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GLOBAL SUPERCONVERGENCE ESTIMATES OF FINITE ELEMENT METHOD FOR SCHRÖDINGER EQUATION*

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Abstract

In this paper, we shall study the initial boundary value problem of Schrödinger equation. The second order gradient superconvergence estimates for the problem are obtained solving by linear finite elements.

Key words: Finite element, superconvergence estimates, interpolation, Schrödinger equation.

1. Introduction

Consider the following initial boundary value problem of Schrödinger equation

$$\begin{cases} u_t - i\Delta u = f, & \forall\ (x,y;t) \in \Omega \times [0,T] \\ u = 0, & \forall\ (x,y;t) \in \partial\Omega \times [0,T] \\ u(x,y;0) = u_0(x,y), & \forall\ (x,y) \in \Omega, t = 0, \end{cases} \tag{1.1}$$

where $\Omega = [0,1]^2$, $u_t = \partial u/\partial t$, $T > 0$ is a constant. The equivalent variational form of (1.1) is: for all $t \in [0,T]$, find $u(t) \in H_0^1(\Omega)$ satisfies the following variational equation:

$$\begin{cases} (u_t, v) + i(\nabla u, \nabla v) = (f, v), & \forall v \in H_0^1(\Omega), \\ a(u(0), v) = a(u_0, v), & \forall v \in H_0^1(\Omega), \end{cases} \tag{1.2}$$

where $(w,v) = \int_\Omega w\bar{v}dx$ denotes the inner product of $L^2(\Omega)$ and $a(u,v) = (\nabla u, \nabla v), i$ be the imaginary unit. We assume that the functions are complex-valued and Hibert spaces are complex spaces.

Let T^h be a quasiuniform rectangulation of Ω with mesh size $h > 0$ and $S^h(\Omega) \subset H_0^1(\Omega)$ be the corresponding piecewise bilinear polynomia space. Then the semidiscrete finite element approximation problem is: for all $t \in [0,T]$, find $u_h(t) \in S^h(\Omega)$ such that

$$\begin{cases} (u_{ht}, v) + ia(u_h, v) = (f, v), & \forall v \in S^h(\Omega), \\ u_h(0) = i_h u_0, & t = 0. \end{cases} \tag{1.3}$$

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Schrödinger equation (1.1) is an important equation in quantum mechanics. The finite element method was studied and a second order convergence was obtained for the linear finite elements in [1]. In this paper, we shall still study the supercovergence analysis for Schrödinger equation solving by bilinear elements and we obtained a second order gradient superconvergence estimate by using integral identities. The remainder of this paper is organized as follows. In section 2, we consider the semidiscrete approximate problem (1.3). In section 3, we shall discuss time discrete approximation scheme.

2. Superconvergence Analysis for Semidiscrete Approximation problem

In this section, we shall discuss the high accuracy analysis for semidiscrete problem (1.3). Let $i_h : C(\Omega) \longrightarrow S^h(\Omega)$ be the bilinear interpolation operator. From Lin[3], we have following results.

Lemma 2.1. *(i). If $u \in H^3(\Omega)$, then*

$$|(\nabla(u - i_h u), \nabla v)| \le Ch^2 \|u\|_3 \|v\|_1, \quad \forall v \in S^h; \tag{2.1}$$

(ii). If $u \in H^4(\Omega)$, then

$$|(\nabla(u - i_h u), \nabla v)| \le Ch^2 \|u\|_4 \|v\|, \quad \forall v \in S^h. \tag{2.2}$$

Lemma 2.2. *If $u_t \in H^3(\Omega)$, then*

$$|((u_t - i_h u_t), v)| \le Ch^2 \|u_t\|_3 \|v\|, \quad \forall v \in S^h. \tag{2.3}$$

Theorem 2.1. *Assume that u and u_h be the solutions of (1.1) and (1.3), respectively, $u_{tt} \in H^3(\Omega), u_t \in H^4(\Omega)$, then there holds*

$$\|u_{ht}(t) - i_h u_t(t)\| \le Ch^2 \Big(\|u_t(0)\|_3 + \|u(0)\|_4 + \int_0^t (\|u_{tt}(s)\|_3 + \|u(s)\|_4) ds \Big). \tag{2.4}$$

Proof. Let $\theta = u_h - i_h u$, then from (1.2) and (1.3)

$$(\theta_t, v) + i(\nabla\theta, \nabla v) = (u_t - i_h u_t, v) + i(\nabla(u - i_h u), \nabla v). \tag{2.5}$$

To estimate θ_t, we first note that, by setting $t = 0, \theta(0) = 0$, and $v = \theta_t(0)$ in (2.5), we get by using (2.2) and (2.3)

$$\|\theta_t(0)\| \le Ch^2 (\|u_t(0)\|_3 + \|u(0)\|_4). \tag{2.6}$$

Differentiating (2.5) with respect to t, we obtain

$$(\theta_{tt}, v) + i(\nabla\theta_t, \nabla v) = (u_{tt} - i_h u_{tt}, v) + i(\nabla(u_t - i_h u_t), \nabla v), \tag{2.7}$$

and hence with $v = \theta_t$,

$$(\theta_{tt}, \theta_t) + i(\nabla\theta_t, \nabla\theta_t) = (u_{tt} - i_h u_{tt}, \theta_t) + i(\nabla(u_t - i_h u_t), \nabla\theta_t). \tag{2.8}$$

Noticing that $(\nabla\theta_t, \nabla\theta_t) \geq 0$ and comparing the real parts of (2.8), by lemma 2.1 and lemma 2.2, we find

$$\frac{1}{2}\frac{d}{dt}\|\theta_t\|^2 = Re(\theta_{tt}, \theta_t) \leq Ch^2(\|u_{tt}\|_3 + \|u_t\|_4)\|\theta_t\|,$$

or

$$\frac{d}{dt}\|\theta_t\| \leq Ch^2(\|u_{tt}\|_3 + \|u_t\|_4).$$

After integration from 0 to t, it yields

$$\|\theta_t\| \leq \|\theta_t(0)\| + Ch^2\int_0^t(\|u_{tt}\|_3 + \|u_t\|_4)ds, \tag{2.9}$$

which yields the result by using (2.6).

Theorem 2.2. *Suppose that u and u_h be the solutions of* (1.1) *and* (1.3)*, respectively, $u_t \in H^3(\Omega), u \in H^4(\Omega)$, then we have following Superconvergence estimate*

$$\|u_h(t) - i_h u(t)\|_1 \leq Ch^2, \tag{2.10}$$

where $C = C(u)$ independent of h.

Proof. Let $\theta = u_h - i_h u$. Since θ_t belongs to S^h, we may choose $v = \theta_t$ in (2.4). Noting that $(\theta_t, \theta_t) \geq 0$, comparing the imaginary parts of (2.5) and using (2.1) and (2.3), we find

$$\frac{1}{2}\frac{d}{dt}\|\nabla\theta\|^2 = Re(\nabla\theta, \nabla\theta_t) \leq Ch^2(\|u_t\|_3 + \|u\|_4)\|\theta_t\|, \tag{2.11}$$

or by theorem 2.1

$$\begin{aligned}\frac{1}{2}\frac{d}{dt}\|\nabla\theta\|^2 \leq& Ch^4(\|u_t\|_3 + \|u\|_4)^2 + \|\theta_t\|^2 \leq Ch^4(\|u_t\|_3 + \|u\|_4)^2\\ &+ Ch^4(\|u_t(0)\|_3 + \|u(0)\|_4 + \int_0^t(\|u_{tt}(s)\|_3 + \|u(s)\|_4)ds.\end{aligned}$$

After integration from 0 to t, we deduce that

$$\|\nabla\theta\|^2 \leq \|\nabla\theta(0)\|^2 + C(u)h^4, \tag{2.12}$$

where

$$\begin{aligned}C(u) =& C\Big\{(\|u_t(0)\|_3 + \|u(0)\|_4)^2 + \int_0^t\{(\|u_t(s)\|_3 + \|u(s)\|_4)^2\\ &+ \int_0^s(\|u_{tt}(\tau)\|^2 + \|u(\tau)\|_4^2)d\tau\}ds\Big\}.\end{aligned}$$

Since $\theta(0) = 0$, hence

$$\|\theta(t)\|_1^2 \leq C(u)h^4,$$

which complete the proof.

3. Superconvergence Estimates for Time Discrete Approximate Scheme

We now turn to the time discrete approximation scheme, Crank-Nicolson-Galerkin scheme. Let τ be the time step and U^n the approximation in $S^h$of $u(t)$ at $t = t_n = n\tau$. Replaced the time derivative in (1.3) by a backward difference quotient

$$\bar{\partial}_t U^n = \tau^{-1}(U^n - U^{n-1}).$$

Defined U^n in S^h recursively by

$$\begin{cases} (\bar{\partial}_t U^n, v) + i(\nabla(U^n + U^{n-1})/2, \nabla v) = (f(t_{n-\frac{1}{2}}), v), & \forall v \in S^h(\Omega), \\ U^0 = i_h u_0, & t = 0. \end{cases} \tag{3.1}$$

Theorem 3.1. *With u and U^n the solutions of* (1.1) *and* (3.1)*, respectively, then*

$$\begin{aligned} \|U^n - i_h u(t_n)\|_1 \le & Ch^2\Big(\|u(0)\|_4 + \int_0^{t_n} (\|u_t(s)\|_3 + \tau\|u(s)\|_4) ds \\ & + C\tau^2 \int_0^{t_n} (\|u_{ttt}(s)\| + \|\Delta u_{tt}(s)\|) ds. \end{aligned} \tag{3.2}$$

Proof. Let $\theta^n = U^n - i_h u(t_n)$, then

$$(\bar{\partial}_t \theta^n, v) + i(\nabla(\theta^n + \theta^{n-1})/2, \nabla v) = (\eta_1^n, v) + i(\Delta\eta_2^n, v) + (\eta_3^n, v) + i(\nabla\eta_4^n, \nabla v), \tag{3.3}$$

where

$$\begin{aligned} &\eta_1^n = u_t(t_{n-\frac{1}{2}}) - \bar{\partial}_t u(t_n), \quad \eta_2^n = u(t_{n-\frac{1}{2}}) - \frac{1}{2}(u(t_n) + u(t_{n-1})), \\ &\eta_3^n = \bar{\partial}_t u(t_n) - \bar{\partial}_t i_h u(t_n), \quad \eta_4^n = \frac{1}{2}\Big(u(t_n) + u(t_{n-1}) - i_h(u(t_n) + u(t_{n-1}))\Big). \end{aligned}$$

Choosing $v = (\theta^n + \theta^{n-1})/2$ in (3.3), since

$$(\nabla(\theta^n + \theta^{n-1})/2, \nabla(\theta^n + \theta^{n-1})/2) \ge 0,$$

we find

$$\begin{aligned} &\frac{1}{2}\tau^{-1}(\|\theta^n\|^2 - \|\theta^{n-1}\|^2) = Re(\bar{\partial}_t \theta^n, (\theta^n + \theta^{n-1})/2) \\ &\quad \le (\|\eta_1^n\| + \|\nabla\eta_2^n\|)\|\theta^n + \theta^{n-1}\|/2 + |(\eta_3^n, (\theta^n + \theta^{n-1})/2)| + |(\nabla\eta_4^n, \nabla(\theta^n + \theta^{n-1})/2)| \end{aligned} \tag{3.4}$$

and

$$\begin{aligned} \|\eta_1^j\| = & \frac{1}{2}\tau^{-1}\Big\| \int_{t_{j-1}}^{t_{j-\frac{1}{2}}} (s - t_{j-1})^2 u_{ttt}(s) ds + \int_{t_{j-\frac{1}{2}}}^{t_j} (s - t_j)^2 u_{ttt}(s) ds \Big\| \\ \le & C\tau \int_{t_{j-1}}^{t_j} \|u_{ttt}(s)\| ds. \end{aligned} \tag{3.5}$$

We obtain

$$\sum_{j=1}^{n}\|\eta_1^j\| = C\tau\int_0^{t_n}\|u_{ttt}(s)\|ds. \tag{3.6}$$

Further

$$\|\triangle\eta_2^j\| = \Big\|\triangle\Big(u(t_{j-\frac{1}{2}}) - \frac{1}{2}(u(t_j)+u(t_{j-1}))\Big)\Big\| \le C\tau\int_{t_{j-1}}^{t_j}\|\triangle u_{tt}(s)\|ds,$$

so that

$$\sum_{j=1}^{n}\|\triangle\eta_2^j\| \le C\tau\int_0^{t_n}\|\triangle u_{tt}(s)\|ds. \tag{3.7}$$

By Lemma 2.1 and Lemma 2.2,

$$\begin{aligned}|(\eta_3^j, v)| &= (\bar{\partial}_t u(t_j) - \bar{\partial}_t i_h u(t_j), v)\\ &= \tau^{-1}|(u(t_j)-u(t_{j-1}) - i_h(u(t_j)-u(t_{j-1})), v)|\\ &\le Ch^2\tau^{-1}\|u(t_j)-u(t_{j-1})\|_3\|v\|,\end{aligned} \tag{3.8}$$

and

$$\sum_{j=1}^{n}\|u(t_j)-u(t_{j-1})\|_3 \le \sum_{j=1}^{n}\int_{t_{j-1}}^{t_j}\|u_t(s)\|_3 ds = \int_0^{t_n}\|u_t(s)\|_3 ds. \tag{3.9}$$

Similarly

$$|(\nabla\eta_4^j, \nabla v)| \le Ch^2\|u(t_j)+u(t_{j-1})\|_4\|v\|, \tag{3.10}$$

and

$$\sum_{j=1}^{n}\|u(t_j)+u(t_{j-1})\|_4 \le 2\sum_{j=0}^{n}\|u(t_j)\|_4 \le \|u(0)\|_4 + \int_0^{t_n}(\|u_t(s)\|_4 + \tau^{-1}\|u(s)\|_4)ds. \tag{3.11}$$

By (3.4) and (3.9), (3.10)

$$\begin{aligned}\|\theta^n\|^2 - \|\theta^{n-1}\|^2 \le &\Big(\tau(\|\eta_1^n\| + \|\nabla\eta_2^n\|) + Ch^2\|u(t_n)-u(t_{n-1})\|_3\\ &+ Ch^2\tau\|u(t_n)+u(t_{n-1})\|_4\Big)(\|\theta^n\| + \|\theta^{n-1}\|).\end{aligned}$$

After cancellation of a common factor,

$$\begin{aligned}\|\theta^n\| \le &\|\theta^{n-1}\| + \tau\|\eta_1^n\| + \tau\|\Delta\eta_2^n\|\\ &+ Ch^2(\|u(t_n)-u(t_{n-1})\|_3 + \tau\|u(t_n)+u(t_{n-1})\|_4).\end{aligned}$$

After repeated application and by (3.4) and (3.5), this yields that

$$\begin{aligned}\|\theta^n\| \le &\tau\sum_{j=1}^{n}\|\eta_1^j\| + \tau\sum_{j=1}^{n}\|\Delta\eta_2^j\|\\ &+ Ch^2\Big(\sum_{j=1}^{n}\|u(t_j)-u(t_{j-1})\|_3 + \tau\sum_{j=1}^{n}\|u(t_j)+u(t_{j-1})\|_4\Big).\end{aligned}$$

Or using (3.6), (3.7), (3.9) and (3.11)

$$\begin{aligned}\|\theta^n\| \leq & Ch^2\Big(\|u(0)\|_4 + \int_0^{t_n}(\|u_t(s)\|_3 + \tau\|u_t(s)\|_4 + \|u(s)\|_4)ds\Big) \\ & + C\tau^2\int_0^{t_n}(\|u_{ttt}(s)\| + \|\triangle u_{tt}(s)\|)ds,\end{aligned}$$

which complete the proof.

From theorem 3.1 we have following result.

Theorem 3.2. *Let u and U^n be the solutions of* (1.1) *and* (3.1)*, respectively, then there holds*

$$\|\bar{\theta}^n\|_1 \leq C_1(u)h^2 + C_2(u)\tau^2, \tag{3.12}$$

where $\bar{\theta}^n = (\theta^n + \theta^{n-1})/2$, $C_1(u)$ and $C_2(u)$ are independent of h.

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