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The Highest Superconvergence of the Tri-linear Element for Schrödinger Operator with Singularity

Wenming He[1] · **Zhimin Zhang**[2] · **Ren Zhao**[2]

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Abstract In this paper, the eigenvalues for Schrödinger operator with singularity are analyzed. A special piecewise uniform rectangular partition is constructed and it has been proven that, under this partition, the tri-linear rectangular finite element method has the highest possible superconvergence rate for eigenvalue.

Keywords Schrödinger operator · Richardson extrapolation · The highest superconvergence

Mathematics Subject Classification 65N25 · 65N30 · 65N15

1 Introduction

Richardson extrapolations for FEMs for elliptic problem have been presented since 1970's (see, e.g. [1,9,10,12,18,23–26], for an incomplete list of references). Interested readers are referred to the survey article by Blum [8]. In this paper, we are mainly concerned with Richardson extrapolation of finite element methods for second-order elliptic eigenvalue problem.

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✉ Wenming He
he_wenming@aliyun.com

Zhimin Zhang
zzhang@math.wayne.edu

Ren Zhao
rzhao@math.wayne.edu

1 Department of Mathematics, Wenzhou University, Wenzhou 320035, Zhejiang, People's Republic of China

2 Department of Mathematics, Wayne State University, Detroit, MI 48202, USA

Consider the following Helmholtz problem:

$$\begin{cases} -\Delta u = \lambda \rho u, & \text{in } \Omega = (0,1)^2, \\ u = 0, & \text{on } \partial\Omega, \\ \int_\Omega u^2 dx = 1, \end{cases} \tag{1}$$

where $\rho \in H^5(\Omega)$. By applying Richardson extrapolation to the bi-linear element for the problem (1), Lin et al. (see [24]) had the following highest superconvergence result:

$$|\lambda_*^h - \lambda| \leq ch^4, \tag{2}$$

where $\lambda_*^h = \frac{4\lambda^{h/2} - \lambda^h}{3}$ and $u \in H^5(\Omega)$ is assumed.

Schrödinger type operators are of great importance in the field of partial differential equations. In particular, the spectrum of Schrödinger operators attracts tremendous attention for the study of the non-relativistic Born–Oppenheimer approximation of the Schrödinger operators for electrons moving in a lattice of atoms. Modeling such electrons is a critical part of the implementation of the "Density Functional Theory" in Quantum Chemistry [7,16,21]. In addition, Hamiltonian systems with true inverse square potentials arise in relativistic quantum mechanics from the square of the Dirac operator on an electron [19]. Therefore, it is crucial to explore equations involving such operators in different areas of physics and to investigate approximations of solutions to such equations. Many work have been done on approximating Schrödinger type operators numerically. For instance, the problem of optimal approximation of eigenfunctions of Schrödinger operators with isolated inverse square potentials, as well as the solutions to equations involving such operators, were considered (see [20,22]). However, to our best knowledge, no superconvergence result of the FEM has been published for Schrödinger operators. The purpose of this work is to fill in this blank and to obtain the highest possible superconvergence result for eigenvalues of the linear Schrödinger operators.

The rest of the paper is organized as follows. In Sect. 2, we provide some preliminaries and state the main theorem of this paper. In Sect. 3, we decompose the proof of our main results into several steps and present a proof for each step. In the last section, we complete the proof of the main theorem.

2 Preliminaries

For the sake of simplicity and clarity, we only consider the tri-linear element for the following Schrödinger problem:

$$\begin{cases} -\Delta u + \phi(x)u = \lambda u, & \text{in } \Omega = (-a,a)^3, \\ u = 0, & \text{on } \partial\Omega. \end{cases} \tag{3}$$

Here $a > 0$, $\phi(x) \in C^\infty(\Omega \setminus \{(0,0,0)\})$, and there exists a positive constant c and $|\beta| \leq 2$ such that $\frac{|\phi(x)|}{|x|^\beta} \leq c$. It is observed that $u(x)$ is singular at point $(0,0,0)$ and does not belong to the Sobolev space $H^5(\Omega)$.

Definition 1 (See [11]) Suppose $p \in (1, +\infty)$ and assume J is a positive integer, $\varepsilon < \frac{1}{2}$ is a positive constant. Denote a family of weight functions by

$$\omega = \{\omega_\alpha = \omega_\alpha(x), \quad x \in \Omega, |\alpha| \leq J\}, \tag{4}$$

where ω_α are weight functions. We define the weighted Sobolev space

$$W^{J,p}(\Omega,\omega)=\{u\in L^p(\Omega,\omega_\alpha)|D^\alpha u\in L^p(\Omega,\omega_\alpha),\quad |\alpha|\le J\}. \tag{5}$$

Here, $W^{J,p}(\Omega,\omega)$ is a normed linear space when equipped with the norm

$$\|u\|_{W^{J,p}(\Omega,\omega)}=\left(\sum_{|\alpha|\le J}\int_\Omega |D^\alpha u|^p\omega_\alpha^p(x)dx\right)^{1/p}, \tag{6}$$

where $\omega_\alpha(x)=|x|^{|\alpha|}$. We also define

$$\|u\|_{W^{J,\infty}(\Omega,\omega)}=\sum_{|\alpha|\le J}\text{ess sup}_{x\in\Omega}|D^\alpha u(x)\omega_\alpha(x)|, \tag{7}$$

where essential supremum means the lowest upper bound over Ω excluding subsets of Ω of Lebesgue measure zero.

Remark 1 The regularity of eigenfunctions u for Schrödinger operators with periodic potentials was studied in [20], where it was proved that $u\in W^{\infty,\infty}(\Omega\setminus\kappa)$ where κ is a set of all singular points and $\rho(x)$ denotes the distance between x and κ and

$$W^{\infty,\infty}(\Omega\setminus\kappa)=\{v:\rho^{|\alpha|}\partial^\alpha v\in L^\infty(\Omega\setminus\kappa),\quad \forall\alpha\in Z_+^3\}. \tag{8}$$

However, for the problem (3), $u(x)$ does not belong to weighted Sobolev space $W^{\infty,\infty}(\Omega\setminus\{(0,0,0)\})$ for the reason that there exist the singularities near corners or edges, which have been discussed and treated in [13,17,27–32]. In this article, we will only discuss the singularity of $u(x)$ at the point $(0,0,0)$ and assume that $u\in W^{5,\infty}(\Omega,\omega)$. The weak form of (3) is to find $u\in H_0^1(\Omega,\phi)$ satisfying

$$\begin{cases}A(u,v)=\lambda(u,v),\quad \forall v\in H_0^1(\Omega,\phi),\\(u,u)=1,\end{cases} \tag{9}$$

where

$$H^1(u,\phi)=\left(\int_\Omega\left[\sum_{i=1}^3\frac{\partial u}{\partial x_i}\frac{\partial u}{\partial x_i}+\phi(x)u^2(x)\right]dx\right)^{\frac{1}{2}}, \tag{10}$$

and

$$A(u,v)=\int_\Omega\left[\sum_{i=1}^3\frac{\partial u(x)}{\partial x_i}\frac{\partial v(x)}{\partial x_i}+\phi(x)u(x)v(x)\right]dx,\quad (u,v)=\int_\Omega u(x)v(x)dx. \tag{11}$$

In this paper, a more general bilinear form $A_E(\cdot,\cdot)$ is defined by

$$A_E(u,v)=\int_E\left[\sum_{i=1}^3\frac{\partial u(x)}{\partial x_i}\frac{\partial v(x)}{\partial x_i}+\phi(x)u(x)v(x)\right]dx, \tag{12}$$

where E is a bounded domain and functions $u,v\in H^1(E,\phi)$. Define $B(y,r)$ by

$$B(y,r)=\{x:|y-x|\le r\}. \tag{13}$$

Throughout this paper, standard notations for the classical Sobolev spaces and their norms are used. The letter c or C denotes a generic constant which is independent of u and N but may not be the same at each occurrence, where $2N$ denotes the number of nodes that the partition $\mathcal{T}_N$, presented in Sect. 2.1, needs in x_i $(i=1,2,3)$ direction.

2.1 A Special Rectangular Partition for the Problem(3)

Graded mesh has been widely used in finite element method (see [5,6,14,19,20]). For example, Hunsicker et al. (see [19]) proposed a graded partition to obtain the optimal convergence of the linear element for Schrödinger operators with periodic potentials. In this subsection, we construct a special graded partition which is the tensor-product of a one-dimensional graded piecewise uniform partition. Assume that l is a positive integer and N denotes the number of partitions in $[0, a]$ satisfying

$$2^l \leq N \leq 2^{l+1} - 1. \tag{14}$$

We describe the partition as follows.

(i) For $0 \leq p \leq l$, we define

$$b_p = \begin{cases} \frac{a2^{4p}}{\sum_{i=0}^{l-1} 2^{4i} + (N-2^l+1)2^{3l}}, & \text{if } 0 \leq p \leq l-1, \\ \frac{a(N-2^l+1)2^{3l}}{\sum_{i=0}^{l-1} 2^{4i} + (N-2^l+1)2^{3l}}, & \text{if } p = l, \end{cases} \tag{15}$$

and

$$a_p = \begin{cases} b_p, & \text{if } p = 0, \\ \sum_{j=0}^{p} b_j, & \text{if } p \geq 1. \end{cases} \tag{16}$$

(ii) Decompose $[-a, a]$ into

$$[-a, a] = \bigcup_{p=0}^{l} D_p, \tag{17}$$

where

$$D_p = \begin{cases} [-a_0, 0] \cup [0, a_0], & \text{if } p = 0, \\ \left[-a_p, a_{p-1}\right] \cup \left[a_{p-1}, a_p\right], & \text{if } p \geq 1. \end{cases} \tag{18}$$

(iii) We get $\mathcal{T}_{N_{x_1}}$ by splitting D_p into 2^{p+1} intervals with grid size $\frac{a2^{3p}}{\sum_{i=0}^{l-1} 2^{4i} + (N-2^l+1)2^{3l}}$ equally if $0 \leq p \leq l-1$, and $2(N - 2^l + 1)$ uniform partitions with grid size $\frac{a2^{3l}}{\sum_{i=0}^{l-1} 2^{4i} + (N-2^l+1)2^{3l}}$ equally if $p = l$. Similarly, we construct $\mathcal{T}_{N_{x_2}}$ and $\mathcal{T}_{N_{x_3}}$.

Denote the resulting partitions in x_i $(1 \leq i \leq 3)$ direction as $\mathcal{T}_{N_{x_i}}$. The final rectangular mesh is defined by $\mathcal{T}_N = \mathcal{T}_{N_{x_1}} \times \mathcal{T}_{N_{x_2}} \times \mathcal{T}_{N_{x_3}}$.

We choose $a = 1, l = 1, N = 3$ to demonstrate the idea of the mesh construction. The graph for x_1 direction is shown in Fig. 1, and the graded graph is depicted in Fig. 2.

The following results hold true for $\mathcal{T}_N$.

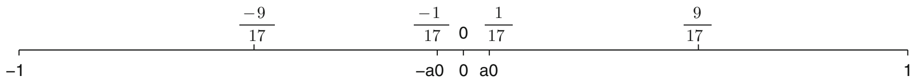

Fig. 1 $\mathcal{T}_{N_{x_1}}$: graded mesh in x_1 direction on $[-1, 1]$

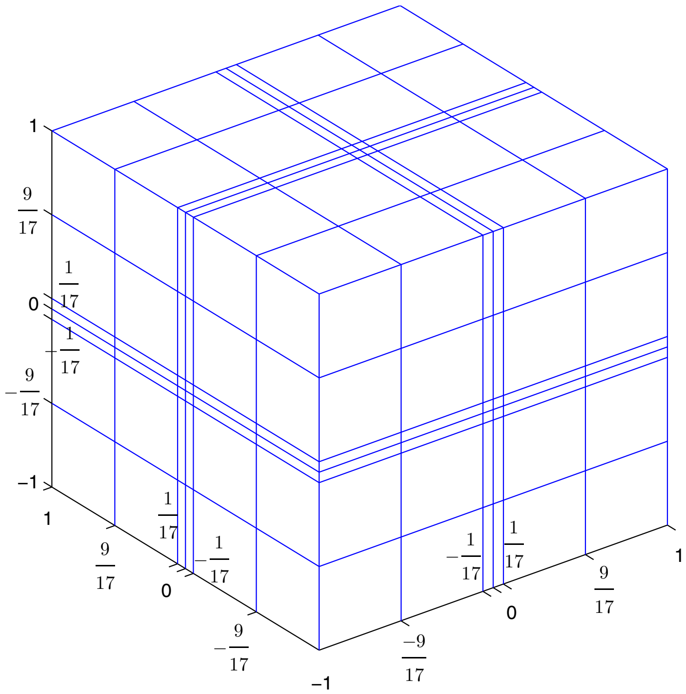

Fig. 2 $\mathcal{T}_N$: graded mesh on $[-1,1]^3$

1. It is obvious that the partition size of $\mathcal{T}_N$ is different in different regions. Set

$$\Omega_p = \begin{cases} \emptyset, & \text{if } p = -1, \\ \prod_{i=1}^{3} \bigcup_{j=0}^{p} D_j, & \text{if } 0 \le p \le l, \end{cases} \tag{19}$$

and

$$\mathcal{T}_{N,p} = \{e : e \subset \Omega_p \setminus \Omega_{p-1}, \quad e \in \mathcal{T}_N\}. \tag{20}$$

We get

$$h_p = b_p 2^{-p} \le c 2^{4(p-l)-p}. \tag{21}$$

Here h_p denotes the grid size of $\mathcal{T}_{N,p}$. Note the fact that the distance between the singular point $(0,0,0)$ and $\Omega_p \setminus \Omega_{p-1}$ is equal to $a_{p-1} = \sum_{j=0}^{p-1} b_j$, and the combination of (15) and (21) implies

$$h_0 \le c 2^{-4l}, \tag{22}$$

and for any $1 \le p \le l$,

$$h_p^4 a_{p-1}^{-3} \le c 2^{16(p-l)-4p} 2^{12(l-p)} = c 2^{-4l}. \tag{23}$$

It is worth to point out that (22) and (23) will play a critical role in the proof of our main results.

2.2 Main Result

Assume that $\overline{\mathcal{T}}_{2N}$ is obtained by splitting every segment of $\mathcal{T}_N$ into eight equal rectangular partitions. Let

$$S^N = \{v \in C(\Omega) : v|_e \in (P_1)^3, \quad \forall e \in \mathcal{T}_N\}$$

and

$$S^{2N} = \{v \in C(\Omega) : v|_e \in (P_1)^3, \quad \forall e \in \mathcal{T}_{2N}\}$$

be the associated tri-linear finite element spaces for $\mathcal{T}_N$ and $\mathcal{T}_{2N}$, respectively. Denote $S_0^N = S^N \cap H_0^1(\Omega)$ and $S_0^{2N} = S^{2N} \cap H_0^1(\Omega, \phi)$. We obtain the tri-linear finite element solution $(\lambda_N, u_N) \in \mathbb{R}^+ \times S_0^N$ and $(\lambda_{2N}, u_{2N}) \in \mathbb{R}^+ \times S_0^{2N}$ for problem (3) from

$$\begin{cases} A(u_N, v) = \lambda_N (u_N, v), \quad \forall v \in S_0^N, \\ (u_N, u_N) = 1, \end{cases} \tag{24}$$

and

$$\begin{cases} A(u_{2N}, v) = \lambda_{2N} (u_{2N}, v), \quad \forall v \in S_0^{2N}, \\ (u_{2N}, u_{2N}) = 1. \end{cases} \tag{25}$$

Using Richardson extrapolation, we obtain the following numerical approximation λ_*^N of λ by

$$\lambda_*^N = \frac{4\lambda_{2N} - \lambda_N}{3}. \tag{26}$$

The main result of this paper states as follows.

Theorem 1 *Let $W^{J,p}(\Omega, \omega)$ be defined as (5). Assume $u \in W^{5,\infty}(\Omega, \omega)$. Then*

$$|\lambda_*^N - \lambda| \le c 2^{-4l} l^2. \tag{27}$$

The following corollary is a direct result from (14) and (27).

Corollary 1 *Under the same assumption of Theorem 1,*

$$|\lambda_*^N - \lambda| \le c N^{-4} |\ln N|^2. \tag{28}$$

Remark 2 Note that (2) is the highest order superconvergent result. For any rectangular partition $\mathcal{T}_h$ with grid size h, we have

$$h \ge c N^{-1}, \tag{29}$$

hence for any linear element, there does not exist $\varepsilon > 0$ independent of N such that

$$|\lambda_*^h - \lambda| \le c N^{-4-\varepsilon}.$$

Combining the above analysis implies that (28) is the best possible error bound in terms of N up to a factor of $|\ln N|^2$.

3 Main Analysis

In the section, we will take the following steps to prove Theorem 1.

(i) We will first show that $\lambda_*^N - \lambda$ can be written into

$$\lambda_*^N - \lambda = \frac{4\lambda_{2N}(u - I_{2N}u, u_{2N}) - \lambda_N(u - I_N u, u_N)}{3} + \frac{4A(I_{2N}u - u, u_{2N}) - A(I_N u - u, u_N)}{3} + \frac{4\lambda_{2N}(u - R_{2N}u, \overline{u}_{2N} - u_{2N}) - \lambda_N(u - R_N u, \overline{u}_N - u_N)}{3}, \quad (30)$$

where $\overline{u}_N, \overline{u}_{2N}, R_N u \in S_0^N$ and $R_{2N}u \in S_0^{2N}(x)$ are respectively defined by

$$\overline{u}_N = \frac{u_N}{(u, u_N)}, \quad \overline{u}_{2N} = \frac{u_{2N}}{(u, u_{2N})}, \quad (31)$$

and

$$A(R_N u, v) = A(u, v), \forall v \in S_0^N, \quad (32)$$

and

$$A(R_{2N}u, v) = A(u, v), \forall v \in S_0^{2N}.$$

(ii) The following convergence estimation will be proved secondly.

$$|\lambda - \lambda_N| + \|u - u_N\|_{L^2(\Omega)} + \|u - R_N u\|_{L^2(\Omega)} + \|u_N - \overline{u}_N\|_{L^2(\Omega)} + \|u - I_N u\|_{L^2(\Omega)} \leq c2^{-2l} l. \quad (33)$$

(iii) We then give a proof of the following estimation:

$$|4A(I_{2N}u - u, u_{2N}) - A(I_N u - u, u_N)| + |4(u - I_{2N}u, u_{2N}) - (u - I_N u, u_N)| \leq c2^{-4l} l^2. \quad (34)$$

(iv) Based on (30), (33) and (34), we complete the proof of (27).

3.1 Analysis I

We now give a proof of (30). Note that from (9), (31) and (32), we have

$$\lambda = \lambda(u, \overline{u}_N) = A(u, \overline{u}_N) = A(R_N u, \overline{u}_N) = \lambda_N(R_N u, \overline{u}_N), \quad (35)$$

and the combination of (24), (31) and (32) will give

$$\begin{aligned}
\lambda_N &= \lambda_N(u, \overline{u}_N) = \lambda_N(R_N u, \overline{u}_N) + \lambda_N(u - R_N u, \overline{u}_N) \\
&= \lambda_N(R_N u, \overline{u}_N) + \lambda_N(u - R_N u, u_N) + \lambda_N(u - R_N u, \overline{u}_N - u_N) \\
&= \lambda_N(R_N u, \overline{u}_N) + \lambda_N(u - I_N u, u_N) + \lambda_N(I_N u - R_N u, u_N) + \lambda_N(u - R_N u, \overline{u}_N - u_N) \\
&= \lambda_N(R_N u, \overline{u}_N) + \lambda_N(u - I_N u, u_N) + A(I_N u - R_N u, u_N) + \lambda_N(u - R_N u, \overline{u}_N - u_N) \\
&= \lambda_N(R_N u, \overline{u}_N) + \lambda_N(u - I_N u, u_N) + A(I_N u - u, u_N) + \lambda_N(u - R_N u, \overline{u}_N - u_N).
\end{aligned}$$

The above two equalities imply that $\lambda_N - \lambda$ can be decomposed into

$$\lambda_N - \lambda = \lambda_N(u - R_N u, \overline{u}_N - u_N) + \lambda_N(u - I_N u, u_N) + A(I_N u - u, u_N).$$

Similarly,

$$\lambda_{2N} - \lambda = \lambda_{2N}(u - R_{2N}u, \overline{u}_{2N} - u_{2N}) + \lambda_{2N}(u - I_{2N}u, u_{2N}) + A(I_{2N}u - u, u_{2N}).$$

From the above two identities, together with (26), we get the desired result (30).

3.2 Analysis II

Now we proceed to prove the convergence estimation (33). Firstly, we introduce the following convergence estimate.

Lemma 1 *Under the assumption that $u \in W^{2,\infty}(\Omega, \omega)$,*

$$\|u - I_N u\|_{H^1(\Omega,\phi)} + \|u - u_N\|_{H^1(\Omega,\phi)} \le c2^{-l} l^{\frac{1}{2}}. \tag{36}$$

Proof Assume that $I_N u$, the modified degree trilinear Lagrange "interpolant" associated to the mesh $\mathcal{T}_N$, satisfies

$$I_N u(x) = \begin{cases} u(x), & \text{if } x \text{ is a node satisfying } x \neq 0, \\ 0, & \text{if } x = 0. \end{cases} \tag{37}$$

Let Ω_p and $\mathcal{T}_{N,p}$ be defined by (19) and (20), respectively. We first observe the following decomposition:

$$\|u - I_N u\|^2_{H^1(\Omega,\phi)} = \|\nabla(u - I_N u)\|^2_{L^2(\Omega)} + \int_\Omega \phi(x)(u - I_N u)^2(x)dx. \tag{38}$$

Now, we need to estimate the two terms on the right-hand side of (38). Assume that $\Omega_{-1} = \emptyset$. For the first term, we can split it as

$$\|\nabla(u - I_N u)\|^2_{L^2(\Omega)} = \sum_{p=0}^{l} \|\nabla(u - I_N u)\|^2_{L^2(\Omega_p \backslash \Omega_{p-1})}. \tag{39}$$

By (22), we have

$$\|\nabla(u - I_N u)\|^2_{L^2(\Omega_0)} \le \|u\|^2_{H^1(\Omega_0)} \le c\|u\|^2_{W^{1,\infty}(\Omega_0,\omega)} \int_{\Omega_0} \frac{1}{|x|^2} dx \le ch_0 \le c2^{-4l}. \tag{40}$$

Denote the volume of Ω_p by V_{Ω_p} and by (23) for all $1 \le p \le l$,

$$\begin{aligned} &\|\nabla(u - I_N u)\|^2_{L^2(\Omega_p \backslash \Omega_{p-1})} \le cV_{\Omega_p} h_p^2 \|u\|^2_{W_2^\infty(\Omega_p \backslash \Omega_{p-1})} \\ &\le ca_{p-1}^3 h_p^2 a_{p-1}^{-4} \|u\|^2_{W_2^\infty(\Omega_p \backslash \Omega_{p-1},\omega)} \le ch_p^2 a_{p-1}^{-1} \le c2^{8(p-l)-2p} 2^{4(l-p)} \le c2^{-2l}. \end{aligned}$$

Inserting the above two estimates into (39), we obtain

$$\|\nabla(u - I_N u)\|^2_{L^2(\Omega)} \le c2^{-2l} l, \tag{41}$$

Assume that $\Omega_{-1} = \emptyset$. For the second term in (38), we decompose it as

$$\int_\Omega \phi(x)(u - I_N u)^2(x)dx = \sum_{p=0}^{l} \int_{\Omega_p \backslash \Omega_{p-1}} \phi(x)(u - I_N u)^2(x)dx. \tag{42}$$

Then (22) gives

$$\left|\int_{\Omega_0}\phi(x)(u-I_Nu)^2(x)dx\right| \le \|u\|^2_{L^\infty(\Omega_0,\omega)}\|\phi^2\|_{L^1(\Omega_0)} \le c\|u\|^2_{L^\infty(\Omega_0,\omega)}ch_0$$
$$\le c\|u\|^2_{L^\infty(\Omega_0,\omega)}c2^{-4l} \le c2^{-4l}, \tag{43}$$

and (23) implies, for all $1 \le p \le l$,

$$\left|\int_{\Omega_p\backslash\Omega_{p-1}}\phi(x)(u-I_Nu)^2(x)dx\right| \le ca_{p-1}^{-2}V_{\Omega_p}\|u-I_Nu\|^2_{L^\infty(\Omega_p\backslash\Omega_{p-1})}$$
$$\le ca_{p-1}^{-2}a_{p-1}^3h_p^4\|u\|^2_{W_2^\infty(\Omega_p\backslash\Omega_{p-1})} \le ca_{p-1}h_p^4a_{p-1}^{-4}\|u\|^2_{W^{2,\infty}(\Omega_p\backslash\Omega_{p-1},\omega)}$$
$$\le ch_p^4a_{p-1}^{-3}\|u\|^2_{W^{2,\infty}(\Omega_p\backslash\Omega_{p-1},\omega)} \le c2^{-4l}. \tag{44}$$

Combining (42) and the above two estimates, we get

$$\int_\Omega \phi(x)(u-I_Nu)^2(x)dx \le c2^{-4l}l. \tag{45}$$

Thus, inserting (41) and (45) into (38), we have

$$\|u-I_Nu\|_{H^1(\Omega,\phi)} \le c2^{-l}l^{\frac{1}{2}}. \tag{46}$$

This implies the desired result in (36).

According to the estimates for the errors in eigenvalue and eigenvector approximation presented by Babuska et al. (see [3,4]) , we now give a proof of (33) based on Lemma 1. Similar to (46), we have

$$\|u-I_Nu\|_{L^2(\Omega)} \le c2^{-2l}l. \tag{47}$$

The following result is showed by Babuska et al. (see [3,4]):

$$|\lambda-\lambda_N| + \|u-u_N\|_{L^2(\Omega)} + \|u-R_Nu\|_{L^2(\Omega)} + \|u_N-\overline{u}_N\|_{L^2(\Omega)}$$
$$\le \|u-u_N\|^2_{H^1(\Omega,\phi)}. \tag{48}$$

By (36) and (48), we get

$$|\lambda-\lambda_N| + \|u-u_N\|_{L^2(\Omega)} + \|u-R_Nu\|_{L^2(\Omega)} + \|u_N-\overline{u}_N\|_{L^2(\Omega)} \le c2^{-2l}l.$$

This, together with (47), gives the desired result in (33).

3.3 Analysis III

Now we are ready to give a proof of (34) and the following steps will be used to approach (34).

(i) Assume that $k(i) = i+1$ if $i = 1$ or 2, and $k(i) = 1$ if $i = 3$. Suppose $D_i = \frac{\partial}{\partial x_i}$, $e \in \mathcal{T}_N$ satisfies $e \subset \Omega\backslash\Omega_0$, and let $h_e^{x_{k(i)}}$ and h_e denote the grid size of $e \in \mathcal{T}_N$ in $x_{k(i)}$ direction and e, respectively. We shall prove the following two expansion identities (a) and (b):

$$(a)\quad \int_e \frac{\partial(u-I_N u)(x)}{\partial x_i}\frac{\partial v(x)}{\partial x_i}dx \quad = -\frac{1}{3}\int_e \left(h_e^{x_{k(i)}}\right)^2 D^2_{k(i)} D_i u(x) D_i v(x) dx$$
$$+\int_e F(x_{k(i)})\left[D^4_{k(i)} D_i u(x) D_i v(x) + 4 D^3_{k(i)} D_i u(x) D_i D_{k(i)} v(x)\right] dx, \tag{49}$$
$$(b)\quad \int_e (u-I_N u)(x) v(x) dx = -\sum_{i=1}^{3}\frac{(h_e^{x_i})^2}{3}\int_e D_i^2 u(x) v(x) dx$$
$$+\,o(h_e^4)\left[\|u\|_{H^3(e)}\|v\|_{H^1(e)} + \|u\|_{H^4(e)}\|v\|_{L^2(e)}\right], \tag{50}$$

where $x_e = (x_{1,e}, x_{2,e}, x_{3,e})$ is the center of e, $x = (x_1, x_2, x_3)$ and $B(x_i) = \frac{1}{2}[(x_i - x_{i,e})^2 - (h_e^{x_i})^2]$, $\quad F(x_i) = \frac{1}{6}B^2(x_i)$ $(i = 1, 2, 3)$.

(ii) We then give a proof of the following superconvergence estimate:

$$\|I_N u - u_N\|_{H^1(\Omega,\phi)} \le c2^{-2l} l. \tag{51}$$

(iii) Based on (49), (50) and (51), we give a proof of (34).

3.3.1 *Proof of* (49) *and* (50)

Let us first consider (49). For any $v \in S^N$,

$$\begin{aligned}
\int_e D_i(u-I_N u)(x) D_i v(x) dx &= -\int_e B'(x_{k(i)}) D_{k(i)}(D_i(u-I_N u)(x) D_i v(x)) dx \\
&= \int_e B(x_{k(i)}) D^2_{k(i)}(D_i(u-I_N u)(x) D_i v(x)) dx \\
&= \int_e B(x_{k(i)}) D^2_{k(i)} D_i u(x) D_i v(x) dx \\
&\quad + 2\int_e B(x_{k(i)}) D_{k(i)} D_i(u-I_N u)(x) D_i D_{k(i)} v(x) dx \\
&=: K_1 + K_2.
\end{aligned} \tag{52}$$

Note that

$$\begin{aligned}
K_1 &= \int_e \left[F''(x_{k(i)}) - (h_e^{x_{k(i)}})^2/3\right] D^2_{k(i)} D_i u(x) D_i v(x) dx \\
&= \int_e F(x_{k(i)}) D^4_{k(i)} D_i u(x) D_i v(x) dx + 2\int_e F(x_{k(i)}) D^3_{k(i)} D_i u(x) D_{k(i)} D_i v(x) dx \\
&\quad - \frac{(h_e^{x_{k(i)}})^2}{3}\int_e D^2_{k(i)} D_i u(x) D_i v(x) dx,
\end{aligned} \tag{53}$$

and

$$\begin{aligned}
K_2 &= 2\int_e F''(x_{k(i)}) D_i D_{k(i)}(u-I_N u)(x) D_i D_{k(i)} v(x) dx \\
&\quad - \frac{2(h_e^{x_{k(i)}})^2}{3}\int_e D_i D_{k(i)}(u-I_N u)(x) D_i D_{k(i)} v(x) dx \\
&= -2\int_e F'(x_{k(i)}) D_i D^2_{k(i)} u(x) D_i D_{k(i)} v(x) dx \\
&= 2\int_e F(x_{k(i)}) D_i D^3_{k(i)} u(x) D_i D_{k(i)} v(x) dx.
\end{aligned} \tag{54}$$

Inserting (53) and (54) into (52), we get the desired result (49). A proof of (50) can be obtained in a similar way.

3.3.2 Proof of (51)

We decompose $I_N u - u_N$ into

$$I_N u - u_N = (I_N u - R_N u) + (R_N u - u_N). \tag{55}$$

We first estimate the first term in the right-hand side. By (32), we have

$$\begin{aligned} &A(I_N u - R_N u, I_N u - R_N u) = A(I_N u - u, I_N u - R_N u) \\ &= \sum_{p=0}^{l} A_{\Omega_p \backslash \Omega_{p-1}}(I_N u - u, I_N u - R_N u) =: \sum_{p=0}^{l} T_p. \end{aligned} \tag{56}$$

We first estimate T_0. From (40) and (43) it follows that

$$\begin{aligned} \left| A_{\Omega_0}(I_N u - u, I_N u - R_N u) \right| &\leq c\|I_N u - u\|_{H^1(\Omega_0,\phi)} \|I_N u - R_N u\|_{H^1(\Omega_0,\phi)} \\ &\leq c 2^{-2l} \|I_N u - R_N u\|_{H^1(\Omega_0,\phi)}. \end{aligned} \tag{57}$$

Next we estimate T_p $(1 \leq p \leq l)$. By (49), we derive

$$\begin{aligned} &\int_{\Omega_p \backslash \Omega_{p-1}} \frac{\partial (u - I_N u)(x)}{\partial x_i} \frac{\partial (I_N u - R_N u)(x)}{\partial x_i} dx \\ &\leq c h_p^2 a_{p-1}^{\frac{3}{2}} \|u\|_{W_3^\infty(\Omega_p \backslash \Omega_{p-1})} \|I_N u - R_N u\|_{H^1(\Omega_p \backslash \Omega_{p-1})} \\ &\leq c h_p^2 a_{p-1}^{\frac{3}{2}-3} \|u\|_{W^{3,\infty}(\Omega_p \backslash \Omega_{p-1},\omega)} \|I_N u - R_N u\|_{H^1(\Omega_p \backslash \Omega_{p-1})} \\ &\leq c 2^{2\times 4(p-l)-p)} 2^{\frac{-3}{2}\times 4(p-l)} \|I_N u - R_N u\|_{H^1(\Omega_p \backslash \Omega_{p-1})} \\ &\leq c 2^{-2l} \|I_N u - R_N u\|_{H^1(\Omega_p \backslash \Omega_{p-1})}. \end{aligned} \tag{58}$$

Note that

$$\begin{aligned} &\left| \int_{\Omega_p \backslash \Omega_{p-1}} \phi(x)(I_N u - u)(x)(I_N u - R_N u)(x) dx \right| \\ &\leq c\|I_N u - R_N u\|_{H^1(\Omega,\phi)} \left(\int_{\Omega_p \backslash \Omega_{p-1}} \phi(x)(I_N u - u)^2(x) dx \right)^{\frac{1}{2}} \\ &\leq c\|I_N u - R_N u\|_{H^1(\Omega,\phi)} a_{p-1}^{-1} h_p^2 a_{p-1}^{\frac{3}{2}} \|u\|_{W_2^\infty(\Omega_p \backslash \Omega_{p-1})} \\ &\leq c\|I_N u - R_N u\|_{H^1(\Omega,\phi)} a_{p-1}^{-1} h_p^2 a_{p-1}^{\frac{3}{2}} a_{p-1}^{-2} \|u\|_{W^{2,\infty}(\Omega,\omega)} \\ &\leq c\|I_N u - R_N u\|_{H^1(\Omega,\phi)} h_p^2 a_{p-1}^{\frac{-3}{2}} \leq c 2^{-2l} \|I_N u - R_N u\|_{H^1(\Omega,\phi)}. \end{aligned} \tag{59}$$

Plugging (58) and (59) into the equality (56), we have

$$T_p \leq c 2^{-2l} \|I_N u - R_N u\|_{H^1(\Omega,\phi)}. \tag{60}$$

Hence,

$$\|I_N u - R_N u\|^2_{H^1(\Omega,\phi)} = \sum_{p=0}^{l} T_p \le c2^{-2l} l \|I_N u - R_N u\|_{H^1(\Omega,\phi)}. \tag{61}$$

Furthermore, by (61), we arrive at

$$\|I_N u - R_N u\|_{H^1(\Omega,\phi)} \le c2^{-2l} l. \tag{62}$$

We now proceed to estimate the second term of the right-hand side of (55). By (32), one has

$$\begin{aligned}
&A(R_N u - u_N, R_N u - u_N) = A(R_N u, R_N u - u_N) - A(u_N, R_N u - u_N)\\
&= A(u, R_N u - u_N) - \lambda_N (u_N, R_N u - u_N)\\
&= \lambda(u, R_N u - u_N) - \lambda_N (u_N, R_N u - u_N)\\
&= (\lambda - \lambda_N)(u, R_N u - u_N) + \lambda_N (u - u_N, R_N u - u_N).
\end{aligned}$$

This estimate, together with (33), gives

$$\begin{aligned}
\|R_N u - u_N\|^2_{H^1(\Omega,\phi)} &\le |\lambda - \lambda_N| \times |(u, R_N u - u_N)| + |\lambda_N| \times |(u - u_N, R_N u - u_N)|\\
&\le c2^{-2l} l c2^{-2l} l + c2^{-2l} l c2^{-2l} l \le c2^{-4l} l^2.
\end{aligned}$$

Therefore,

$$\|R_N u - u_N\|_{H^1(\Omega,\phi)} \le c2^{-2l} l. \tag{63}$$

Combining the estimates (55), (62) and (63) gives the desired result (51).

3.3.3 Proof of (34)

One observes that $\int_\Omega \frac{\partial(u - I_N u)}{\partial x_i} \frac{\partial u_N}{\partial x_i} dx$ can be decomposed into

$$\int_\Omega \frac{\partial(u - I_N u)}{\partial x_i} \frac{\partial u_N}{\partial x_i} dx = \int_{\Omega_0} + \int_{\Omega \setminus \Omega_0} \frac{\partial(u - I_N u)}{\partial x_i} \frac{\partial u_N}{\partial x_i} dx. \tag{64}$$

We now estimate the two terms of the right-hand side. At first, by (51), we have

$$\begin{aligned}
&\left| \int_{\Omega_0} \frac{\partial(u - I_N u)}{\partial x_i} \frac{\partial u_N}{\partial x_i} dx \right|\\
&\le c\|u - I_N u\|_{H^1(\Omega_0)} \left(\|u - I_N u\|_{H^1(\Omega_0)} + \|I_N u - u_N\|_{H^1(\Omega_0)} + \|u\|_{H^1(\Omega_0)} \right)\\
&\le c\left(\int_{\Omega_0} |x|^{-2} dx \right)^{\frac{1}{2}} \left[\left(\int_{\Omega_0} |x|^{-2} dx \right)^{\frac{1}{2}} + 2^{-2l} l \right] \le c2^{-2l} 2^{-2l} l \le c2^{-4l} l.
\end{aligned} \tag{65}$$

To estimate $\sum_{e \subset \Omega \setminus \Omega_0} \int_e \frac{\partial(u - I_N u)}{\partial x_i} \frac{\partial u_N}{\partial x_i} dx$, we split it into

$$\begin{aligned}
&\sum_{e \subset \Omega \setminus \Omega_0} \int_e \frac{\partial(u - I_N u)}{\partial x_i} \frac{\partial u_N}{\partial x_i} dx\\
&= \sum_{e \subset \Omega \setminus \Omega_0} \int_e \frac{\partial(u - I_N u)}{\partial x_i} \frac{\partial(u_N - I_N u)}{\partial x_i} dx + \sum_{e \subset \Omega \setminus \Omega_0} \int_e \frac{\partial(u - I_N u)}{\partial x_i} \frac{\partial I_N u}{\partial x_i} dx.
\end{aligned} \tag{66}$$

We first estimate the first item of the right-hand side. It follows from (51) that

$$\left|\sum_{e\subset\Omega\setminus\Omega_0}\int_e \frac{\partial(u-I_Nu)}{\partial x_i}\frac{\partial(u_N-I_Nu)}{\partial x_i}dx\right| \le c2^{-4l}l^2. \tag{67}$$

Next we estimate the second item of the right-hand side. By (49), we have the following decomposition for $\sum_{e\subset\Omega_p\setminus\Omega_{p-1}}\int_e \frac{\partial(u-I_Nu)}{\partial x_i}\frac{\partial I_Nu}{\partial x_i}dx$ for all $1\le p\le l$:

$$\begin{aligned}\sum_{e\subset\Omega_p\setminus\Omega_{p-1}}\int_e \frac{\partial(u-I_Nu)}{\partial x_i}\frac{\partial I_Nu}{\partial x_i}dx &= -\frac{1}{3}\sum_{e\subset\Omega_p\setminus\Omega_{p-1}}\int_e \left(h_e^{x_{k(i)}}\right)^2 D_{k(i)}^2 D_i u(x) D_i I_N u(x)dx\\ &\quad+\sum_{e\subset\Omega_p\setminus\Omega_{p-1}}\int_e F(x_{k(i)})D_{k(i)}^4 D_i u(x)D_i I_N u(x)dx\\ &\quad+4\sum_{e\subset\Omega_p\setminus\Omega_{p-1}}\int_e F(x_{k(i)})D_{k(i)}^3 D_i u(x) D_i D_{k(i)} I_N u(x)dx\\ &=: I_1+I_2+I_3.\end{aligned} \tag{68}$$

To estimate I_1, we decompose it into

$$\begin{aligned}I_1 &= \frac{1}{3}\sum_{e\subset\Omega_p\setminus\Omega_{p-1}}\int_e \left(h_e^{x_{k(i)}}\right)^2 D_{k(i)}^2 D_i^2 u(x) I_N u(x)dx\\ &= \frac{1}{3}\sum_{e\subset\Omega_p\setminus\Omega_{p-1}}\int_e \left(h_e^{x_{k(i)}}\right)^2 D_{k(i)}^2 D_i^2 u(x)(I_N u-u)(x)dx\\ &\quad+\frac{1}{3}\int_e \left(h_e^{x_{k(i)}}\right)^2 D_{k(i)}^2 D_i^2 u(x)u(x)dx\\ &=: I_{1,1}+I_{1,2}.\end{aligned} \tag{69}$$

Note that

$$\begin{aligned}|I_{1,1}| &\le ch_p^2 a_p^{\frac{3}{2}}\|u\|_{W_4^\infty(\Omega_p\setminus\Omega_{p-1})} ch_p^2 a_p^{\frac{3}{2}}\|u\|_{W^{2,\infty}(\Omega_p\setminus\Omega_{p-1})}\\ &\le ch_p^4 a_p^3 \|u\|_{W_4^\infty(\Omega_p\setminus\Omega_{p-1})}\|u\|_{W_2^\infty(\Omega_p\setminus\Omega_{p-1})}\\ &\le ch_p^4 a_p^3 a_p^{-4}\|u\|_{W^{4,\infty}(\Omega_p\setminus\Omega_{p-1},\omega)} a_p^{-2}\|u\|_{W^{2,\infty}(\Omega_p\setminus\Omega_{p-1},\omega)} \le ch_p^4 a_p^{-3}\le c2^{-4l},\end{aligned}$$

then we obtain

$$|I_1 - I_{1,2}| \le c2^{-4l}.$$

To estimate I_2, we decompose it into

$$\begin{aligned}|I_2| &\le ch_p^4\|u\|_{H^5(\Omega_p\setminus\Omega_{p-1})}\|I_N u\|_{H^1(\Omega_p\setminus\Omega_{p-1})}\\ &\le ch_p^4 a_p^{3/2} a_p^{-5}\|u\|_{W^{5,\infty}(\Omega,\omega)} a_p^{3/2} a_p^{-1}\|u\|_{W^{1,\infty}(\Omega,\omega)} \le ch_p^4 a_p^{-3} \le c2^{-4l}.\end{aligned}$$

Similarly,

$$\begin{aligned}|I_3| &\le ch_p^4\|u\|_{H^4(\Omega_p\setminus\Omega_{p-1})}\sum_{e\subset\Omega_p\setminus\Omega_{p-1}}\|I_N u\|_{H^2(e)}\\ &\le ch_p^4 a_p^{3/2} a_p^{-4}\|u\|_{W^{4,\infty}(\Omega,\omega)} a_p^{3/2}\|u\|_{W_2^\infty(\Omega_p\setminus\Omega_{p-1})}\\ &\le ch_p^4 a_p^3 a_p^{-4} a_p^{-2}\|u\|_{W_2^\infty(\Omega,\omega)} \le ch_p^4 a_p^{-3}\le c2^{-4l}.\end{aligned}$$

Substituting the above three estimates into (68), we derive

$$\sum_{p=1}^{l}\left|\sum_{e\subset\Omega_p\backslash\Omega_{p-1}}\int_e \frac{\partial(u-I_Nu)}{\partial x_i}\frac{\partial I_N u}{\partial x_i}-\frac{1}{3}\left(h_e^{x_{k(i)}}\right)^2 D_{k(i)}^2 D_i^2 u(x)u(x)dx\right|$$
$$\leq c2^{-4l}l. \tag{70}$$

Inserting (67) and (70) into (66), we arrive at

$$\sum_{p=1}^{l}\left|\sum_{e\subset\Omega_p\backslash\Omega_{p-1}}\int_e \left(\frac{\partial(u-I_Nu)}{\partial x_i}\frac{\partial u_N}{\partial x_i}-\frac{1}{3}\left(h_e^{x_{k(i)}}\right)^2 D_{k(i)}^2 D_i^2 u(x)u(x)\right)dx\right|$$
$$\leq c2^{-4l}l. \tag{71}$$

Furthermore, by (64), (65) and (71), one observes that

$$\left|\int_\Omega \frac{\partial(u-I_Nu)}{\partial x_i}\frac{\partial u_N}{\partial x_i}dx-\sum_{p=1}^{l}\sum_{e\subset\Omega_p\backslash\Omega_{p-1}}\int_e \frac{1}{3}\left(h_e^{x_{k(i)}}\right)^2 D_{k(i)}^2 D_i^2 u(x)u(x)dx\right|$$
$$\leq c2^{-4l}l.$$

Similarly,

$$\left|\int_\Omega 4\frac{\partial(u-I_{2N}u)}{\partial x_i}\frac{\partial u_{2N}}{\partial x_i}dx-\sum_{p=1}^{l}\sum_{e\subset\Omega_p\backslash\Omega_{p-1}}\int_e \frac{1}{3}\left(h_e^{x_{k(i)}}\right)^2 D_{k(i)}^2 D_i^2 u(x)u(x)dx\right|$$
$$\leq c2^{-4l}l.$$

Combining the above two estimates, we have

$$\left|\int_\Omega \left[4\frac{\partial(u-I_{2N}u)}{\partial x_i}\frac{\partial u_{2N}}{\partial x_i}-\frac{\partial(u-I_Nu)}{\partial x_i}\frac{\partial u_N}{\partial x_i}\right]dx\right|\leq c2^{-4l}l^2. \tag{72}$$

We now turn to the estimation of $4\int_\Omega \phi(x)(u-I_{2N}u)(x)u_{2N}(x)dx-\int_\Omega \phi(x)(u-I_Nu)(x)u_N(x)dx$. We split $\int_\Omega \phi(x)(u-I_Nu)u_N(x)dx$ into

$$\int_\Omega \phi(x)(u-I_Nu)(x)u_N(x)dx$$
$$=\int_\Omega \phi(x)(u-I_Nu)(x)(u_N-I_Nu)(x)dx+\int_\Omega \phi(x)(u-I_Nu)(x)I_Nu(x)dx$$
$$=:\ J_1+J_2. \tag{73}$$

By (62),

$$|J_1|\leq c2^{-4l}l^2. \tag{74}$$

To estimate J_2, one observes that

$$\left|\int_{\Omega_0}\phi(x)(u-I_Nu)(x)I_Nu(x)dx\right|\leq c\int_{\Omega_0}|x|^{-2}dx\|u-I_Nu\|_{L^\infty(\Omega_0)}\|I_Nu\|_{L^\infty(\Omega_0)}$$
$$\leq ch_0^1\|u\|_{W^{1,\infty}(\Omega,\omega)}\|u\|_{W^{1,\infty}(\Omega,\omega)}\leq c2^{-4l}. \tag{75}$$

Set $\mu(x) = \phi(x) I_N u(x)$ and assume $p \geq 1$. We have the following decomposition

$$\begin{aligned}
&\int_{\Omega_p \setminus \Omega_{p-1}} \phi(x)(u - I_N u)(x) I_N u(x) dx \\
&= \int_{\Omega_p \setminus \Omega_{p-1}} (u - I_N u)(x) I_N \mu(x) dx + \int_{\Omega_p \setminus \Omega_{p-1}} (u - I_N u)(x)(\mu - I_N \mu)(x) dx \\
&=: B_1 + B_2. \qquad (76)
\end{aligned}$$

By (50), B_1 can be decomposed into

$$\begin{aligned}
B_1 &= \sum_{e \subset \Omega_p \setminus \Omega_{p-1}} \int_e (u - I_N u)(x) I_N \mu(x) dx \\
&= - \sum_{e \subset \Omega_p \setminus \Omega_{p-1}} \sum_{i=1}^{3} \frac{(h_e^{x_i})^2}{3} \int_e D_i^2 u(x) I_N \mu(x) dx \\
&\quad + \sum_{e \subset \Omega_p \setminus \Omega_{p-1}} o(h_e^4) \left[\|u\|_{H^3(e)} \|\mu\|_{H^1(e)} + \|u\|_{H^4(e)} \|\mu\|_{L^2(e)} \right] \\
&= - \sum_{e \subset \Omega_p \setminus \Omega_{p-1}} \sum_{i=1}^{3} \frac{(h_e^{x_i})^2}{3} \int_e D_i^2 u(x) (I_N \mu - \phi u)(x) dx \\
&\quad - \sum_{e \subset \Omega_p \setminus \Omega_{p-1}} \sum_{i=1}^{3} \frac{(h_e^{x_i})^2}{3} \int_e D_i^2 u(x) \phi(x) u(x) dx \\
&\quad + \sum_{e \subset \Omega_p \setminus \Omega_{p-1}} o\left(h_e^4\right) \left[\|u\|_{H^3(e)} \|\mu\|_{H^1(e)} + \|u\|_{H^4(e)} \|\mu\|_{L^2(e)} \right] \\
&=: B_{1,1} + B_{1,2} + B_{1,3}. \qquad (77)
\end{aligned}$$

So we need to estimate the three terms in the right-hand side. Note that $\mu = \phi I_N u$ implies

$$\begin{aligned}
&\|I_N \mu - \phi u\|_{L^2(\Omega_p \setminus \Omega_{p-1})} \leq \|I_N \mu - \mu\|_{L^2(\Omega_p \setminus \Omega_{p-1})} + \|\phi(I_N u - u)\|_{L^2(\Omega_p \setminus \Omega_{p-1})} \\
&\leq c h_p^2 a_p^{\frac{3}{2}} \|\mu\|_{W_2^\infty(\Omega_p \setminus \Omega_{p-1})} + c h_p^2 a_p^{\frac{3}{2}} \|\phi\|_{L^\infty(\Omega_p \setminus \Omega_{p-1})} \|\nabla^2 u\|_{L^\infty(\Omega_p \setminus \Omega_{p-1})} \\
&\leq c h_p^2 a_p^{\frac{3}{2}} a_p^{-4} + c h_p^2 a_p^{\frac{3}{2}} a_p^{-2} a_p^{-2} \leq c h_p^2 a_p^{-\frac{5}{2}}. \qquad (78)
\end{aligned}$$

Combining (23) and (78) gives

$$\begin{aligned}
|B_{1,1}| &\leq c h_p^2 \|u\|_{H^2(\Omega_p \setminus \Omega_{p-1})} \|I_N \mu - \phi u\|_{L^2(\Omega_p \setminus \Omega_{p-1})} \\
&\leq c h_p^2 a_p^{\frac{3}{2}-2} c h_p^2 a_p^{-\frac{5}{2}} \leq c h_p^4 a_p^{-3} \leq c 2^{-4l}.
\end{aligned}$$

Similarly, we have

$$\begin{aligned}
|B_{1,3}| &\leq c h_p^4 [\|u\|_{H^3(\Omega_p \setminus \Omega_{p-1})} \|\mu\|_{H^1(\Omega_p \setminus \Omega_{p-1})} + \|u\|_{H^4(\Omega_p \setminus \Omega_{p-1})} \|\mu\|_{L^2(\Omega_p \setminus \Omega_{p-1})}] \\
&\leq c h_p^4 a_p^{-3} \leq c 2^{-4l}.
\end{aligned}$$

Substituting the above two estimates into (77), one observes that

$$|B_1 - B_{1,2}| \leq c 2^{-4l}. \qquad (79)$$

By the same arguments in the proof of (79), we get

$$|B_2| \leq c2^{-4l}. \tag{80}$$

Thus, we derive

$$\left| \int_{\Omega_p \backslash \Omega_{p-1}} \phi(x)(u - I_N u)(x) I_N u(x) dx + \sum_{e \subset \Omega_p \backslash \Omega_{p-1}} \sum_{i=1}^{3} \frac{(h_e^{x_i})^2}{3} \int_e D_i^2 u(x) \phi(x) u(x) dx \right| \leq c2^{-4l},$$

where we have used (76), (79) and (80). Inserting (74) and the above estimate into (73), we arrive at

$$\left| \int_{\Omega} [\phi(x)(u - I_N u)(x) I_N u(x) dx + \sum_{p=1}^{l} \sum_{e \subset \Omega_p \backslash \Omega_{p-1}} \sum_{i=1}^{3} \frac{(h_e^{x_i})^2}{3} \int_e D_i^2 u(x) \phi(x) u(x) dx \right| \leq c2^{-4l} l.$$

Similarly,

$$\left| \int_{\Omega} [4\phi(x)(u - I_{2N} u)(x) I_{2N} u(x) dx + \sum_{p=1}^{l} \sum_{e \subset \Omega_p \backslash \Omega_{p-1}} \sum_{i=1}^{3} \frac{(h_e^{x_i})^2}{3} \int_e D_i^2 u(x) \phi(x) u(x) dx \right| \leq c2^{-4l} l.$$

Finally, substituting the above two estimates into (73), we get

$$\left| 4 \int_{\Omega} \phi(x)(u - I_{2N} u)(x) u_{2N}(x) dx - \int_{\Omega} \phi(x)(u - I_N u)(x) u_N(x) dx \right| \leq c2^{-4l} l^2.$$

This estimate, together with (72), completes the proof of (34).

4 Proof of Main Theorem

Based on the above analysis, we are ready to give a proof of Theorem 1. Similar to (33), we have

$$|\lambda - \lambda_{2N}| + \|u - I_{2N} u\|_{L^2(\Omega)} + \|u - u_{2N}\|_{L^2(\Omega)} + \|u - R_{2N} u\|_{L^2(\Omega)} + \|u_{2N} - \overline{u}_{2N}\|_{L^2(\Omega)} \leq c2^{-2l} l.$$

This, together with (33), gives

$$\begin{aligned} &|4\lambda_{2N}(u - I_{2N} u, \overline{u}_{2N} - u_{2N}) + \lambda_N(u - I_N u, \overline{u}_N - u_N)| \\ &\leq c \left[\|u - I_{2N} u\|_{L^2(\Omega)} \|\overline{u}_{2N} - u_{2N}\|_{L^2(\Omega)} + \|u - I_N u\|_{L^2(\Omega)} \|\overline{u}_N - u_N\|_{L^2(\Omega)} \right] \\ &\leq c2^{-4l} l^2. \end{aligned} \tag{81}$$

Combining (30), (34) and (81), we have the desired result in (27) and this completes the proof of our main theorem.

Table 1 Error of bi-linear element over $\mathcal{T}_N$

N	$\|\lambda_N - \lambda\|$	$\|\lambda_N - \lambda\|N^2$	$\|\lambda_{2N} - \lambda\|$	$\|\lambda_*^N - \lambda\|$	$\|\lambda_*^N - \lambda\|N^4$
12	0.021229	3.052	0.005486	0.000238	4.942
13	0.018807	3.178	0.004724	0.000030	0.847
14	0.016332	3.201	0.004066	0.000023	0.870
15	0.014197	3.194	0.003540	0.000012	0.625

5 Numerical Example

Consider the following Khon–Sham problem

$$\left(-\frac{1}{2}\Delta - \frac{1}{|x|}\right)u = \lambda u \quad x \in \Re^3, \quad \int_{\Re^3} u^2 dx = 1. \tag{82}$$

It is observed that the minimal eigenvalue λ for the problem (82), which denotes the ground-state energy of the hydrogen atom, is equal to -0.5 (see [15]).

Note that the ground state charge density goes down exponentially (see [1,15]), (82) can be approached by the following problem

$$\begin{cases} \left(-\frac{1}{2}\Delta - \frac{1}{|x|}\right)u = \lambda u & x \in \Omega \\ u = 0, & x \in \partial\Omega, \end{cases} \tag{83}$$

where Ω is a bounded domain.

In this paper, we choose $\Omega = [-12, 12]^3$. Let λ_N and λ_{2N} denote the minimal eigenvalues for the problem (24) and (25), respectively. Set

$$\lambda_*^N = \frac{4\lambda_{2N} - \lambda_N}{3}. \tag{84}$$

The numerical results are shown in Table 1. From the data, it can be concluded that there exist two constants c_1 and c_2, independent of N, such that

$$c_1 N^{-2} \le |\lambda_N - \lambda| \le c_2 N^{-2},$$

and

$$c_1 N^{-4} \le |\lambda_*^N - \lambda| \le c_2 N^{-4}.$$

Furthermore, numerical data in Table 1 also indicates that λ_*^N behaves better than our theoretical error estimate by a factor $|\ln N|^2$.

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