013) https://doi.org/10.1007/s10483-013-1713-x
- [31] WHEELER, M. F. and WHITEMAN, J. R. Superconvergence of recovered gradients of discrete time/piecewise linear Galerkin approximations for linear and nonlinear parabolic problems. Numerical Methods for Partial Differential Equations, 10(3), 271–294 (1994)
- [32] LIN, Q. and LIU, X. Q. Global superconvergence estimates of finite element method for Schrödinger equation. Journal of Computational Mathematics, $16(6)$, 521–526 (1998)
- [33] SHI, D. Y., WANG, P. L., and ZHAO, Y. M. Superconvergence analysis of anisotropic linear triangular finite element for nonlinear Schrödinger equation. Applied Mathematics Letters, 38, 129–134 (2014)
- [34] TIAN, Z. K., CHEN, Y. P., and WANG J. Y. Superconvergence analysis of bilinear finite element for the nonlinear Schrödinger equation on the rectangular mesh. Advances in Applied Mathematics and Mechanics, $10(2)$, 468-484 (2018)
- [35] WANG, J. Y., HUANG, Y. Q., TIAN, Z. K., and ZHOU, J. Superconvergence analysis of finite element method for the time-dependent Schrödinger equation. Computers and Mathematics with Applications, 71(10), 1960–1972 (2016)
- [36] ZHOU, L. L., XU, Y., ZHANG, Z. M., and CAO, W. X. Superconvergence of local discontinuous Galerkin method for one-dimensional linear Schrödinger equations. Journal of Scientific Comput $ing, 73(2/3), 1290-1315 (2017)$
- [37] HU, H. L., CHEN, C. M., and PAN, K. J. Time-extrapolation algorithm (TEA) for linear parabolic problems. Journal of Computational Mathematics, 32(2), 183–194 (2014)