Hindawi
Mathematical Problems in Engineering
Volume 2021, Article ID 1049917, 11 pages
https://doi.org/10.1155/2021/1049917

Research Article

The Local and Parallel Finite Element Scheme for Electric Structure Eigenvalue Problems

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Received 30 April 2021; Revised 26 June 2021; Accepted 25 July 2021; Published 20 August 2021

Academic Editor: Qiang Guo

In this paper, an efficient multiscale finite element method via local defect-correction technique is developed. This method is used to solve the Schrödinger eigenvalue problem with three-dimensional domain. First, this paper considers a three-dimensional bounded spherical region, which is the truncation of a three-dimensional unbounded region. Using polar coordinate transformation, we successfully transform the three-dimensional problem into a series of one-dimensional eigenvalue problems. These one-dimensional eigenvalue problems also bring singularity. Second, using local refinement technique, we establish a new multiscale finite element discretization method. The scheme can correct the defects repeatedly on the local refinement grid, which can solve the singularity problem efficiently. Finally, the error estimates of eigenvalues and eigenfunctions are also proved. Numerical examples show that our numerical method can significantly improve the accuracy of eigenvalues.

1. Introduction

As an important equation in quantum mechanics, Schrödinger eigenvalue problems have important physical background modern electronic structure computations [1, 2]. Thus, finite element methods for solving this problem become an important topic which has attracted the attention of mathematical and physical fields: a priori error estimate is discussed in [3], some posteriori error estimates and adaptive algorithms have been studied in [4–7], and, in addition, it also includes two-scale method [8–12] and the extrapolation methods [13–16].

It is worth noting that some researchers [5, 6, 17] constructed a series of efficient algorithms to solve PDE eigenvalue problems with angular singularity. For elliptic boundary value problem, Xu and Zhou [18] combined two-grid finite element discretization scheme with the local defect correction to propose a general and powerful parallel-computing technique. This technique has been used and developed by many scholars, for instance, it can be used to solve Stokes equation (see [19, 20]), Especially, Xu and Zhou [21], Dai and Zhou [22], and Bi et al. [23–25] developed this method and established local and parallel three-scale finite element discretizations for symmetric elliptic singular eigenvalue problems.

As a matter of fact, due to the influence of Coulomb potentials, the convergence order of three-dimensional numerical methods and the computational efficiency of numerical methods will further deteriorate [26]. Therefore, one of the most direct and effective methods is to transform the three-dimensional problem into one-dimensional problem. Inspired by [27–29] and others references, it is necessary to further study the high-precision numerical method for singular problems. Therefore, in this paper, we turn to discuss finite element multiscale discretization based on local defect correction. We further apply local defect-correction technique proposed by Xu and Zhou to Schrödinger eigenvalue problems, and our work has the following features. (1) We first extend local and parallel three-scale finite element discretizations for symmetric eigenvalue problems established by Dai and Zhou [22] to solve Schrödinger eigenvalue problem. (2) Based on [23], we establish a new multiscale finite element discretization method by local refinement, and this scheme repeatedly makes defect correction on finer and finer local meshes to make up for accuracy loss caused by abrupt changes of local mesh size in three-scale scheme. (3) For the two-scale algorithms in [8, 10], we prove the local error estimates of eigenfunctions. (4) Our scheme is simple and easy to carry out, and theoretical analysis and numerical experiment verify its efficiency to solve the singular Schrödinger eigenvalue problem.

The rest of this paper is organized in the following way. in Section 2, we will briefly introduce Schrödinger eigenvalue problem and the associated dimension reduction scheme. In Section 3, we will establish the multiscale finite element method. The error estimates of eigenvalues and eigenfunctions will be studied in Section 4. Several numerical experiments are presented in Section 5 to demonstrate the accuracy and efficiency of our algorithm. Some concluding remarks are given in Section 6.

2. Dimension Reduction Scheme

Consider the Schrödinger eigenvalue problem:

$$-\frac{1}{2}\Delta\psi + V\psi = \lambda\psi, \quad \text{in } \mathbb{R}^3, \tag{1}$$

$$\lim_{|x|\longrightarrow\infty} \psi = 0, \tag{2}$$

where V is the effective potential and $x = (x_1, x_2, x_3) \in \mathbb{R}^3$.

Applying a truncation from a unbounded domain $\mathbb{R}^3$ to a bounded spherical domain $\mathbb{B}^3 :=\{x \in \mathbb{R}^3 : |x| < R\}$, we find

$$\begin{aligned} -\frac{1}{2}\Delta\psi + V\psi &= \lambda\psi, \quad \text{in } \mathbb{B}^3,\\ \psi &= 0, \quad \text{on } \partial\mathbb{B}^3. \end{aligned} \tag{3}$$

Using the spherical coordinate transformation [27], problems (1) and (2) are equivalent to

$$-\frac{1}{2}\partial_t\left((t+1)^2\partial_t u_k\right) + \frac{k(k+1)}{2}u_k + \frac{R^2}{4}(t+1)^2 V_0(r)u_k = \lambda_k \frac{R^2}{4}(t+1)^2 u_k, \tag{4}$$

$$u_k(1) = 0. \tag{5}$$

This problem has singularities towards $t = -1$.

Next, we introduce the weighted Sobolev spaces on $\Omega := (-1, 1)$:

$$\begin{aligned} L^2_\omega(\Omega) &:= \left\{v : \int_\Omega \omega v^2 \mathrm{d}t < \infty\right\},\\ H^1_{\omega,k}(\Omega) &:= \{v : \partial_t^m v \in L^2_\omega(\Omega) \text{if } k = 0, \partial_t^m v \in L^2_{\omega^m}(\Omega) \text{if } k\\ &\geq 1, m = 0, 1, v(1) = 0\}, \end{aligned} \tag{6}$$

with $\omega(t) := (t+1)^2$. For simplicity of notations in the reminder, we omit the subscript k in u_k and λ_k and denote $H^1_{\omega,k}(\Omega)$ by $H^1_\omega(\Omega)$ for short.

The variational form of (4) and (5) is to find $\lambda \in \mathbb{R}$ and nonzero $u \in H^1_\omega(\Omega)$, satisfying

$$a(u, v) = \lambda b(u, v), \quad \forall v \in H^1_\omega(\Omega), \tag{7}$$

where

$$\begin{aligned} a(u, v) &= \int_\Omega \frac{1}{2}(t+1)^2 u'v' + \frac{k(k+1)}{2}uv + \frac{R^2}{4}(t+1)^2\\ &\quad (V_0(r) + \mu)uv\mathrm{d}t, \end{aligned} \tag{8}$$

$$b(u, v) = \int_\Omega \frac{R^2}{4}(t+1)^2 uv\mathrm{d}t,$$

with $\mu > 0$. According to Theorem 1 in [27], $a(\cdot,\cdot)$ and $b(\cdot,\cdot)$ define the inner product in $H^1_\omega(\Omega)$ and $L^2_\omega(\Omega)$, respectively. Let $\|\cdot\|_a$ and $\|\cdot\|_b$ be the norm induced by the inner products $a(\cdot,\cdot)$ and $b(\cdot,\cdot)$. Let $\|\cdot\|_a$ and $\|\cdot\|_b$.

For $D \subset \Omega_0 \subset \Omega$, we use $D \subset\subset \Omega_0$ to mean that $\mathrm{dist}(\partial D \backslash \partial\Omega, \partial\Omega_0 \backslash \partial\Omega) > 0$.

Assume that $\pi_h(\Omega) = \{\tau\}$ is a mesh of Ω with mesh-size function $h(x)$ whose value is the diameter h_τ of the element τ containing x, and $h(\Omega) = \max_{x\in\Omega} h(x)$ is the mesh diameter of $\pi_h(\Omega)$. We write $h(\Omega)$ as h for simplicity. Let $V_h(\Omega) \subset C(\overline{\Omega})$, defined on $\pi_h(\Omega)$, be a space of piecewise polynomials, and $V^0_h(\Omega) = V_h(\Omega) \cap H^1_\omega(\Omega)$. Given $G \subset \Omega$, we define $\pi_h(G)$ and $V_h(G)$ to be the restriction of $\pi_h(\Omega)$ and $V_h(\Omega)$ to G, respectively, and

$$\begin{aligned} V^0_h(G) &= \left\{v \in V^0_h(\Omega) : v|_{\partial G \backslash \partial\Omega} = 0\right\},\\ V^h_0(G) &= \left\{v \in V^0_h(\Omega) : \mathrm{supp}\, v \backslash \partial\Omega \subset\subset G\right\}. \end{aligned} \tag{9}$$

For any $G \subset \Omega$ mentioned in this paper, we assume that it aligns with $\pi_h(\Omega)$ when necessary.

In this part, C denotes a positive constant independent of h, which may not be the same constant in different places. For simplicity, we use the symbol $x \lesssim y$ to mean that $x \leq Cy$.

We adopt the following assumptions similar as in [18] for meshes and finite element space.

(A0) There exists $\nu \geq 1$ such that $h(\Omega)^\nu \lesssim h(x), \forall x \in \Omega$.

(A1) There exists $r \geq 1$ such that, for $w \in H^1_\omega(\Omega) \cap H^{1+t}(\Omega)$,

$$\inf_{v \in V^0_h(\Omega)} \left(\left\| h^{-1}(w - v) \right\|_b + \|w - v\|_a \right) \lesssim h^t \|w\|_{1+t}, \quad 0 \leq t \leq r. \tag{10}$$

(A2) *Inverse Estimate.* For any $v \in V_h(\Omega_1)$, $\|v\|_{a,\Omega_1} \lesssim \|h^{-1} v\|_{b,\Omega_1}$.

(A3) *Superapproximation.* For $G \subset \Omega_1$, let $\widetilde{\omega} \in C^\infty(\overline{\Omega})$ with supp $\widetilde{\omega} \backslash \partial\Omega \subset\subset G$. Then, for any $w \in V_h(G)$, there exists $v \in V^0_h(G)$ such that $\|h^{-1}(\widetilde{\omega} w - v)\|_{a,G} \lesssim \|w\|_{a,G}$.

The finite element approximation of (7) is given; find $\lambda_h \in C$ and $u_h \in V^0_h(\Omega)$, $\|u_h\|_a = 1$, satisfying

$$a(u_h, v) = \lambda_h b(u_h, v), \quad \forall v \in V^0_h(\Omega). \tag{11}$$

Define the solution operator T: $L^2_\omega(\Omega) \longrightarrow H^1_\omega(\Omega)$ and T_h: $L^2_\omega(\Omega) \longrightarrow V^0_h(\Omega)$ as follows:

$$a(Tg, v) = b(g, v), \quad \forall v \in H^1_\omega(\Omega), \tag{12}$$

$$a(T_h g, v) = b(g, v), \quad \forall v \in V^0_h(\Omega). \tag{13}$$

Problems (7) and (11) have the equivalent operator forms (14) and (15), respectively:

$$Tu = \lambda^{-1} u, \tag{14}$$

$$T_h u_h = \lambda_h^{-1} u_h. \tag{15}$$

The following regularity assumption is needed in theoretical analysis. For any $f \in L^2_\omega(\Omega)$, $Tf \in H^1_\omega(\Omega) \cap H^{1+\gamma}(\Omega)$ satisfies

$$\|Tf\|_{1+\gamma} \leq C_\Omega \|f\|_b. \tag{16}$$

According to [30] and Section 5.5 in [31], the above assumption is reasonable.

For some $G \subset \Omega$, we need the following local regularity assumption.

R(G): for any $f \in L^2_\omega(G)$, there exists a $\phi \in H^1_\omega(G) \cap H^{1+\gamma}(G)$ satisfying

$$\begin{aligned} a(\phi, v) &= b(f, v), \quad \forall v \in H^1_\omega(G), \\ \|\phi\|_{1+\gamma,G} &\leq C_G \|f\|_{b,G}, \end{aligned} \tag{17}$$

where C_Ω and C_G are two priori constants.

Define the Ritz projection P_h: $H^1_\omega(\Omega) \longrightarrow V^0_h(\Omega)$ by

$$a(u - P_h u, v) = 0, \quad \forall v \in V^0_h(\Omega). \tag{18}$$

Then, $T_h = P_h T$ (see [32]).

Let $M(\lambda)$ be the space spanned by all generalized eigenfunctions corresponding to λ of T, $M_h(\lambda)$ be the space spanned by all generalized eigenfunctions corresponding to all eigenvalues of T_h that converge to λ.

We also need the lemma as follows (see [8, 10]).

Lemma 1. *Let (λ, u) be an eigenpair of (7). Then, for all $w \in H^1_0(\Omega)$, $w \neq 0$,*

$$\frac{a(w, w)}{b(w, w)} - \lambda = \frac{a(w - u, w - u)}{b(w, w)} - \lambda \frac{b(w - u, w - u)}{b(w, w)}. \tag{19}$$

The a priori error estimates of the finite element approximations (11) can be found in [3, 32].

Lemma 2. *Assume that $M(\lambda) \subset H^{r+s}(\Omega)$ $(0 < s < 1)$. Then,*

$$\left| \lambda_h - \lambda \right| \lesssim h^{2r+2s-2}, \tag{20}$$

and let $u_h \in M_h(\lambda)$ with $\|u_h\|_b = 1$; then, there is $u \in M(\lambda)$ such that

$$\begin{aligned} \left\| u_h - u \right\|_a &\lesssim h^{r+s-1}, \\ \left\| u_h - u \right\|_b &\lesssim h^{r+s-1+\gamma}. \end{aligned} \tag{21}$$

The authors in [18, 33] studied the local behavior of finite element. The following results are given in [18].

Lemma 3. *Suppose that $f \in L^2_\omega(\Omega)$ and $G \subset\subset \Omega_0 \subset \Omega$. If $w \in V_h(\Omega_0)$ satisfies*

$$a(w, v) = b(f, v), \quad \forall v \in V^h_0(\Omega_0), \tag{22}$$

then

$$\|w\|_{a,G} \lesssim \|w\|_{b,\Omega_0} + \|f\|_{b,\Omega_0}. \tag{23}$$

Proof. Let $p \geq 2\nu - 1$ be an integer, and let

$$D \subset\subset \Omega_p \subset\subset \Omega_{p-1} \subset\subset \cdots \subset\subset \Omega_1 \subset\subset \Omega_0. \tag{24}$$

Choose $D_1 \subset \Omega$ satisfying $D \subset\subset D_1 \subset\subset \Omega_p$ and $\widetilde{\omega} \in C^\infty(\overline{\Omega})$ such that supp $\widetilde{\omega} \subset\subset \Omega_p$ and $\widetilde{\omega} \equiv 1$ on $\overline{D_1}$. Then, from (A3), there exists $v \in V^h_0(\Omega_p)$ such that

$$\left\| \widetilde{\omega}^2 w - v \right\|_{a,\Omega_p} \lesssim h_{\Omega_0} \|w\|_{a,\Omega_p}, \tag{25}$$

so we have

$$a\left(w, \widetilde{\omega}^2 w - v\right) \lesssim h_{\Omega_0} \|w\|^2_{a,\Omega_p}, \tag{26}$$

$$|b(f, v)| \lesssim \|f\|_{b,\Omega_0} \|v\|_{b,\Omega_p} \lesssim \|f\|_{b,\Omega_0} \left(h_{\Omega_0} \|w\|_{a,\Omega_p} + \|\widetilde{\omega} w\|_{a,\Omega} \right). \tag{27}$$

Since $v \in V^h_0(\Omega_p) \subset V^h_0(\Omega_0)$, the definition w implies

$$a\left(w, \widetilde{\omega}^2 w\right) = a\left(w, \widetilde{\omega}^2 w - v\right) + b(f, v). \tag{28}$$

A simple calculation shows that

$$a(\widetilde{\omega} w, \widetilde{\omega} w) \lesssim a\left(w, \widetilde{\omega}^2 w\right) + \|w\|^2_{b,\Omega_0}, \quad \forall w \in H^1_\omega(\Omega). \tag{29}$$

It follows from (26)–(29) that

$$\begin{aligned}\|\widetilde{\omega}w\|_{a,\Omega}^2 &\lesssim a\left(w,\widetilde{\omega}^2 w\right)+\|w\|_{b,\Omega_0}^2\\ &= a\left(w,\widetilde{\omega}^2 w - v\right)+\|w\|_{b,\Omega_0}^2 + b(f,v)\\ &\lesssim h_{\Omega_0}\|w\|_{a,\Omega_p}^2 + \|w\|_{b,\Omega_0}^2 + \|f\|_{b,\Omega_0}\left(h_{\Omega_0}\|w\|_{1,\Omega_p}+\|\widetilde{\omega}w\|_{a,\Omega}\right),\end{aligned} \tag{30}$$

and thus,

$$\|w\|_{a,D} \lesssim h_{\Omega_0}^{1/2}\|w\|_{a,\Omega_p} + \|w\|_{b,\Omega_0} + \|f\|_{b,\Omega_0}. \tag{31}$$

Similarly, we can obtain

$$\|w\|_{a,\Omega_j} \lesssim h_{\Omega_0}^{1/2}\|w\|_{a,\Omega_{j-1}} + \|w\|_{b,\Omega_0} + \|f\|_{b,\Omega_0}, \quad j=1,2,\ldots,p. \tag{32}$$

By using (31) and (32), we get from (A0) and (A2) and inverse estimate that

$$\begin{aligned}\|w\|_{a,D} &\lesssim h_{\Omega_0}^{(p+1)/2}\|w\|_{a,\Omega_0} + \|w\|_{b,\Omega_0} + \|f\|_{b,\Omega_0}\\ &\lesssim h_{\Omega_0}^{(p+1)/2}\left\|h^{-1}w\right\|_{b,\Omega_0} + \|w\|_{b,\Omega_0} + \|f\|_{b,\Omega_0}\\ &\lesssim \|w\|_{b,\Omega_0} + \|f\|_{b,\Omega_0}.\end{aligned} \tag{33}$$

This completes the proof. □

Lemma 4. *Suppose that $G \subset\subset \Omega_0 \subset \Omega$. Then, the following estimates are valid:*

$$h^{\gamma}\left\|u-P_h u\right\|_{a,\Omega} + \left\|u-P_h u\right\|_{b,\Omega} \lesssim h^{\gamma} \inf_{v\in V_h^0(\Omega)} \|u-v\|_{a,\Omega}, \tag{34}$$

$$\left\|u-P_h u\right\|_{a,G} \lesssim \inf_{v\in V_h^0(\Omega)} \|u-v\|_{a,\Omega_0} + h^{\gamma}\left\|u-P_h u\right\|_{a,\Omega}. \tag{35}$$

Proof. By (15), we obtain

$$\left\|T_h\left(\lambda_h u_h - \lambda u\right)\right\|_a \lesssim \left\|\lambda_h u_h - \lambda u\right\|_b. \tag{36}$$

By the definitions of T, T_h, and P_h, we deduce that

$$\begin{aligned}\lambda T u &= u,\\ \lambda T_h u &= P_h u.\end{aligned} \tag{37}$$

Let $P_h^{\Omega_0}$ be the finite element projection onto $V_0^h(\Omega_0)$; then,

$$a\left(P_h u - P_h^{\Omega_0}u, v\right) = 0, \quad \forall v \in V_0^h(\Omega_0). \tag{38}$$

According to Lemma 3, we have

$$\left\|P_h u - P_h^{\Omega_0}u\right\|_{a,G} \lesssim \left\|P_h u - P_h^{\Omega_0}u\right\|_{b,\Omega_0}. \tag{39}$$

Then, by using (14) and (39), we conclude that

$$\begin{aligned}\left\|u-P_h u\right\|_{a,D} &\lesssim \left\|u - P_h^{\Omega_0}u + P_h^{\Omega_0}u - P_h u\right\|_{a,D}\\ &\lesssim \inf_{v\in V_h^0(\Omega)} \|u-v\|_{a,\Omega_0} + \left\|u-P_h u\right\|_{b,\Omega}.\end{aligned} \tag{40}$$

Thus, we derive (35) from (39). □

3. Multiscale Discretizations Based on Local Defect Correction

Consider the eigenvalue problem (7) which has an isolated singular point $t=-1$ (e.g., see Figure 1).

Let $D \subset\subset \Omega$ be a given subdomain containing the singular point z, and we introduce domains:

$$\Omega \supset \Omega_1 \supset \Omega_2 \supset \cdots \supset \Omega_l \supset \supset D. \tag{41}$$

Let $\pi_H(\Omega)$ be a shape-regular grid, which is made up of simplices, with size $H \in (0,1)$, $\pi_w(\Omega)$ be a refined mesoscopic shape-regular grid (from $\pi_H(\Omega)$), and $\pi_h(\Omega_i)$ be a locally refined grid (from $\pi_{h_{i-1}}(\Omega_{i-1})$) that satisfies $h_{-1}=H$, $h_0 = w, h_i \ll h_{i-1}\,(i=0,1,\ldots,l)$ (Figure 1 shows $\pi_H(\Omega)$, $\pi_w(\Omega)$, and $\pi_{h_1}(\Omega_1)$. Let $V_H^0(\Omega), V_w^0(\Omega)$, and $\left\{V_{h_i}^0(\Omega_i)\right\}_1^l$ be finite element spaces of degree less than or equal to r defined on $\pi_H(\Omega)$, $\pi_w(\Omega)$, and $\left\{\pi_{h_i}(\Omega_i)\right\}_1^l$, respectively.

Based on algorithm B_0 in [22], we establish the following three-scale discretization scheme.

Scheme 1. (three-scale discretizations based on local defect correction).

Step 1: solve (7) on a globally coarse grid $\pi_H(\Omega)$; find $\lambda_H \in \mathscr{C}, u_H \in V_H^0(\Omega)$ such that $\|u_H\|_0 = 1$ and

$$a\left(u_H, v\right) = \lambda_H b\left(u_H, v\right), \quad \forall v \in V_H^0(\Omega). \tag{42}$$

Step 2: solve two linear boundary value problems on a globally mesoscopic grid $\pi_w(\Omega)$; find $u^w \in V_w^0(\Omega)$ such that

$$a\left(u^w, v\right) = \lambda_H b\left(u_H, v\right), \quad \forall v \in V_w^0(\Omega), \tag{43}$$

and then, compute the Rayleigh quotient $\lambda^w = a(u^w, u^w)/b(u^w, u^w)$.

Step 3: solve two linear boundary value problems on a locally fine grid $\pi_{h_1}(\Omega_1)$; find $e^{h_1} \in V_{h_1}^0(\Omega_1)$ such that

$$a\left(e^{h_1}, v\right) = \lambda^w b\left(u^w, v\right) - a\left(u^w, v\right), \quad \forall v \in V_{h_1}^0(\Omega_1). \tag{44}$$

Step 4: set

$$u^{w,h_1} = \begin{cases} u^w + e^{h_1}, & \text{on } \overline{\Omega}_1,\\ u^w, & \text{in } \Omega\setminus\overline{\Omega}_1,\end{cases} \tag{45}$$

and compute the Rayleigh quotient:

$$\lambda^{w,h_1} = \frac{a\left(u^{w,h_1}, u^{w,h_1}\right)}{b\left(u^{w,h_1}, u^{w,h_1}\right)}. \tag{46}$$

We use $(\lambda^{w,h_1}, u^{w,h_1})$ obtained by Scheme 1 as the approximate eigenpair of (7).

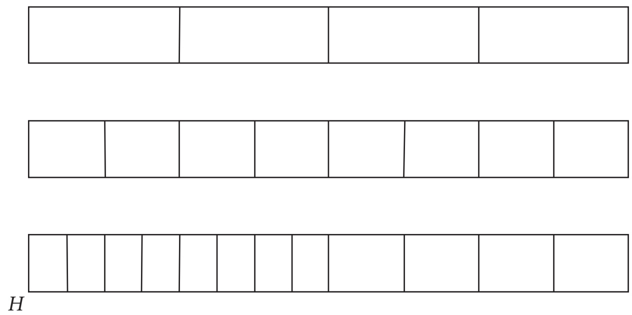

Figure 1: Finite element meshes.

It is obvious that (λ^w, u^w) in Scheme 1 can be viewed as approximate eigenpairs obtained by the two-grid discretization scheme in [8, 10] from $\pi_H(\Omega)$ and $\pi_w(\Omega)$.

Using Scheme 1, abrupt changes of mesh size will appear near $\partial\Omega_1$. Influenced by the technique on the transition layer proposed by [23], we repeatedly use the local defect-correction technique to establish the following multiscale discretization scheme.

Scheme 2. (multiscale discretizations based on local defect correction).

Step 1: the same as that of Step 1 of Scheme 1.

Step 2: the same as that of Step 2 of Scheme 1.

Step 3: $u^{w,h_0} \Leftarrow u^w$ and $\lambda^{w,h_0} \Leftarrow \lambda^w$.

Step 4: for $i = 1, 2, \ldots, l$, execute Step 5 and Step 6.

Step 5: solve linear boundary value problems on locally fine grid $\pi_{h_i}(\Omega_i)$; find $e^{h_i} \in V^0_{h_i}(\Omega_i)$ such that

$$a\left(e^{h_i}, v\right) = \lambda^{w,h_{i-1}} b\left(u^{w,h_{i-1}}, v\right) - a\left(u^{w,h_{i-1}}, v\right), \quad \forall v \in V^0_{h_i}(\Omega_i). \tag{47}$$

Step 6: set

$$u^{w,h_i} = \begin{cases} u^{w,h_{i-1}} + e^{h_i}, & \text{on } \overline{\Omega}_i, \\ u^{w,h_{i-1}}, & \text{in } \Omega \setminus \overline{\Omega}_i, \end{cases} \tag{48}$$

and compute

$$\lambda^{w,h_i} = \frac{a\left(u^{w,h_i}, u^{w,h_i}\right)}{b\left(u^{w,h_i}, u^{w,h_i}\right)}. \tag{49}$$

We use $(\lambda^{w,h_l}, u^{w,h_l})$ obtained by Scheme 2 as the approximate eigenpair of (7).

4. Theoretical Analysis

Next, we shall discuss the error estimates of Schemes 1 and 2. In our analysis, we introduce an auxiliary grid $\pi_{h_i}(\Omega)$ which is defined globally and denote the corresponding finite element space of degree $\leq r$ by $V^0_{h_i}(\Omega)$ $(i = 1, 2, \ldots, l)$. We also assume that $\pi_{h_i}(\Omega_i)$ and $V^0_{h_i}(\Omega_i)$ are the restrictions of $\pi_{h_i}(\Omega)$ and a subspace of $V^0_{h_i}(\Omega)$ to Ω_i, respectively, and

$$V^0_H(\Omega) \subset V^0_w(\Omega) \subset V^0_{h_1}(\Omega) \subset V^0_{h_2}(\Omega) \subset \cdots \subset V^0_{h_l}(\Omega). \tag{50}$$

For D and Ω_i stated at the beginning of Section 3, let $G_i \subset \Omega$ and $F \subset \Omega$ satisfy $D \subset\subset F \subset\subset G_i \subset\subset \Omega_i$ $(i = 1, 2, \ldots, l)$.

Theorem 1. *Assume that $M(\lambda) \subset H^{r+s}(\Omega) \cap H^{r+1}(\Omega/\overline{D})$ and $(1 < r+s,\ 0 \leq s < 1)$, and H is properly small. Then, there exists $u \in M(\lambda)$ such that*

$$\left\|u^w - u\right\|_a \lesssim H^{r+s-1+\gamma} + w^{r+s-1}, \tag{51}$$

$$\left\|u^w - u\right\|_b \lesssim H^{r+s-1+\gamma}, \tag{52}$$

$$\left\|u^w - u\right\|_{a,\Omega\setminus\overline{F}} \lesssim H^{r+s-1+\gamma} + w^r, \tag{53}$$

$$\left|\lambda^w - \lambda\right| \lesssim H^{2r+2s-2+2\gamma} + w^{2r+2s-2}. \tag{54}$$

Proof. Let $u \in M(\lambda)$ such that $u - u_H$ satisfies Lemma 2. From (12) and (13), Step 2 of Scheme 1, (14), and Lemmas 2 and 4, we derive that

$$\begin{aligned} \left\|u^w - u\right\|_a &= \left\|\lambda_H T_w u_H - \lambda T u\right\|_a \\ &\leq \left\|\lambda_H T_w u_H - \lambda T_w u\right\|_a + \left\|\lambda T_w u - \lambda T u\right\|_a \\ &\lesssim \left\|\lambda_H u_H - \lambda u\right\|_b + \lambda \left\|P_w T u - T u\right\|_a \\ &\lesssim H^{r+s-1+\gamma} + w^{r+s-1}, \end{aligned} \tag{55}$$

and then, (51) follows. By Lemmas 2 and 4,

$$\begin{aligned} \left\|u^w - u\right\|_{a,\Omega/\overline{D}} &\lesssim \left\|\lambda_H u_H - \lambda u\right\|_b + \lambda \left\|P_w T u - T u\right\|_{a,\Omega/\overline{D}} \\ &\lesssim H^{r+s-1+\gamma} + w^r, \end{aligned} \tag{56}$$

and then, (53) follows. By calculation,

$$\begin{aligned} \left\|u^w - u\right\|_b &= \left\|\lambda_H T_w u_H - \lambda T u\right\|_b \\ &\leq \left\|\lambda_H T_w u_H - \lambda T_w u\right\|_b + \left\|\lambda T_w u - \lambda T u\right\|_b \\ &\lesssim \left\|\lambda_H u_H - \lambda u\right\|_b + \lambda \left\|P_w T u - T u\right\|_b \\ &\lesssim H^{r+s-1+\gamma} + w^{r+s-1+\gamma} \\ &\lesssim H^{r+s-1+\gamma}, \end{aligned} \tag{57}$$

and then, (52) follows. From (19), we have

$$\lambda^w - \lambda = \frac{a\left(u^w - u, u^w - u\right)}{b\left(u^w, u^w\right)} - \lambda \frac{b\left(u^w - u, u^w - u\right)}{b\left(u^w, u^w\right)}. \tag{58}$$

Note that u_H and u^w just approximate the same eigenfuntion u. The combination of (51), (52), and (58) yields (54).

Theorem 2 is a critical result in this paper, which develops the results of Theorem 3.3 in [22]. □

Theorem 2. *Assume that $R(\Omega_i)$ holds $(i = 1, 2, \ldots, l)$, $u \in M(\lambda)$. Then,*

$$\left\|u^{w,h_l}-P_{h_l}u\right\|_a \lesssim \left\|u-P_{h_l}u\right\|_{b,\Omega_l}+h_{l-1}^{\gamma}\left\|P_{h_l}u-u^{w,h_{l-1}}\right\|_{a,\Omega_l} +\left\|\lambda u-\lambda^{w,h_{l-2}}u^{w,h_{l-2}}\right\|_{b,\Omega_l}+\left\|\lambda^{w,h_{l-1}}u^{w,h_{l-1}}-\lambda u\right\|_b +\left\|u^{w,h_{l-1}}-P_{h_l}u\right\|_{a,\Omega\setminus\overline{G_l}}+\left\|u^{w,h_{l-1}}-u\right\|_{a,\Omega_l\setminus\overline{F}},\quad l\geq 1. \tag{59}$$

Proof. Due to the inequality

$$\left\|u^{w,h_l}-P_{h_l}u\right\|_{a,\Omega} \lesssim \left\|u^{w,h_l}-P_{h_l}u\right\|_{a,D}+\left\|u^{w,h_l}-P_{h_l}u\right\|_{a,G_l\setminus\overline{D}} +\left\|u^{w,h_l}-P_{h_l}u\right\|_{a,\Omega\setminus\overline{G_l}}, \tag{60}$$

we shall estimate $\|u^{w,h_l}-P_{h_l}u\|_{a,D}$, $\|u^{w,h_l}-P_{h_l}u\|_{a,G_l\setminus\overline{D}}$, and $\|u^{w,h_l}-P_{h_l}u\|_{a,\Omega\setminus\overline{G_l}}$, respectively.

First, we proceed to estimate $\|u^{w,h_l}-P_{h_l}u\|_{a,D}$. From (18), (47), and (48), we derive

$$\begin{aligned} a\left(u^{w,h_l}-P_{h_l}u,v\right) &= a\left(u^{w,h_l},v\right)-a\left(P_{h_l}u,v\right)\\ &= a\left(u^{w,h_{l-1}}+e^{h_l},v\right)-a(u,v)\\ &= \lambda^{w,h_{l-1}}b\left(u^{w,h_{l-1}},v\right)-\lambda b(u,v),\quad \forall v\in V_{h_l}^0(\Omega_l). \end{aligned} \tag{61}$$

It is obvious that

$$\lambda^{w,h_{l-1}}b\left(u^{w,h_{l-1}},v\right)-\lambda b(u,v) =\left(\lambda^{w,h_{l-1}}-\lambda\right)b(u,v)+\lambda^{w,h_{l-1}}b\left(u^{w,h_{l-1}}-u,v\right),\quad \forall v\in H_0^1(\Omega), \tag{62}$$

which together with (61) yields

$$a\left(u^{w,h_l}-P_{h_l}u,v\right)=\left(\lambda^{w,h_{l-1}}-\lambda\right)b(u,v) +\lambda^{w,h_{l-1}}b\left(u^{w,h_{l-1}}-u,v\right),\quad \forall v\in V_{h_l}^0(\Omega_l). \tag{63}$$

Since $(u^{w,h_l}-P_{h_l}u)|_{\Omega_l}\in V_{h_l}(\Omega_l)$ and $V_0^{h_l}(\Omega_l)\subset V_{h_l}^0(\Omega_l)$, from the above formula and Lemma 3, we deduce that

$$\left\|u^{w,h_l}-P_{h_l}u\right\|_{a,D}\lesssim \left\|u^{w,h_l}-P_{h_l}u\right\|_{b,\Omega_l}+\left|\lambda^{w,h_{l-1}}-\lambda\right|+\left\|u^{w,h_l}-u\right\|_{b,\Omega_l}. \tag{64}$$

By calculation, we have

$$\begin{aligned} \left\|u^{w,h_l}-P_{h_l}u\right\|_{b,\Omega_l} &\leq \left\|u^{w,h_{l-1}}-P_{h_l}u\right\|_{b,\Omega_l}+\left\|e^{h_l}\right\|_{b,\Omega_l}\\ &\leq \left\|u-P_{h_l}u\right\|_{b,\Omega_l}+\left\|u-u^{w,h_{l-1}}\right\|_{b,\Omega_l}+\left\|e^{h_l}\right\|_{b,\Omega_l}. \end{aligned} \tag{65}$$

Substituting the above relation in (64), we obtain

$$\left\|u^{w,h_l}-P_{h_l}u\right\|_{a,D}\lesssim \left|\lambda^{w,h_{l-1}}-\lambda\right|+\left\|u^{w,h_{l-1}}-u\right\|_{b,\Omega_l} +\left\|u-P_{h_l}u\right\|_{b,\Omega_l}+\left\|e^{h_l}\right\|_{b,\Omega_l}. \tag{66}$$

To estimate $\|e^{h_l}\|_{b,\Omega_l}$, we use the Aubin–Nitsche duality argument. For any given $f\in L_2(\Omega_l)$, consider the boundary value problem; find $\varphi\in H_\Gamma^1(\Omega_l)\colon=\left\{v\in H_\omega^1(\Omega_l)\colon v|_{\partial\Omega_l\setminus\{-1\}}=0\right\}$ such that

$$a(\varphi,v)=b(f,v),\quad \forall v\in H_\Gamma^1(\Omega_l). \tag{67}$$

Let φ be the generalized solution of (67) and φ_{h_l} and $\varphi_{h_{l-1}}$ be finite element solutions of (67) in $V_{h_l}^0(\Omega_l)$ and $V_{h_{l-1}}^0(\Omega_l)$, respectively. Then,

$$\begin{aligned} \left\|\varphi-\varphi_{h_l}\right\|_{a,\Omega_l}&\lesssim h_l^{\gamma}\|f\|_{b,\Omega_l},\\ \left\|\varphi-\varphi_{h_{l-1}}\right\|_{a,\Omega_l}&\lesssim h_{l-1}^{\gamma}\|f\|_{b,\Omega_l}. \end{aligned} \tag{68}$$

From (47) and (48), we obtain

$$a\left(u^{w,h_l},\varphi_{h_l}\right)=\lambda^{w,h_{l-1}}b\left(u^{w,h_{l-1}},\varphi_{h_l}\right). \tag{69}$$

Then, by the definitions of φ, φ_{h_l}, and e^{h_l}, we deduce that

$$\begin{aligned} b\left(e^{h_l},f\right) &= a\left(e^{h_l},\varphi\right)=a\left(e^{h_l},\varphi_{h_l}\right)=a\left(u^{w,h_l}-u^{w,h_{l-1}},\varphi_{h_l}\right)\\ &= a\left(P_{h_l}u-u^{w,h_{l-1}},\varphi_{h_l}\right)+a\left(u^{w,h_l},\varphi_{h_l}\right)-a\left(P_{h_l}u,\varphi_{h_l}\right)\\ &= a\left(P_{h_l}u-u^{w,h_{l-1}},\varphi_{h_l}\right)+\lambda^{w,h_{l-1}}b\left(u^{w,h_{l-1}},\varphi_{h_l}\right)\\ &\quad -\lambda b\left(u,\varphi_{h_l}\right)\\ &= a\left(P_{h_l}u-u^{w,h_{l-1}},\varphi_{h_l}-\varphi\right)+a\left(P_{h_l}u-u^{w,h_{l-1}},\varphi-\varphi_{h_{l-1}}\right)\\ &\quad +a\left(P_{h_l}u-u^{w,h_{l-1}},\varphi_{h_{l-1}}\right)+\lambda^{w,h_{l-1}}b\left(u^{w,h_{l-1}},\varphi_{h_l}\right)\\ &\quad -\lambda b\left(u,\varphi_{h_l}\right)\\ &\lesssim h_{l-1}^{\gamma}\left\|P_{h_l}u-u^{w,h_{l-1}}\right\|_{a,\Omega_l}\|f\|_{0,\Omega_l}+a\left(P_{h_l}u-u^{w,h_{l-1}},\varphi_{h_{l-1}}\right)\\ &\quad +\lambda^{w,h_{l-1}}b\left(u^{w,h_{l-1}},\varphi_{h_l}\right)-\lambda b\left(u,\varphi_{h_l}\right). \end{aligned} \tag{70}$$

Step 2 of Scheme 2 shows that

$$a\left(u^{w,h_0},\varphi_{h_0}\right)=\lambda^{w,h_{-1}}b\left(u^{w,h_{-1}},\varphi_{h_0}\right), \tag{71}$$

namely, for $l=1$,

$$a\left(u^{w,h_{l-1}},\varphi_{h_{l-1}}\right)=\lambda^{w,h_{l-2}}b\left(u^{w,h_{l-2}},\varphi_{h_{l-1}}\right), \tag{72}$$

for $l>1$, the above formula follows from (47) and (48). Therefore,

$$\begin{aligned} a\left(P_{h_l}u-u^{w,h_{l-1}},\varphi_{h_{l-1}}\right) &= a\left(u-u^{w,h_{l-1}},\varphi_{h_{l-1}}\right)\\ &= \lambda b\left(u,\varphi_{h_{l-1}}\right)-a\left(u^{w,h_{l-1}},\varphi_{h_{l-1}}\right)\\ &= \lambda b\left(u,\varphi_{h_{l-1}}\right)-\lambda^{w,h_{l-2}}b\left(u^{w,h_{l-2}},\varphi_{h_{l-1}}\right)\\ &\lesssim \left\|\lambda u-\lambda^{w,h_{l-2}}u^{w,h_{l-2}}\right\|_{b,\Omega_l}\|f\|_{b,\Omega_l}. \end{aligned} \tag{73}$$

It is clear that

$$\left|\lambda^{w,h_{l-1}}b\left(u^{w,h_{l-1}},\varphi_{h_l}\right)-\lambda b\left(u,\varphi_{h_l}\right)\right|\lesssim \left\|\lambda^{w,h_{l-1}}u^{w,h_{l-1}}-\lambda u\right\|_{b,\Omega_l} \|f\|_{b,\Omega_l}. \tag{74}$$

Substituting the above two formulae in (70), we derive

$$\left|b\left(e^{h_l}, f\right)\right| \lesssim \left(h_{l-1}^{\gamma}\left\|P_{h_l}u - u^{w,h_{l-1}}\right\|_{a,\Omega_l} + \left\|\lambda u - \lambda^{w,h_{l-2}}u^{w,h_{l-2}}\right\|_{b,\Omega_l} + \left\|\lambda^{w,h_{l-1}}u^{w,h_{l-1}} - \lambda u\right\|_{b}\right)\|f\|_{b,\Omega_l}. \tag{75}$$

Thus, we obtain

$$\left\|e^{h_l}\right\|_{a,\Omega_l} \lesssim h_{l-1}^{\gamma}\left\|P_{h_l}u - u^{w,h_{l-1}}\right\|_{a,\Omega_l} + \left\|\lambda u - \lambda^{w,h_{l-2}}u^{w,h_{l-2}}\right\|_{b,\Omega_l} + \left\|\lambda^{w,h_{l-1}}u^{w,h_{l-1}} - \lambda u\right\|_{b}. \tag{76}$$

Substituting (76) in (66), we obtain

$$\left\|u^{w,h_l} - P_{h_l}u\right\|_{a,D} \lesssim \left\|u - P_{h_l}u\right\|_{b,\Omega_l} + h_{l-1}^{\gamma}\left\|P_{h_l}u - u^{w,h_{l-1}}\right\|_{a,\Omega_l} + \left\|\lambda u - \lambda^{w,h_{l-2}}u^{w,h_{l-2}}\right\|_{b,\Omega_l} + \left|\lambda^{w,h_{l-1}} - \lambda\right| + \left\|u^{w,h_{l-1}} - u\right\|_{b}. \tag{77}$$

Similarly, since $(G_l/\overline{D}) \subset\subset \Omega_l$, we deduce

$$\left\|u^{w,h_l} - P_{h_l}u\right\|_{a,D} \lesssim \left\|u - P_{h_l}u\right\|_{b,\Omega_l} + h_{l-1}^{\gamma}\left\|P_{h_l}u - u^{w,h_{l-1}}\right\|_{a,\Omega_l} + \left\|\lambda u - \lambda^{w,h_{l-2}}u^{w,h_{l-2}}\right\|_{b,\Omega_l} + \left|\lambda^{w,h_{l-1}} - \lambda\right| + \left\|u^{w,h_{l-1}} - u\right\|_{b}. \tag{78}$$

The remainder is to analyze $\|u^{w,h_l} - P_{h_l}u\|_{a,\Omega\setminus\overline{G}}$. From (48), we see that

$$\left\|u^{w,h_l} - P_{h_l}u\right\|_{a,\Omega\setminus\overline{\Omega}_l} = \left\|u^{w,h_{l-1}} - P_{h_l}u\right\|_{a,\Omega\setminus\overline{\Omega}_l}, \tag{79}$$

which leads to

$$\begin{aligned}&\left\|u^{w,h_l} - P_{h_l}u\right\|_{a,\Omega\setminus\overline{G_l}}\\ &\leq \left\|u^{w,h_l} - P_{h_l}u\right\|_{a,\Omega\setminus\overline{\Omega}_l} + \left\|u^{w,h_{l-1}} - P_{h_l}u\right\|_{a,\Omega_l\overline{G_l}} + \left\|e^{h_l}\right\|_{a,\Omega_l\setminus\overline{G_l}}\\ &\lesssim \left\|u^{w,h_{l-1}} - P_{h_l}u\right\|_{a,\Omega\setminus\overline{G_l}} + \left\|e^{h_l}\right\|_{a,\Omega_l\setminus\overline{G_l}}.\end{aligned} \tag{80}$$

It follows from (7), (47), and (62) that

$$\begin{aligned}a\left(e^{h_l}, v\right) &= \lambda^{w,h_{l-1}}b\left(u^{w,h_{l-1}}, v\right) - a\left(u^{w,h_{l-1}}, v\right) - \lambda b(u, v) + a(u, v)\\ &= \left(\lambda^{w,h_{l-1}} - \lambda\right)b(u, v) + \lambda^{w,h_{l-1}}b\left(u^{w,h_{l-1}} - u, v\right)\\ &\quad - a\left(u^{w,h_{l-1}} - u, v\right), \quad \forall v \in V_h^0(\Omega_l).\end{aligned} \tag{81}$$

Then, by Lemma 3, we have

$$\left\|e^{h_l}\right\|_{a,\Omega_l/\overline{G_l}} \lesssim \left\|e^{h_l}\right\|_{b,\Omega_l/\overline{F}} + \left|\lambda^{w,h_{l-1}} - \lambda\right| + \left\|u^{w,h_{l-1}} - u\right\|_{a,\Omega_l/\overline{F}}, \tag{82}$$

where $F \subset \Omega$ satisfies $D \subset\subset F \subset\subset G_l$. Substituting (82) in (80), we obtain

$$\left\|u^{w,h_l} - P_{h_l}u\right\|_{a,\Omega/\overline{G_l}} \lesssim \left\|u^{w,h_{l-1}} - P_{h_l}u\right\|_{a,\Omega/\overline{G_l}} + \left\|e^{h_l}\right\|_{b,\Omega/\overline{F}} + \left|\lambda^{w,h_{l-1}} - \lambda\right| + \left\|u^{w,h_{l-1}} - u\right\|_{a,\Omega/\overline{F}}. \tag{83}$$

It follows from substituting (76) in the above inequality that

$$\begin{aligned}\left\|u^{w,h_l} - P_{h_l}u\right\|_{a,\Omega/\overline{G_l}} \lesssim{}& \left\|u^{w,h_{l-1}} - P_{h_l}u\right\|_{a,\Omega/\overline{G_l}} + h_{l-1}^{\gamma}\left\|P_{h_l}u - u^{w,h_{l-1}}\right\|_{a,\Omega_l}\\ &+ \left\|\lambda u - \lambda^{w,h_{l-2}}u^{w,h_{l-2}}\right\|_{b,\Omega_l} + \left\|\lambda^{w,h_{l-1}}u^{w,h_{l-1}} - \lambda u\right\|_{b}\\ &+ \left|\lambda^{w,h_{l-1}} - \lambda\right| + \left\|u^{w,h_{l-1}} - u\right\|_{b,\Omega/\overline{F}}.\end{aligned} \tag{84}$$

Combining (60), (77), (78), and (84), finally, we obtain (59). □

Theorem 3. *Assume that the conditions of Theorem 1 hold. Then, there exists $u \in M(\lambda)$ such that*

$$\left\|u^{w,h_1} - u\right\|_{a,\Omega} \lesssim h_1^{r+s-1} + w^r + H^{r+s-1+\gamma}, \tag{85}$$

$$\left\|u^{w,h_1} - u\right\|_{b,\Omega} \lesssim w^r + H^{r+s-1+\gamma}, \tag{86}$$

$$\left\|u^{w,h_1} - u\right\|_{a,\Omega/\overline{F}} \lesssim w^r + H^{r+s-1+\gamma}, \tag{87}$$

$$\left|\lambda^{w,h_1} - \lambda\right| \lesssim h_1^{2r+2s-2} + w^{2r} + H^{2r+2s-2+2\gamma}. \tag{88}$$

Proof. Let $u \in M(\lambda)$ such that $u - u_H$ satisfies Lemma 2. From Theorem 2, we know $l = 1$, $h_{-1} = H, h_0 = w$, $u^{w,h_0} = u^w$, $\lambda^{w,h_0} = \lambda^w$, $u^{w,h_{-1}} = u_H$, and $\lambda^{w,h_{-1}} = \lambda_H$; thus, we obtain

$$\begin{aligned}\left\|u^{w,h_1} - P_{h_1}u\right\|_{a,\Omega} \lesssim{}& \left\|u - P_{h_1}u\right\|_{0,\Omega_1} + w^{\gamma}\left\|P_{h_1}u - u^w\right\|_{a,\Omega_1}\\ &+ \left\|\lambda u - \lambda_H u_H\right\|_{b,\Omega_1} + \left\|\lambda^w u^w - \lambda u\right\|_{b}\\ &+ \left\|u^w - P_{h_1}u\right\|_{a,\Omega\setminus\overline{G_1}} + \left\|u^w - u\right\|_{a,\Omega_1\setminus\overline{F}}.\end{aligned} \tag{89}$$

Using Lemma 4, Theorem 1, and Lemma 2 to estimate the terms at the right-hand side of the above formula gives

$$\begin{aligned}\left\|u^{w,h_1} - P_{h_1}u\right\|_{a,\Omega} &\lesssim h_1^{r+s-1+\gamma} + w^{\gamma}w^{r+s-1} + H^{r+s-1+\gamma} + w^{r+s-1+\gamma}\\ &\quad + \left(w^{r+s-1+\gamma} + w^r\right) + \left(w^{r+s-1+\gamma} + w^r\right)\\ &\lesssim H^{r+s-1+\gamma} + w^r.\end{aligned} \tag{90}$$

Combining (35) and (39) yields (85), (86), and (87). From (19), we have

$$\lambda^{w,h_1} - \lambda = \frac{a\left(u^{w,h_1} - u, u^{w,h_1} - u\right)}{b\left(u^{w,h_1}, u^{w,h_1}\right)} - \lambda\frac{b\left(u^{w,h_1} - u, u^{w,h_1} - u\right)}{b\left(u^{w,h_1}, u^{w,h_1}\right)}. \tag{91}$$

Table 1: $V=-(1/r)$.

DOF_H	DOF_w	λ_H	λ^w	λ^{w,h_1}	λ^{w,h_2}	λ^{w,h_3}	λ^{w,h_4}
4	16	−0.3558419	−0.4662707	−0.4903221	−0.4963517	−0.4975584	−0.4976819
8	64	−0.4320788	−0.4974509	−0.4993601	−0.4997939	−0.4998737	−0.4998816
16	256	−0.4735824	−0.4998515	−0.4999630	−0.4999897	−0.4999946	−0.4999951
32	1024	−0.4918086	−0.4999910	−0.4999978	−0.4999994	−0.4999997	−0.4999997
4	16	−0.10798797	−0.12015585	−0.12343262	−0.12435602	−0.12457107	−0.12462204
8	64	−0.11060517	−0.12445755	−0.12476411	−0.12484341	−0.12486019	−0.12486334
16	256	−0.12023285	−0.12497717	−0.12499349	−0.12499748	−0.12499831	−0.12499849
32	1024	−0.12372913	−0.12499867	−0.12499966	−0.12499990	−0.12499995	−0.12499996

Table 2: $V=(r^2/2)$.

DOF_H	DOF_w	λ_H	λ^w	λ^{w,h_1}	λ^{w,h_2}	λ^{w,h_3}	λ^{w,h_4}
4	16	2.3568087	1.7807519	1.5673755	1.5176295	1.5145651	1.5142457
8	64	1.6871072	1.5041081	1.5010234	1.5002569	1.5001762	1.5001727
16	256	1.5588758	1.5002540	1.5000634	1.5000159	1.5000109	1.5000107
32	1024	1.5155354	1.5000157	1.5000039	1.5000010	1.5000007	1.5000007
4	16	3.0744959	2.6046912	2.5284162	2.5069841	2.5039841	2.5036625
8	64	3.0722770	2.5418424	2.5142338	2.5054025	2.5045811	2.5045358
16	256	2.5890816	2.5004065	2.5001018	2.5000260	2.5000149	2.5000137
32	1024	2.5245263	2.5000247	2.5000062	2.5000016	2.5000009	2.5000008

Combining (85), (86), and (91) yields (88). □

Theorem 4. *Under the conditions of Theorem 1, we further assume that $R(\Omega_i)$ holds ($i=1,2,\ldots,l$), and*

$$w^r=\mathcal{O}\left(H^{r+s-1+\gamma}\right),\quad h_l^{r+s-1}\gtrsim H^{r+s-1+\gamma}. \tag{92}$$

Then, there exists $u\in M(\lambda)$ such that

$$\left\|u^{w,h_l}-u\right\|_{a,\Omega}\lesssim h_l^{r+s-1}, \tag{93}$$

$$\left\|u^{w,h_l}-u\right\|_{b,\Omega}\lesssim H^{r+s-1+\gamma}, \tag{94}$$

$$\left\|u^{w,h_l}-u\right\|_{a,\Omega\setminus\overline{F}}\lesssim H^{r+s-1+\gamma}, \tag{95}$$

$$\left|\lambda^{w,h_l}-\lambda\right|\lesssim h_l^{2r+s+s-2}. \tag{96}$$

Proof. Let $u\in M(\lambda)$ such that $u-u_H$ satisfies Lemma 2. The proof of (93)–(96) is completed by induction. When $l=1$, Scheme 2 is actually Scheme 1. Hence, from Theorems 1 and 3 and (92), we know that (93)–(96) hold for $l=0,1$.

Suppose (93)–(96) hold for $l-2$ and $l-1$, i.e.,

$$\begin{aligned}
\left\|u^{w,h_{l-2}}-u\right\|_{a,\Omega}&\lesssim h_{l-2}^{r+s-1},\\
\left\|u^{w,h_{l-2}}-u\right\|_{b,\Omega}&\lesssim H^{r+s-1+\gamma},\\
\left\|u^{w,h_{l-2}}-u\right\|_{a,\Omega\setminus\overline{F}}&\lesssim H^{r+s-1+\gamma},\\
\left|\lambda^{w,h_{l-2}}-\lambda\right|&\lesssim h_{l-2}^{2r+s+s-2},\\
\left\|u^{w,h_{l-1}}-u\right\|_{a,\Omega}&\lesssim h_{l-1}^{r+s-1},\\
\left\|u^{w,h_{l-1}}-u\right\|_{b,\Omega}&\lesssim H^{r+s-1+\gamma},\\
\left\|u^{w,h_{l-1}}-u\right\|_{a,\Omega\setminus\overline{F}}&\lesssim H^{r+s-1+\gamma},\\
\left|\lambda^{w,h_{l-1}}-\lambda\right|&\lesssim h_{l-1}^{2r+s+s-2}.
\end{aligned} \tag{97}$$

Next, we shall prove that (93)–(96) hold for l. Using the above formula and Lemma 4 to estimate the terms at the right-hand side of (59) gives

$$\begin{aligned}
\left\|u^{w,h_l}-P_{h_l}u\right\|_{a,\Omega}&\lesssim h_l^{r+s-1+\gamma}+h_{l-1}^{\gamma}\left(h_l^{r+s-1}+h_{l-1}^{r+s-1}\right)+H^{r+s-1+\gamma}\\
&\quad+H^{r+s-1+\gamma}+\left(H^{r+s-1+\gamma}+h_l^{r}\right)+H^{r+s-1+\gamma}\\
&\lesssim H^{r+s-1+\gamma}.
\end{aligned} \tag{98}$$

The combination of (35), (39), and (98) yields (93), (94), and (95). From (19), we have

Table 3: $V = r$.

DOF_H	DOF_w	λ_H	λ^w	λ^{w,h_1}	λ^{w,h_2}	λ^{w,h_3}	λ^{w,h_4}
4	16	2.2305059	1.9209211	1.8729501	1.8611124	1.8601497	1.8600937
8	64	1.9785415	1.8584870	1.8564450	1.8559369	1.8558894	1.8558874
16	256	1.8939159	1.8559226	1.8557987	1.8557678	1.8557648	1.8557646
32	1024	1.8658088	1.8557673	1.8557596	1.8557577	1.8557575	1.8557575
4	16	2.9297073	2.7099046	2.6801814	2.6714983	2.6700907	2.6699643
8	64	2.8582383	2.6735285	2.6699339	2.6688537	2.6686711	2.6686594
16	256	2.7093909	2.6680156	2.6678766	2.6678430	2.6678375	2.6678370
32	1024	2.6792284	2.6678409	2.6678323	2.6678303	2.6678299	2.6678299

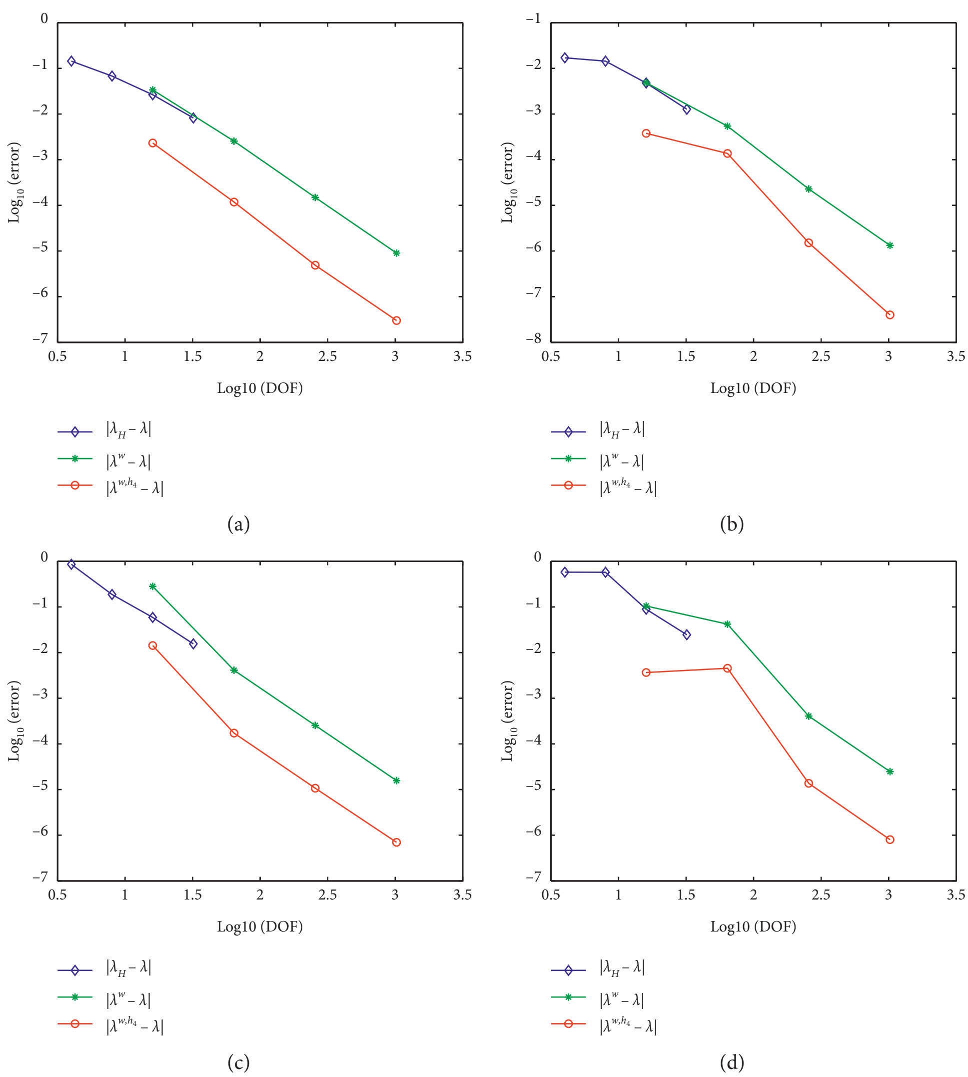

Figure 2: Continued.

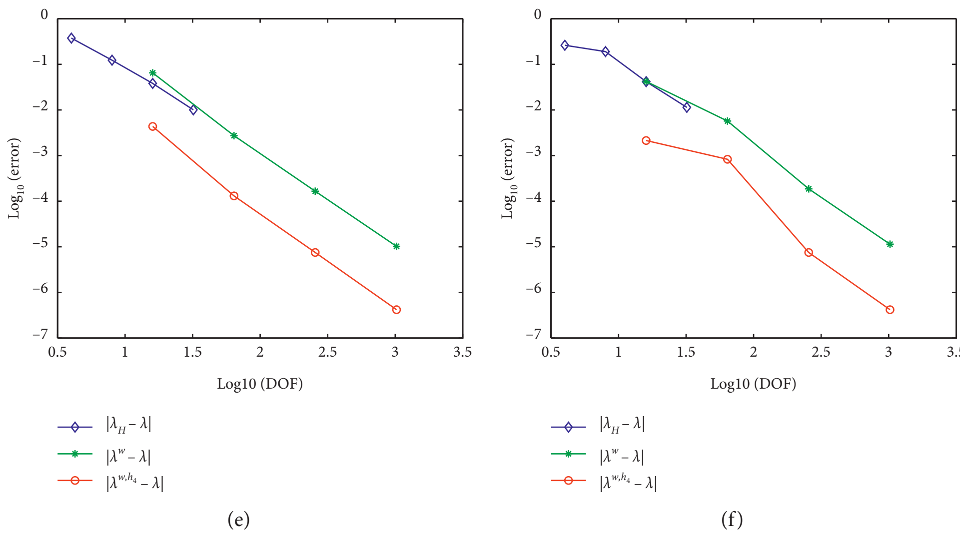

FIGURE 2: Error curve of numerical eigenvalues obtained by multiscale Scheme 2. (a) $V = -(1/r), \lambda = -0.5$. (b) $V = -(1/r), \lambda = -0.125$. (c) $V = -(r^2/2), \lambda = 1.5$. (d) $V = (r^2/2), \lambda = 2.5$. (e) $V = r, \lambda = 1.855757081489$. (f) $V = r, \lambda = 2.667829482852$.

$$\lambda^{w,h_l} - \lambda = \frac{a\left(u^{w,h_l} - u, u^{w,h_l} - u\right)}{b\left(u^{w,h_l}, u^{w,h_l}\right)} - \lambda \frac{b\left(u^{w,h_l} - u, u^{w,h_l} - u\right)}{b\left(u^{w,h_l}, u^{w,h_l}\right)}. \tag{99}$$

The combination of (93), (94), and (99) yields (96). □

5. Numerical Experiments

We will report some numerical experiments by using linear finite element and quadratic spectral element on uniform meshes. In our numerical experiments, we use Scheme 2 to solve the problem such that $\Omega_i = (-1, -1 + (1/2^i) \times (3/2))$, $i = 0, 1, 2, \ldots$, and locally fine grids have the same degree of freedom as that of globally mesoscopic grid (see Tables 1–3).

In our experiments, the parameter μ is taken to be 1. We set $R = 40$ for the eigenvalue problem with $V = -(1/r)$ and $l = 1$ and $R = 15$ for the other cases. The coarse mesh size and the mesoscopic mesh size satisfy $\omega = H^2$ which means $\mathrm{DOF}_w = \mathrm{DOF}_H^2$.

We use MATLAB 2011b under the package of Chen (see [34]) to solve the problem, and the numerical results are shown in Tables 1–3. This tables corresponds to the results of different potential energy V. From these tables, we can see that, without increasing degree of freedom on locally fine grids, the first local defect correction can largely improve the accuracy of the eigenvalue, and the local defect corrections that follows can gradually improve the accuracy of the eigenvalue by overcoming the singularity at the origin. Here, we set

$$\mathrm{DOF}_w = \mathrm{DOF}_{\Omega_i}, \quad i = 1, 2, \ldots. \tag{100}$$

In Figure 2, we also plot the error curve of numerical eigenvalues obtained by multiscale Scheme 2. It can be seen that using coarse finite element space with the mesh size H, the error of the finite element eigenvalues is around poor accuracy 10^{-2}. After performing the two-grid iteration, the error of the finite element eigenvalues can be increased from 10^{-2} to 10^{-5}. The final mutiscale iteration can improve the error up to $10^{-6} \sim 10^{-7}$. These figures show the accuracy and effectiveness of our numerical scheme.

6. Conclusion

In this paper, we developed a efficient multiscale finite element method for solving the Schrödinger eigenvalue problem with three-dimensional domain. Our scheme can correct the defects repeatedly on the local refinement grid, which can solve the singularity problem efficiently. The error estimates of eigenvalues and eigenfunctions are proved. Some numerical examples are presented to verify the effectiveness of our numerical method.

Data Availability

The data used to support the findings of this study are included within the article.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

Acknowledgments

The research was supported by NSFC (nos. 62062018, 11901135, and 11961009), Guizhou Province University Science and Technology top talents project (no. KY[2018] 047), Guizhou Key Laboratory of Big Data Statistics Analysis (no. BDSA20200102), and foundation of Guizhou Science and Technology Department (no. [2020]1Y015).

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