

## GLOBAL SUPERCONVERGENCE ESTIMATES OF FINITE ELEMENT METHOD FOR SCHRÖDINGER EQUATION\*

Qin Lin

(Institute of Systems Science, Academia Sinica, Beijing 100080, China)

Xiao-qi Liu

(Department of Mathematics, Xiangtan Teachers College, Hunan 411201, China)

### 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

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

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:

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

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 Hilbert spaces are complex spaces.

Let  $T^h$  be a quasiuniform rectangulation of  $\Omega$  with mesh size  $h > 0$  and  $S^h(\Omega) \subset H_0^1(\Omega)$  be the corresponding piecewise bilinear polynomials 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

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

---

\* Received December 26, 1995.

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 superconvergence 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  $i_h : C(\Omega) \rightarrow S^h(\Omega)$  be the bilinear interpolation operator. From Lin<sup>[3]</sup>, we have following results.

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

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

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

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

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

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

**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

$$\|u_{ht}(t) - i_h u_t(t)\| \leq Ch^2 \left( \|u_t(0)\|_3 + \|u(0)\|_4 + \int_0^t (\|u_{tt}(s)\|_3 + \|u(s)\|_4) ds \right). \quad (2.4)$$

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

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

To estimate  $\theta_t$ , 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)

$$\|\theta_t(0)\| \leq Ch^2 (\|u_t(0)\|_3 + \|u(0)\|_4). \quad (2.6)$$

Differentiating (2.5) with respect to  $t$ , we obtain

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

and hence with  $v = \theta_t$ ,

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