FINITE ELEMENT APPROXIMATIONS TO THE DISCRETE SPECTRUM OF THE SCHRÖDINGER OPERATOR WITH THE COULOMB POTENTIAL

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Abstract. In the present paper, the authors consider the Schrödinger operator $H$ with the Coulomb potential defined in $\mathbb{R}^3_m$, where $m$ is a positive integer. Both bounded domain approximations to multielectron systems and finite element approximations to the helium system are analyzed. The spectrum of $H$ becomes completely discrete when confined to bounded domains. The error estimate of the bounded domain approximation to the discrete spectrum of $H$ is obtained. Since numerical solution is difficult for a higher-dimensional problem of dimension more than three, the finite element analyses in this paper are restricted to the $S$-state of the helium atom. The authors transform the six-dimensional Schrödinger equation of the helium $S$-state into a three-dimensional form. Optimal error estimates for the finite element approximation to the three-dimensional equation, for all eigenvalues and eigenfunctions of the three-dimensional equation, are obtained by means of local regularization. Numerical results are shown in the last section.

Key words. spectrum approximation, Schrödinger equation, weighted norm, local regularization, finite element method

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1. Introduction. The multielectron Coulomb problem in quantum mechanics cannot be solved in a finite form. Nevertheless it challenges and stimulates many mathematicians and physicists to devote themselves to developing efficient methods for solving the system.

Several successful approximation techniques in quantum physics/chemistry have been developed for this problem. They include the Hartree–Fock method [15], the finite difference method [19], [35], the correlation-function hyperspherical-harmonic method [18], [24], and various variational approximations. For the Hartree–Fock method, every electron is considered independently to be in a central electric field formed by the nucleus and other electrons. The finite difference method needs a rectangular domain in $\mathbb{R}^N$ and uniform grids. The double and triple basis set methods (which are variational methods indeed) are very powerful for the eigenvalue problem of the helium atom. Kono and Hattori (see [21], [22]) used two sets of basis functions $r_1^{\rho_1}r_2^{\rho_2}e^{-\xi r_1 - \eta r_2} A (\xi \text{ terms})$ and $r_1^{\rho_1}r_2^{\rho_2}e^{-\zeta (r_1 + r_2)/A} (\zeta \text{ terms})$ to calculate the energy levels for the $S$, $P$, and $D$ states of the helium atom. ($A$ is an appropriate angular factor.) The former set of functions is expected to describe the whole wave function roughly, while the latter is expected to describe the short- and middle-range correlation effects. Their calculations yield 9–10 significant digits for $S$ states. Klein-dienst, Lächow, and Merckens [20] and Drake and Yan [12] applied the double basis set method to $S$-states of helium. Their basis functions are $r_1^{\rho_1}r_2^{\rho_2}e^{-\xi r_1 - \eta r_2}$ and $r_1^{\rho_1}r_2^{\rho_2}e^{-\xi r_1 - \eta r_2}$. Drake and Yan employed truncations to ensure numerical stability and convergence. By complete optimization of the exponential scale factors $\xi_1$, $\eta_1$, $\xi_2$, and $\eta_2$, they achieved more than 15 significant digits. Recently, Drake, Cas-sar, and Nistor [13] obtained 21 significant digits for the ground state of helium by the triple basis set method. Korobov [23] even obtained 25 significant digits for the ground state of helium. That work can be used as a benchmark for other approaches.

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for three-body systems. All three of these excellent works in variational methods promote the development of few-body problems in quantum mechanics.

The finite element method (FEM) is used initially in elastic mechanics and fluid mechanics. It uses local interpolation functions to approximate the unknown function (see [8] and [36]), and thus can describe the local properties of wave functions. Therefore, we can expect to obtain good approximations to the energy. Important works on FEM applied to atomic and molecular problems first appeared in 1975 (see [3]). They were devoted to one- or two-dimensional problems [3], [4], [14], [16], [30]. In 1985, Levin and Schertzer [25] published the first work applying FEM to three-dimensional problems. They calculated the ground state of the helium atom. Most of the works applying FEM to three-body problems have appeared since 1990 (i.e., [1], [6], [31], [37]). All of the cited works obtained very good results.

To apply FEM to quantum mechanics, we should consider three aspects of the problem. The first is the spectrum approximation of the whole space Schrödinger operator by the operator defined on some bounded domain. The second is the error estimate for FEM approximation. The third is the real computation of approximate solutions. To the best of our knowledge, we have not found any work analyzing the first two aspects.

In this paper, we consider the first aspect for the system of an arbitrary atom. But as for the finite element aspect, since any problem of dimension more than three is a great challenge for both modern numerical methods and computers, we restrict the finite element analysis and computation to the \( S \)-state of the helium atom. In fact, we can transform the \( 3m \)-dimensional Schrödinger equation (see [38] for \( m = 2, 3 \)) into a \( 3(m - 1) \)-dimensional form rigorously, and theoretical analysis of the FEM applied to the simplified equation can be obtained similarly, in view of the argument of sections 3, 4, and 5 in the present paper. However, real computations are very difficult to carry out because of numerous degrees of freedom. Our numerical results on the lithium atom (the Schrödinger equation is nine-dimensional) will appear in another paper [39].

The present paper consists of three parts. First, we consider the bounded domain approximation of the \( 3m \)-dimensional Schrödinger equation \((m\) is the number of electrons in an ion). The spectrum of the Schrödinger operator \( H \) consists of the discrete spectrum included in \((-a, 0)\) (for some \( a > 0 \)) and the continuous spectrum \([0, +\infty)\). We show that the spectrum of \( H \) becomes completely discrete if it is restricted to bounded domains. In section 2, we show that for any eigenvalue of the whole space problem and for any \( \epsilon > 0 \), assuming the bounded domain large enough, there is an eigenpair of the bounded domain problem such that the errors of both the eigenvalue and the eigenfunction are smaller than \( \epsilon \). Secondly, we analyze the finite element approximation of the \( S \)-state of the helium atom. In section 3, the six-dimensional Schrödinger equation is transformed into a three-dimensional form, and some Hilbert spaces with weighted inner products and norms are defined. Because we cannot say that the solutions of both the three-dimensional equation and the six-dimensional one are continuous, the technique of local regularization [25] is used to prove the convergence of the finite element scheme. In section 4, we describe the three-dimensional local regularization operator in detail. In section 5, an equivalent variational equation of the three-dimensional equation and its FEM approximation are given for the helium atom of the \( S \)-state. The optimal order error estimate of the finite element scheme is obtained. Thirdly, we have calculated approximate solutions by the finite element scheme. In section 6, we give the numerical results from two kinds of FEM approximations to the three-dimensional energy equation. The results are better than
existing finite element results. Furthermore, from the figures we can see that our approximate wave functions coincide very well with many physical properties well known to physicists, and with many essential physical assumptions in quantum mechanics which are not added into our computations a priori.

The difficulties appear in three aspects: 1. the proof of the continuity and coercivity of the bilinear forms in the variational equations with the presence of the singularities in the Coulomb potential, 2. the proof of the convergency of the finite element scheme while the variational spaces are not standard Sobolev spaces, and 3. obtaining precise results in presence of numerous unknowns and singular integrals.

Through the paper, \( C \) represents the generic constant independent of minded parameters; the symbol \( \iff \) means “be equivalent to.” We use atomic units except where explicitly explained, i.e., Bohr radius \( a_0 \) for length, Rydberg (Hartree only in section 6) for energy. We consider the nonrelativistic and spin-independent case.

2. Discrete spectrum approximations of the Schrödinger operator in bounded domains. Let \( m > 0 \) be an integer, \( N = 3m \). The Schrödinger equation of an \( m \)-electron ion is

\[
H \psi = E \psi \quad \text{in } \mathbb{R}^N,
\]

where

\[
H \psi = -\Delta \psi + V \psi,
\]

\[
\Delta \psi = \sum_{i=1}^{m} \left( \frac{\partial^2}{\partial x_i^2} + \frac{\partial^2}{\partial y_i^2} + \frac{\partial^2}{\partial z_i^2} \right),
\]

\[
V = -\sum_{i=1}^{m} \frac{2Z}{r_i} + \sum_{1 \leq i < j \leq m} \frac{2}{r_{ij}};
\]

\((x_i, y_i, z_i)\) are the coordinates of the \( i \)th electron, \( r_i = \sqrt{x_i^2 + y_i^2 + z_i^2} \) is the distance between the \( i \)th electron and the nucleus, \( 1 \leq i \leq m \); and \( r_{ij} = [(x_i - x_j)^2 + (y_i - y_j)^2 + (z_i - z_j)^2]^{1/2} \) is the distance between the \( i \)th electron and the \( j \)th electron, \( 1 \leq i < j \leq m \). \( Z \) is the charge number of the nucleus.

It is well known that \( H \) is self-adjoint and bounded below (Theorem 10.33 and the analysis on p. 323 of [34]). Its spectrum \( \sigma(H) \) is included in \( \mathbb{R}^1 \). Furthermore, the continuous spectrum of \( H \) is \([0, +\infty)\), and \( \forall s \in \sigma(H) \cap (-\infty, 0) \), \( s \) is an eigenvalue of \( H \) (see Theorems 10.30 and 10.31 in [34]).

**Lemma 2.1.** Let \( 1 \leq p < 2, 3/2 < q < 2, 1 \leq q_1 < \min(3, \frac{Nq}{N-2q}) \). Then there exists a constant \( C \) such that \( \forall v \in H^1(\mathbb{R}^N), u \in W^{2,q}(\mathbb{R}^N), \)

\[
\frac{u}{r_i}, \quad \frac{u}{r_{ij}} \in L^{q_1}(\mathbb{R}^N),
\]

and

\[
\left\{ \begin{array}{l}
\int_{\mathbb{R}^N} \frac{v}{r_i} \, dx, \quad \int_{\mathbb{R}^N} \frac{v}{r_{ij}} \, dx \leq C \|v\|_{2,\mathbb{R}^N}^2,

\frac{u}{r_i} \|_{0,q_1,\mathbb{R}^N}, \quad \frac{u}{r_{ij}} \|_{0,q_1,\mathbb{R}^N} \leq C \|u\|_{2,q,\mathbb{R}^N};
\end{array} \right.
\]

moreover, if \( v \) is compactly supported in \( \mathbb{R}^N \), then

\[
\frac{v}{r_i}, \quad \frac{v}{r_{ij}} \in L^p(\mathbb{R}^N),
\]
and

\begin{equation}
\left\| \frac{v}{r_i} \right\|_{0,p,RN}, \left\| \frac{v}{r_j} \right\|_{0,p,RN} \leq C\|v\|_{1,RN},
\end{equation}

where 1 ≤ i, j ≤ m and i < j.

Proof. (1) ∀x ∈ R^N, set x = (x^{(1)}, \ldots, x^{(m)}), x^{(i)} = (x^{(1)}, \ldots, x^{(i-1)}, x^{(i+1)}, \ldots, x^{(m)}). Define B_i = \{(x_i, y_i, z_i) \mid x_i^2 + y_i^2 + z_i^2 \leq 1\}, i = 1, \ldots, m.

Since \( H^1(B_i) \hookrightarrow L^q(B_i), W^{2,q}(B_i) \hookrightarrow C(B_i), W^{2,q}(R^3) \hookrightarrow W^{1,q}(R^3) \hookrightarrow L^2(R^3), \)

let 0 ≤ t < 2, 0 ≤ s < 3; then ∀v ∈ \( H^1(R^N) \), u ∈ \( W^{2,q}(R^N) \),

\begin{align*}
\int_{R^3 \setminus B_i} \frac{v^2}{r_i^t} dx^{(i)} &\leq \|v\|_{0,R^N}^2 \leq \|v\|_{1,R^N}^2, \\
\int_{B_i} \frac{v^2}{r_i^t} dx^{(i)} &\leq \left( \int_{B_i} v^q dx^{(i)} \right)^{\frac{1}{q}} \left( \int_{B_i} r_i^{-\frac{3}{2}} dx^{(i)} \right)^{\frac{2}{3}} \leq C\|v\|_{0,6,B_i}^2 \leq C\|v\|_{1,B_i}^2, \\
\int_{B_i} \frac{u^2}{r_i^t} dx^{(i)} &\leq \|u\|_{0,\infty,B_i}^2 \int_{B_i} r_i^{-s} dx^{(i)} \leq C\|u\|_{2,q,B_i}^2 \quad \text{for almost every } \tilde{z}^{(i)} \in R^{N-3}.
\end{align*}

Hence

\begin{equation}
\int_{R^3} \frac{v^2}{r_i^t} dx^{(i)} \leq C\|v\|_{1,R^N}^2, \quad \int_{R^3} \frac{u^2}{r_i^t} dx^{(i)} \leq C\|u\|_{2,q,R^N}^2.
\end{equation}

By Tonelli’s theorem [34], integrating (2.6) with respect to the rest variables gives

\begin{equation}
\int_{R^N} \frac{v^2}{r_i} dx \leq C\|v\|_{1,R^N}^2, \quad \int_{R^N} \frac{u^2}{r_i} dx \leq C\|u\|_{2,q,R^N}^2.
\end{equation}

Setting s = \( \frac{N(q-2)+(q-1)\frac{p}{p-1}}{N(q-2)+(q-1)\frac{p}{p-1}} \)q, by (2.7) we have

\begin{align*}
\int_{R^N} \left( \frac{u}{r_i} \right)^q dx &\leq \left( \int_{R^N} \frac{u^2}{r_i} dx \right)^{\frac{q}{2}} \left( \int_{R^N} \frac{u^q}{r_i^{\frac{2q-1}{q}}} dx \right)^{\frac{q-1}{q}} \leq C\|u\|_{2,q,R^N}^q.
\end{align*}

If the support of v ∈ \( H^1(R^N) \) is compact, set R > 0 large enough and define

\( B_i(0,R) = \{(x_i, y_i, z_i) \in R^3 \mid \sqrt{x_i^2 + y_i^2 + z_i^2} \leq R\}, \)

\( \Omega_R = \{(x^{(1)}, \ldots, x^{(m)}) \in R^N \mid \sqrt{x_i^2 + y_i^2 + z_i^2} \leq R, \quad i = 1, 2, \ldots, m\}. \)

Assuming \( \text{supp} v \subset \Omega_R, \) by Hölder’s inequality there exists a positive constant C, depending on R and p, such that

\begin{equation}
\int_{R^3} \left( \frac{v}{r_i} \right)^p dx^{(i)} = \int_{B_i(0,R)} \left( \frac{v}{r_i} \right)^p dx^{(i)} \leq C\|v\|_{0,6,B_i(0,R)}^p \leq C\|v\|_{1,B_i(0,R)}^p.
\end{equation}

Integrating (2.8) with respect to the rest of the variables produces the following:

\begin{equation}
\int_{R^N} \left( \frac{v}{r_i} \right)^p dx^{(i)} \leq C \int_{R^{N-3}} \|v\|_{1,B_i(0,R)}^p dx^{(i)} \leq C\|v\|_{1,R^N}^p.
\end{equation}
(2) For any \(1 \leq i < j \leq m\), let \(\xi^{(i)} = x^{(i)} - x^{(j)}, \xi^{(j)} = (\xi, \eta, \zeta), \) \(x^{(i)} = (x_i, y_i, z_i)\). For any \(v = v(x^{(1)}, \ldots, x^{(m)}) \in H^1(R^N)\), define
\[
v_{ij}(x^{(1)}, \ldots, x^{(i)}, \ldots, x^{(m)}) = v(x^{(1)}, \ldots, x^{(i)} + x^{(j)}, \ldots, x^{(m)}),
\]

By Tonelli’s theorem [34], we have
\[
\int_{R^N} \int_{R^3} v^2(x^{(1)}, \ldots, x^{(i)}, \ldots, x^{(m)})dx^{(i)}d\hat{x}^{(i)} = \int_{R^N} \int_{R^3} v_{ij}^2(x^{(1)}, \ldots, \xi^{(i)}, \ldots, x^{(m)})d\xi^{(i)}d\hat{x}^{(i)} = \int_{R^N} v_{ij}^2dx, \quad \forall v \in H^1(R^N).
\]
Thus \(v_{ij} \in L^2(R^N)\). In the same way, we have
\[
\partial v_{ij} = \partial v_{ij} \partial y_k, \partial v_{ij} \partial z_k \in L^2(R^N), \quad 1 \leq k \leq N, \quad k \neq i, j.
\]
Since \(\frac{\partial v_{ij}}{\partial x_i} = \frac{\partial v_{ij}}{\partial x_j} = \frac{\partial v}{\partial x_i} + \frac{\partial v}{\partial x_j}\), we have
\[
\int_{R^N} \int_{R^3} \left| \frac{\partial v_{ij}}{\partial x_i} \right|^2d\xi^{(i)} = \int_{R^N} \int_{R^3} \left| \frac{\partial v_{ij}}{\partial x_i} \right|^2d\xi^{(i)}d\hat{x}^{(i)} = \int_{R^N} \int_{R^3} \left| \frac{\partial v}{\partial x_i} \right|^2d\xi^{(i)}d\hat{x}^{(i)}.
\]
i.e., \(\frac{\partial v_{ij}}{\partial x_i} \in L^2(R^N)\). Similarly, we have
\[
\frac{\partial v_{ij}}{\partial \eta_i}, \frac{\partial v_{ij}}{\partial \eta_j}, \frac{\partial v_{ij}}{\partial y_j}, \frac{\partial v_{ij}}{\partial z_j} \in L^2(R^N).
\]
Therefore \(v_{ij} \in H^1(R^N)\). In the same way, if \(u \in W^{2,q}(R^N)\), we have \(u_{ij} \in W^{2,q}(R^N)\), 
\(1 \leq i, j \leq m\). By (1), \(v/r_{ij} = v_{ij}/|\xi_{ij}|, u/r_{ij} = u_{ij}/|\xi_{ij}|\) satisfy (2.3)–(2.5).

Let \(\sigma > 0\) be a constant, \(\hat{x} = (\hat{x}^{(1)}, \ldots, \hat{x}^{(m)}) = \sigma x, \hat{x}^{(i)} = (\hat{x}_i, \hat{y}_i, \hat{z}_i), \psi(\hat{x}) = \psi(\sigma x)\) for any \(x \in R^N\). Then (2.1) becomes
\[
-s^2\hat{\Delta} \psi - \sigma \sum_{i=1}^{m} \frac{2Z\psi}{r_i} + \sigma \sum_{1 \leq i < j \leq m} \frac{2\psi}{r_{ij}} = E\psi \quad \text{in} \quad R^N,
\]
where \(\hat{\Delta}\) concerns the derivatives with respect to \(\hat{x}\). Obviously, \(\psi \in H^1(R^N) \iff \hat{\psi} \in H^1(R^N)\). By Lemma 2.1, we can choose \(\sigma, K\) large enough such that
\[
2\sigma \sum_{i=1}^{m} \int_{R^N} \frac{2Z\hat{\psi}^2}{r_i}d\hat{x} \leq \sigma^2 |\hat{\psi}|_{1,R^N}^2 + K |\hat{\psi}|^2 \quad \forall \hat{\psi} \in H^1(R^N).
\]
Let \(\lambda = E + K\); then the variational form of (2.9) is the following: Find \((\lambda, \hat{\psi}) \in R^1 \times H^1(R^N)\) and \(\hat{\psi} \neq 0\) such that
\[
\hat{a}(\hat{\psi}, \hat{\varphi}) = \lambda \int_{R^N} \hat{\psi}\hat{\varphi}d\hat{x} \quad \forall \hat{\varphi} \in H^1(R^N),
\]
where
\[
\hat{a}(\hat{\psi}, \hat{\varphi}) = \sigma^2 \int_{R^N} \hat{\nabla}\hat{\psi} \cdot \hat{\nabla}\hat{\varphi}d\hat{x} + \int_{R^N} \left( -\sum_{i=1}^{m} \frac{2Z\sigma}{r_i} + \sum_{1 \leq i < j \leq m} \frac{2\sigma}{r_{ij}} + K \right) \hat{\psi}\hat{\varphi}d\hat{x}.
\]
It is easy to see that \( \hat{a}(\cdot, \cdot) \) is continuous and coercive on \( H^1(R^N) \) by Lemma 2.1 and (2.10).

The weak form of (2.1) is the following: Find \((\lambda, \psi) \in R^1 \times H^1(R^N) \) and \( \psi \neq 0 \) such that

\[
(2.12) \quad a(\psi, \varphi) = \lambda \int_{R^N} \psi \varphi dx \quad \forall \varphi \in H^1(R^N),
\]

where

\[
a(\psi, \varphi) = \int_{R^N} \nabla \psi \cdot \nabla \varphi dx + \int_{R^N} \left( -\sum_{i=1}^{m} \frac{2Z}{r_i} + \sum_{1 \leq i < j \leq m} \frac{2}{r_{ij}} + K \right) \psi \varphi dx.
\]

By the transform \( a(\psi, \varphi) = \sigma^N \hat{a}(\hat{\psi}, \hat{\varphi}) \) and

\[
\min\{\sigma^N, \sigma^{N-2}\} \|\psi\|_{1,R^N} \leq \|\hat{\psi}\|_{1,R^N} \leq \max\{\sigma^N, \sigma^{N-2}\} \|\psi\|_{1,R^N},
\]

we know that \( a(\cdot, \cdot) \) is continuous and coercive on \( H^1(R^N) \). For the sake of simplicity in notation, we drop the continuity and coercivity constants and write \( \| \cdot \|_{1,R^N} = \sqrt{a(\cdot, \cdot)} \) throughout this paper.

We consider the approximation of (2.12) in a bounded domain. Let \( R > 0 \) be large enough and \( B = B(0, R) \subset R^N \) be the ball with radius \( R \) and center at the origin. The approximation of (2.12) is defined as follows: Find \((\lambda_B, \psi_B) \in R^1 \times H^1_0(B) \) and \( \psi_B \neq 0 \) such that

\[
(2.13) \quad a(\psi_B, \varphi_B) = \lambda \int_{R^N} \psi_B \varphi_B dx \quad \forall \varphi_B \in H^1_0(B).
\]

For all \( \phi_B \in H^1_0(B) \), we extend \( \phi_B \) by zero to the exterior of \( B \) and still denote the extension as \( \phi_B \in H^1(R^N) \). Thus (2.13) is the Galerkin approximation of (2.12). \( a(\cdot, \cdot) \) is continuous and coercive on \( H^1_0(B) \), and the continuity and coercivity constants are independent of the radius \( R \).

**Theorem 2.2.** If the Schrödinger operator \( H \) is restricted to the bounded domain \( B \), then its spectrum is discrete. It has the form

\[
(2.14) \quad 0 < \lambda_{B1} \leq \lambda_{B2} \leq \cdots \to +\infty,
\]

where \( \lambda_{Bi} = \lambda_{Bi+1} \) means that \( \lambda_{Bi} \) is multiple. If \( \psi_B \) is the eigenfunction in (2.13) associated with \( \lambda_B \), then \( \psi_B \in H^2(B) \cap H^1_0(B) \).

**Proof.** Since \( H^1_0(B) \hookrightarrow \hookrightarrow L^2(B) \), by the Lax–Milgram theorem [9], we know that (2.13) has eigenvalues and eigenfunctions. Its spectrum is discrete and has the form of (2.14).

Let \((\lambda_B, \psi_B)\) be an eigenpair of (2.13), i.e.,

\[
(2.15) \quad \begin{cases} 
-\Delta \psi_B - \sum_{i=1}^{m} \frac{2Z \psi_B}{r_i} + \sum_{1 \leq i < j \leq m} \frac{2 \psi_B}{r_{ij}} = E \psi_B & \text{in } B, \\
\psi = 0 & \text{on } \partial B.
\end{cases}
\]

By Lemma 2.1, we have

\[
\frac{\psi_B}{r_i} \quad \frac{\psi_B}{r_{ij}} \in L^p(B), \quad 1 \leq i \leq m, \quad 1 < p < 2.
\]
By the $L^p$ theory of elliptic equations \[17\], $\psi_B \in W^{2,p}(B)$ for any $1 < p < 2$. Then by Lemma 2.1,

$$\frac{\psi_B}{\tau_i}, \frac{\psi_B}{\tau_{ij}} \in L^2(B), \quad 1 \leq i < j \leq m.$$ 

Thus $\psi_B \in H^2(B)$.

**Theorem 2.3.** If $(\lambda, \psi)$ is an eigenpair of (2.12) with $\|\psi\|_{1,R^N} = 1$, then for any $\epsilon > 0$ there exist $R > 0$ and an eigenpair $(\lambda_B, \psi_B)$ of (2.13) such that

\begin{align}
|\lambda - \lambda_B| &< Ce^2, \\
\|\psi - \psi_B\|_{1,R^N} &< C\epsilon,
\end{align}

(2.16) \hspace{1cm} (2.17)

where $\psi_B$ is extended by zero to the exterior of $B$ and $C$ is a positive constant independent of $R$ and $\epsilon$.

**Proof.** By Theorem 10.33 in \[34\] and the coercivity of $a(\cdot, \cdot)$, we know that the discrete spectrum of (2.12) is

$$0 < \lambda_1 \leq \lambda_2 \leq \cdots < K,$$

where $\lambda_i = \lambda_{i+1}$ means that $\lambda_i$ is multiple, and $K$ is the unique accumulation. By the minmax theorem \[10\],

$$\lambda_i \leq \lambda_{Bi}, \quad i = 1, 2, \ldots.$$

Define $V_i, V_{Bi}$ as the eigenspaces associated with $\lambda_i$ and $\lambda_{Bi}$, respectively. We assume $\psi \in V_i$. By the theory of abstract spectrum approximation (p. 699 of \[10\]), there exists $\psi_{Bi} \in V_{Bi}$ such that

\begin{align}
|\lambda_i - \lambda_{Bi}| &\leq C(\varepsilon_B(\lambda_i))^2, \\
\|\psi - \psi_{Bi}\|_{1,R^N} &\leq C\varepsilon_B(\lambda_i),
\end{align}

(2.18) \hspace{1cm} (2.19)

where

\begin{align}
\varepsilon_B(\lambda_i) = \sup_{\psi \in V_i} \inf_{v \in H^1_0(B)} \frac{\|u - v\|_{1,R^N}}{\|\psi\|_{1,R^N}}.
\end{align}

(2.20)
\( C \) is a constant depending on the continuity and coercivity constants of the bilinear form \( a(\cdot, \cdot) \) and \( \lambda_1 \), but is independent of \( R \).

Let \( \{ \psi_1, \ldots, \psi_l \} \) be an orthonormal basis of \( V_i \) with respect to the norm of \( H^1(\mathbb{R}^N) \), and let \( l \) be the multiplicity of \( \lambda_i \). For any \( \epsilon > 0 \), since \( \psi_k \in H^1(\mathbb{R}^N) \), there exists a \( \phi_k \in C_0^\infty(\mathbb{R}^N) \) such that \( \| \psi_k - \phi_k \|_{1,R^N} < \epsilon/l \). Set \( R \) large enough such that \( \cup_{k=1}^l \mathrm{supp} \phi_k \subset B = B(0, R) \); then

\[
\varepsilon _B (\lambda_i) \leq \sum_{k=1}^l \| \psi_k - \phi_k \|_{1,R^N} < \epsilon.
\]

In view of (2.18)–(2.21), we have (2.16) and (2.17). \( \square \)

3. Weighted norms and Hilbert spaces. We consider the eigenvalue problem of the \( S \)-state of the helium atom, i.e., \( Z = m = 2 \). The eigenvalue equations of the Hamiltonian and the square of the angular momentum are

\[
-\Delta_1 \psi - \Delta_2 \psi + \left( \frac{2}{r_{12}} - \frac{4}{r_1} - \frac{4}{r_2} \right) \psi = E \psi, \quad (3.1)
\]

\[
\begin{align*}
\left\{ \begin{array}{l}
\sum_{i=1}^2 \left( y_i \frac{\partial}{\partial z_i} - z_i \frac{\partial}{\partial y_i} \right)^2 + \sum_{i=1}^2 \left( z_i \frac{\partial}{\partial x_i} - x_i \frac{\partial}{\partial z_i} \right)^2 \\
+ \sum_{i=1}^2 \left( x_i \frac{\partial}{\partial y_i} - y_i \frac{\partial}{\partial x_i} \right)^2 + l(l+1) & \end{array} \right\} \psi = 0, \quad (3.2)
\end{align*}
\]

where \( l = 0, 1, \ldots \). Let \( \theta', \phi, \phi' \) be three Euler angles such that \( (r_1, \theta', \phi') \) are the spherical coordinates of the first electron in the fixed system \( \rho - x y z \), \( \phi \) is the inter-electronic angle between the \( r_1 - z \) plane and the \( r_1 - r_2 \) plane, and \( \theta \) is the inter-electronic angle. We introduce the Hylleraas–Breit transform [7]:

\[
\begin{align*}
&x_1 = r_1 \sin \theta' \cos \phi', \\
y_1 = r_1 \sin \theta' \sin \phi', \\
z_1 = r_1 \cos \theta', \\
x_2 = r_2(\sin \theta \cos \theta' \cos \phi \cos \phi' - \sin \theta \sin \phi \sin \phi' + \cos \theta \sin \theta' \cos \phi'), \\
y_2 = r_2(\sin \theta \cos \phi \cos \phi' \sin \phi' + \sin \theta \sin \phi \cos \phi' + \cos \theta \sin \theta' \sin \phi'), \\
z_2 = r_2(\cos \theta \cos \theta' - \sin \theta \sin \theta' \cos \phi).
\end{align*}
\]

We can transform (3.1) and (3.2) into the following forms by (3.3):

\[
L(\psi) - \frac{A_1(\psi)}{r_1^2} - \frac{A_2(\psi)}{r_2^2} = E \psi, \quad (3.4)
\]

\[
\begin{align*}
\left[ \frac{\partial^2}{\partial \theta'^2} + \cot \theta' \frac{\partial}{\partial \theta'} + \frac{1}{\sin^2 \theta'} \left( \frac{\partial^2}{\partial \phi'^2} + \frac{\partial^2}{\partial \phi^2} \right) - \frac{2 \cos \theta' \partial^2}{\sin^2 \theta' \partial \phi \partial \phi'} + l(l+1) \right] \psi &= 0, \quad (3.5)
\end{align*}
\]
Thus any wave function \(\psi\) of the helium atom, \(l = 0\); then (3.5) has only constant solutions. Therefore, we can transform (3.4) of the \(S\)-state into a three-dimensional form

\[
L(u) = Eu.
\]

Assume that \(\Omega \subset X = [0, +\infty) \times [0, +\infty) \times [0, \pi]\) is a bounded domain. \(u = u(r_1, r_2, \theta), v = v(r_1, r_2, \theta)\). We define inner products, norms, and Hilbert spaces as follows:

\[
(u, v)_0 = \int_\Omega uv r_1^2 r_2^2 \sin \theta dr_1 dr_2 d\theta, \quad \|u\|_{0,r,\Omega}^2 = \int_\Omega u^2 r_1^2 r_2^2 \sin \theta dr_1 dr_2 d\theta,
\]

\[
(u, v)_1 = (u, v)_0 + \int_\Omega \left[ r_1^2 r_2^2 \frac{\partial u}{\partial r_1} \frac{\partial v}{\partial r_1} + r_1^2 r_2^2 \frac{\partial u}{\partial r_2} \frac{\partial v}{\partial r_2} + (r_1^2 + r_2^2) \frac{\partial u}{\partial \theta} \frac{\partial v}{\partial \theta} \right] \sin \theta dr_1 dr_2 d\theta,
\]

\[
|u|_{1,r,\Omega}^2 = \int_\Omega r_1^2 r_2^2 \left( \frac{\partial u}{\partial r_1} \right)^2 + r_1^2 r_2^2 \left( \frac{\partial u}{\partial r_2} \right)^2 + (r_1^2 + r_2^2) \left( \frac{\partial u}{\partial \theta} \right)^2 \sin \theta dr_1 dr_2 d\theta,
\]

\[
|u|_{2,r,\Omega}^2 = \left\| \frac{\partial u}{\partial r_1} \right\|_{1,r,\Omega}^2 + \left\| \frac{\partial u}{\partial r_2} \right\|_{1,r,\Omega}^2 + \left\| \frac{\partial u}{\partial \theta} \right\|_{1,r,\Omega}^2,
\]

\[
\|u\|_{i+1,r,\Omega}^2 = \|u\|_{i,r,\Omega}^2 + |u|_{i+1,r,\Omega}^2, \quad i = 0, 1,
\]

\[
H^i_r(\Omega) = \left\{ v \mid \|v\|_{i,r,\Omega} < +\infty \right\}, \quad i = 0, 1,
\]

\[
H^2_r(\Omega) = \left\{ v \mid \|v\|_{2,r,\Omega} < +\infty, \int_\Omega u^2 (r_1^2 + r_2^2) \sin \theta dr_1 dr_2 d\theta < \infty \right\}.
\]

**Lemma 3.1.** Assume that \(\Omega \subset X\) is a bounded domain; then

\[
H^i_r(\Omega) \hookrightarrow H^0_r(\Omega).
\]
Furthermore, if there exists a constant $d_\Omega > 0$, such that for any $(r_1, r_2, \theta) \in \Omega$, $r_1, r_2 \geq d_\Omega$, then

$$H^2_r(\Omega) \hookrightarrow H^1_r(\Omega).$$

**Proof.** (1): Proof of (3.7). Let $x = (x_1, y_1, z_1, x_2, y_2, z_2) = H(r_1, r_2, \theta, \theta', \phi, \phi')$ be the Hylleraas–Breit transform defined by (3.3), and let $\Omega \subset R^6$ be a bounded domain defined by

$$\hat{\Omega} = \{ x | x = H(r_1, r_2, \theta, \theta', \phi, \phi'), (r_1, r_2, \theta) \in \Omega, \; 0 \leq \theta' \leq \pi, \; 0 \leq \phi, \phi' \leq 2\pi \}.$$ 

The Jacobian determinant of (3.3) is

$$\det \left( \frac{\partial(x_1, y_1, z_1, x_2, y_2, z_2)}{\partial(r_1, r_2, \theta, \theta', \phi, \phi')} \right) = r_1^2 r_2^2 \sin \theta \sin \theta'.$$

By direct calculation, we have $||u||^2_{i, r, \Omega} = \frac{1}{2\pi \sin \varphi^i} ||u||^2_{i, \hat{\Omega}}$, where $|| \cdot ||_{i, \hat{\Omega}}$ is the norm of the standard Sobolev space $H^i(\hat{\Omega})$, $i = 0, 1$. It is easy to show that $H^0(\Omega)$ and $H^1(\Omega)$ are Hilbert spaces, and $H^1(\Omega) \hookrightarrow H^0(\Omega)$.

(2): Proof of (3.8). Let $\{v_n\}$ be a bounded sequence in $H^2_r(\Omega)$; then $\{v_n\}, \{\frac{\partial v_n}{\partial r_1}\}, \{\frac{\partial v_n}{\partial r_2}\}$ are bounded uniformly in $H^1(\Omega)$. By (1), we can choose (successively) a subsequence denoted as $\{v_n\}$ too, such that $\{v_n\}, \{\frac{\partial v_n}{\partial r_1}\}, \{\frac{\partial v_n}{\partial r_2}\}$ are Cauchy sequences in $H^0(\Omega)$. Thus $\{v_n\}$ is a Cauchy sequence in the measure

$$\left( \|v_n\|_{0, r, \Omega}^2 + \int_{\Omega} \left( \left| \frac{\partial v_n}{\partial r_1} \right|^2 + \left| \frac{\partial v_n}{\partial r_2} \right|^2 + \left| \frac{\partial v_n}{\partial \theta} \right|^2 \right) r_1^2 r_2^2 \sin \theta \sin \theta' \right)^{1/2} .$$

It is clear that

$$\int_{\Omega} \left| \frac{\partial v_n}{\partial \theta} \right|^2 (r_1^2 + r_2^2) \sin \theta dr_1 dr_2 d\theta \leq \frac{2}{d_\Omega^4 \pi} \int_{\Omega} \left| \frac{\partial v_n}{\partial \theta} \right|^2 r_1^2 r_2^2 \sin \theta dr_1 dr_2 d\theta,$$

and so we have

$$\|v_n\|_{1, r, \Omega}^2 \leq \max \{1, 2/d_\Omega^4\} \left( \|v_n\|_{0, r, \Omega}^2 + \left\| \frac{\partial v_n}{\partial r_1} \right\|_{0, r, \Omega}^2 + \left\| \frac{\partial v_n}{\partial r_2} \right\|_{0, r, \Omega}^2 + \left\| \frac{\partial v_n}{\partial \theta} \right\|_{0, r, \Omega}^2 \right).$$

Therefore $\{v_n\}$ is a Cauchy sequence in $H^1(\Omega)$ and converges. □

**Remark 3.2.** Suppose that $\Omega$ is bounded. For any integer $k > 0$, define

$$P_k(\Omega) = \left\{ p = \sum_{0 \leq l + m + n \leq k} \alpha_{lmn} r_1^l r_2^m \theta^n \mid \alpha_{lmn} \in R^1, (r_1, r_2, \theta) \in \Omega \right\};$$

then $P_k(\Omega) \subset H^2(\Omega) \subset H^2(\Omega)$.

**Lemma 3.3.** Supposing $R > 0$ is a constant, there exists a constant $C$ independent of $R$ such that, for any $f \in H^1([0, R])$,

$$\int_0^R f^2 dx \leq C \max\{R^2, R^{-2}\} \left( \int_0^R x^2 f^2 dx + \int_0^R f^2 dx \right).$$
Proof. For any \( f \in C^1([R/2, R]) \) there exists \( \xi \in [R/2, R] \) such that
\[
f(\xi) = \frac{2}{R} \int_{R/2}^{R} f(x)dx.
\]
Then for any \( x \in [R/2, R] \), by Hölder’s inequality we have
\[
|f(x)| = |f(\xi) + \int_{\xi}^{x} f'(t)dt| \leq \frac{2}{R} \int_{R/2}^{R} |f(t)|dt + \int_{R/2}^{R} |f'(t)|dt
\]
\[
\leq \left( \frac{2}{R} \int_{R/2}^{R} |f(t)|^2dt \right)^{1/2} + \left( \frac{R}{2} \int_{R/2}^{R} |f'(t)|^2dt \right)^{1/2}.
\]
Thus there exists a positive constant \( C \) independent of \( R \) such that
\[
(3.12) \quad |f|_{[0,\infty, [R/2, R]} \leq C \max\{\sqrt{R}, 1/\sqrt{R}\} \|f\|_{[R/2, R]}.
\]
Set \( x_0 \in [R/2, R] \). By (3.12), we have, for any \( x \in [0, R] \) and \( f \in C^\infty([0, R]) \),
\[
(3.13) \quad f^2(x) \leq 2 \left\{ f^2(x_0) + \frac{1}{x_0} f'(x_0) dx \right\} \leq C \left\{ f^2(x_0) + R \int_0^R f'(x_0) dx \right\}
\]
\[
\leq C \max\{R, R^{-3}\} \left( \int_{R/2}^{R} x^2 f^2(x)dx + \int_0^R f'(x)dx \right) \forall x \in [0, R],
\]
where \( C \) is a constant independent of \( R \). We obtain (3.11) for all functions in \( C^\infty([0, R]) \) by integrating both sides of (3.13) over \([0, R]\). Therefore (3.11) is true for all functions in \( H^1([0, R]) \) by the density of \( C^\infty([0, R]) \) in \( H^1([0, R]) \). \( \square \)

Now, we expand each function \( u(r_1, r_2, \theta) \) in some Banach space defined on \( \Omega \) to \( R^3 \setminus \Omega \). Thus \( r_1, r_2, \theta \) are not the distances and the interelectronic angle in the previous sense. For any \( u = u(r_1, r_2, \theta) \), define
\[
(3.14) \quad \|u\|_{0, \Omega}^2 = \int_{\Omega} u^2 r_1^2 r_2^2 |\sin \theta|dr_1 dr_2 d\theta,
\]
\[
(3.15) \quad \|u\|_{1, \Omega}^2 = \int_{\Omega} \left[ \left( \frac{\partial u}{\partial r_1} \right)^2 + \left( \frac{\partial u}{\partial r_2} \right)^2 + \left( \frac{\partial u}{\partial \theta} \right)^2 \right] (r_1^2 + r_2^2) |\sin \theta| dr_1 dr_2 d\theta,
\]
\[
H(\Omega) = \{ u | \|u\|_{0, \Omega}^2 + \|u\|_{1, \Omega}^2 < \infty \}.
\]

Theorem 3.4. Suppose that \( \Omega \subset X \) is a bounded open domain satisfying \( C^1 \)-regularity [2]. There exists a linear operator
\[
E : H(\Omega) \rightarrow H(R^3)
\]
such that, for any \( u \in H(\Omega) \),
\[
(3.16) \quad Eu(r_1, r_2, \theta) = u(r_1, r_2, \theta), \quad \text{almost everywhere in } (r_1, r_2, \theta) \in \Omega,
\]
\[
(3.17) \quad \|Eu\|_{i, R^3} \leq C \|u\|_{i, \Omega}, \quad i = 0, 1,
\]
where \( C \) is a constant depending on \( \Omega \).

Proof. Let \( B(0, 1) \) be the open unit ball in \( R^3 \). Since \( \Omega \) is bounded and \( C^1 \)-regular, there exist a finite number of bounded open sets \( O_0, \ldots, O_M \) such that \( O_0 \subset \subset
\[\Omega, \partial\Omega \subset \bigcup_{i=1}^{M} O_i, \text{ and } \Omega \subset \bigcup_{i=0}^{M} O_i, \text{ and there exist } m + 1 \text{ transforms } (\xi, \eta, \zeta) = \varphi_i(r_1, r_2, \theta) \] such that
\[
\varphi_i(O_1) = B(0, 1), \quad \varphi_i(O_i \cap \partial\Omega) = \Sigma = B(0, 1) \cap \{\zeta = 0\}, \]
\[
\varphi_i(O_i \cap \Omega) = B^+(0, 1) = \{ (\xi, \eta, \zeta) \in B(0, 1) \mid \zeta > 0 \}, \]
\[
\varphi_i \in C^1(\overline{O_i \cap \partial\Omega}), \quad \varphi_i^{-1} \in C^1(\Sigma).
\]

For the convenience of notation, define \(x = (r_1, r_2, \theta)\) and \(\hat{x} = (\xi, \eta, \zeta)\). We choose a partition of unity \(\{\alpha_i\}\) associated with \(\{O_i\}\) satisfying
\[
\alpha_i \in C^\infty_0(O_i), \quad 0 \leq \alpha_i \leq 1, \quad 0 \leq i \leq M, \quad \sum_{i=0}^{M} \alpha_i(x) = 1 \quad \forall x \in \Omega.
\]

(1): Proof for functions \(u \in C^1(\Omega)\). Set \(u_i = u\alpha_i; \text{ then } u = \sum_{i=0}^{M} u_i. \)

\[
(3.18) \quad \left\| \begin{array}{c}
\varphi_i(x) = r_1^2 r_2^2 \sin \theta, \\
\omega_i(x) = (r_1^2 + r_2^2) \sin \theta, \\
v_i(x) = u_i(\varphi_i^{-1}(x)) = u_i(x).
\end{array} \right.
\]

For any \(0 \leq i \leq M, \) since \(\partial_{\psi_i} = \sum_{l=1}^{3} \frac{\partial u_i}{\partial \psi_l} \frac{\partial \psi_l}{\partial x_l}, \) there exists a constant \(C\) depending only on \(\varphi_i\) and \(\varphi_i^{-1}\) such that

\[
(3.19) \quad \int_{B^+(0,1)} |v_i|^2 \varrho_i d\hat{x} = \int_{\partial \Omega \cap O_i} |u_i|^2 \varrho_i d\hat{x} \leq C \| u_i \|_{0, \Omega \cap O_i}^2,
\]
\[
(3.20) \quad \int_{B^+(0,1)} \left| \frac{\partial v_i}{\partial \psi_k} \right|^2 \omega_i d\hat{x} \leq C \sum_{l=1}^{3} \int_{B^+(0,1)} \left| \frac{\partial u_i}{\partial \psi_l} \right|^2 \left| \frac{\partial \psi_l}{\partial \psi_k} \right|^2 \omega_i d\hat{x}
\leq C \sum_{l=1}^{3} \left\| \frac{\partial u_i}{\partial \psi_l} \right\|_{0, \Omega \cap O_i}^2,
\]

where \(J_i = \det(\frac{\partial \psi_i}{\partial x})\) is the Jacobian determinant. Similarly, we have

\[
(3.21) \quad \| u_i \|_{0, \Omega \cap O_i}^2 \leq C \int_{B^+(0,1)} |v_i|^2 \varrho_i d\hat{x},
\]
\[
(3.22) \quad \left\| \frac{\partial u_i}{\partial \psi_k} \right\|_{0, \Omega \cap O_i}^2 \leq C \sum_{l=1}^{3} \int_{B^+(0,1)} \left| \frac{\partial v_i}{\partial \psi_l} \right|^2 \omega_i d\hat{x}.
\]

We expand \(u_0\) by zero to the exterior of \(O_0\) and denote the extension as \(\tilde{u}_0; \) then \(\tilde{u}_0 \in C^1_0(R^3). \) We expand \(v_i(x)\) as follows:

\[
(3.23) \quad \tilde{v}_i(x) = \begin{cases} 
\overline{v}_i(x), & \hat{x} \in B^+(0,1) \cup \Sigma, \\
\frac{4v_i(\xi, \eta, \zeta)}{\zeta - \frac{1}{2}} - 3v_i(\xi, \eta, \zeta), & \hat{x} \in B^-(0,1),
\end{cases}
\]

where \(B^-(0,1) = \{ \hat{x} \in B(0,1) \mid \zeta < 0 \}. \) Obviously, \(\tilde{v}_i \in C^1(B^+(0,1) \cup B^-(0,1)). \) For any multiple index \(\alpha \in \{ (0,0,0), (1,0,0), (0,1,0), (0,0,1) \}\) and \(\hat{x}_0 \in \Sigma, \) we have

\[
\lim_{\hat{x} \to B^+(0,1)} D^\alpha \tilde{v}_i(x) = D^\alpha v_i(\hat{x}_0),
\]
\[
\lim_{\hat{x} \to B^-(0,1)} D^\alpha \tilde{v}_i(x) = \lim_{\hat{x} \to B^-(0,1)} \left[ \begin{array}{c}
4 \left( -\frac{1}{2} \right)^{\alpha_3} 
\end{array} \right. 
D^\alpha v_i \left( \xi, \eta, -\frac{1}{2} \right) + 3(-1)^{\alpha_3+1} D^\alpha v_i(\xi, \eta, -\zeta)
\]
\[
= D^\alpha v_i(\hat{x}_0).
\]
Thus $\tilde{u}_i(x) = \tilde{v}_i(\phi_i(x)) \in C^0_0(O_i)$. Expand $\tilde{u}_i$ by zero to the exterior of $O_i$ and denote the extension by $\tilde{u}_i$ too; then $\tilde{u}_i \in C^0_0(R^3)$. Define $E u = \sum_{i=0}^{M} \tilde{u}_i$; then $(E u)(x) = \sum_{i=0}^{M} u_i(x) = u(x) \forall x \in \Omega$. Combing (3.19)–(3.23) yields (3.16) and (3.17).

(2): Proof for functions $u \in H(\Omega)$. Let $\hat{\Omega}$ be defined as in (3.9). In view of

$$
\|u\|^2_{m,r,\Omega} = \frac{1}{8\pi^2} \|u\|^2_{\hat{\Omega}},
$$

we have $H^i(\Omega) \hookrightarrow H^i(\hat{\Omega}), \ i = 0, 1$, in the sense of isomorphism. Since $C^1(\hat{\Omega})$ is dense in $H^1(\hat{\Omega})$, for any $v(r_1, r_2, \theta) \in H^1(\hat{\Omega})$ there exists $\{v_n(r_1, r_2, \theta)\} \subset C^1(\hat{\Omega})$ such that $v_n(r_1, r_2, \theta)$ converge to $v(r_1, r_2, \theta)$ in $H^1(\hat{\Omega})$, and hence in $H^1(\Omega), \ i = 0, 1$. Since $\frac{\partial v_n}{\partial \xi} = \sum_{i=1}^{6} \frac{\partial v_n}{\partial x_i}, \ \frac{\partial v_n}{\partial x_r}, \ \frac{\partial v_n}{\partial x_{v_r}}$, and $\frac{\partial v_n}{\partial \xi}$ are continuous and bounded, we have $v_n(r_1, r_2, \theta) \subset C^1(\Omega), \ \text{where } \xi = r_1, r_2, \theta, \phi, \phi'$. Thus $C^1(\Omega)$ is dense in $H^1(\Omega), \ i = 0, 1$.

Since $\Omega \subset X, \ C^1(\Omega)$ is dense in $H(\Omega)$ in view of $H(\Omega) \hookrightarrow H_0^1(\Omega)$. There exists a sequence $\{u_n\} \subset C^1(\Omega)$ converging to $u \in H(\Omega)$. By (3.18), $\{E u_n\}$ is a Cauchy sequence in $H(R^3)$ and hence converges to some $w \in H(R^3)$. Set $E u = w$. Since $\|u_n - E u\|_{i,\Omega} = \|E u_n - E u\|_{i,\Omega} \rightarrow 0$, we have $E u = u$, a.e. in $\Omega$. Furthermore,

$$
\|E u\|_{i,\Omega} = \lim_{n \rightarrow \infty} \|E u_n\|_{i,\Omega} \leq C \lim_{n \rightarrow \infty} \|u_n\|_{i,\Omega} = C\|u\|_{i,\Omega}, \ i = 0, 1.
$$

The proof is complete.

We define $\Omega_{r_1,\theta}$ as the projection of $\Omega$ onto the $r_1-\theta$ plane. For any $(r_1, \theta) \in \Omega_{r_1,\theta}$, define

$$
\Omega_{r_2}(r_1, \theta) = \{r_2 \mid (r_1, r_2, \theta) \in \Omega\}.
$$

$\Omega_{r_2,\theta}$ and $\Omega_{r_2}(r_2, \theta)$ are defined in the same way.

**Theorem 3.5.** Let $\Omega \subset X$ be a bounded domain satisfying one of the following two conditions:

(a) $\Omega$ is $C^1$–regular;

(b) the boundary $\partial \Omega$ is Lipschitz continuous, and there exists a constant $d > 0$ such that, for almost every $(r_2, \theta) \in \Omega_{r_2,\theta}$ (respectively, $(r_1, \theta) \in \Omega_{r_1,\theta}$), if $\Omega_r \subset \Omega_{r_1}(r_2, \theta)$ (respectively, $\Omega_{r_2}(r_1, \theta)$) is a maximal simply connected set, then meas$(\Omega_r)$ \geq d.

Furthermore, we assume that there are $f_1, f_2, \ldots, f_M \in (H^m_r(\Omega))^\prime$ satisfying

$$
(3.24) \forall p \in P_{m-1}(\Omega), \sum_{i=1}^{M} f_i(p) = 0 \iff p = 0.
$$

Then there exists a constant $C(\Omega)$ such that

$$
(3.25) \quad \|v\|_{m,r,\Omega} \leq C(\Omega) \left\{|v|_{m,r,\Omega} + \sum_{i=1}^{M} f_i(v)\right\} \forall v \in H^m_r(\Omega), \ m = 1, 2.
$$

**Proof.** (1) In view of (3.7), we can prove (3.25) in the case of $m = 1$ by the argument of Theorem 3.1.1 in [9, p. 115].
(2) Proof of (3.25) in the case of \( m = 2 \). If (3.25) were false, then for any integer \( n > 0 \) there should exist \( v_n \in H^2_\Omega \) such that \( \|v_n\|_{2,r,\Omega} = 1 \) and

\[
|v_n|_{2,r,\Omega} + \left| \sum_{i=1}^{M} f_i(v_n) \right| < \frac{1}{n}.
\]

In view of Theorem 3.4, the definition of \( \| \cdot \|_{2,r,\Omega} \), and (3.25) for \( m = 1 \), there exists a subsequence of \( \{v_n\} \) (also denoted as \( \{v_n\} \)), which is a Cauchy sequence under the following measures:

\[
\| \cdot \|_{0,r,\Omega}, \quad \| \cdot \|_{0,r,\Omega}^\theta,
\]

\[
\left\{ \left( \frac{\partial v_n}{\partial \theta} \right)^2 + \left( \frac{\partial^2 v_n}{\partial r^2} \right)^2 + \left( \frac{\partial^2 v_n}{\partial r \partial \theta} \right)^2 \right\} (r_1^2 + r_2^2) \sin \theta dr_1 dr_2 d\theta \}^{1/2}.
\]

(i) Suppose that \( \Omega \) satisfies the condition (a). We set \( u_n = \frac{\partial v_n}{\partial \theta} \); then \( u_n \in H(\Omega) \).

Choose \( R > 0 \) to be sufficiently large such that \( \Omega \subset [0, R] \times [0, R] \times [0, \pi] \). By Lemma 3.3 and Theorem 3.4, we have

\[
\int_{\Omega_2(r_1, \theta)} \left( \frac{\partial u_n}{\partial \theta} \right)^2 r_1^2 \sin \theta dr_2 \leq \int_0^R (\sum_{i=1}^M f_i(v_n))^2 r_1^2 \sin \theta dr_2 \leq C \left\{ \int_0^R (\sum_{i=1}^M f_i(v_n))^2 r_1^2 \sin \theta dr_2 \right\} \forall (r_1, \theta) \in \Omega_{r_1, \theta},
\]

where \( C \) depends on \( R \). By Lemma 3.3, integrating both sides of the above inequality over \( \Omega_{r_1, \theta} \) produces

\[
\int_0^\pi \left( \frac{\partial u_n}{\partial \theta} \right)^2 r_1^2 \sin \theta dr_2 d\theta \leq C \sum_{i=0}^1 \|u_n\|_{r_i, \Omega}^2 \leq C \sum_{i=0}^1 \|u_n\|_{r_i, \Omega}^2.
\]

Thus \( \{v_n\} \) is a Cauchy sequence under \( [\int_{\Omega} \left( \frac{\partial u_n}{\partial \theta} \right)^2 r_1^2 \sin \theta dr_2 d\theta]^{1/2} \). Similarly, \( \{v_n\} \) is a Cauchy sequence under \( [\int_{\Omega} \left( \frac{\partial u_n}{\partial \theta} \right)^2 r_1^2 \sin \theta dr_2 d\theta]^{1/2} \). Consequently, \( \{v_n\} \) is a Cauchy sequence in \( H^2_\Omega \) by (3.27), and so in \( H^2_\Omega \) by (3.26). Suppose \( v_n \to v \in H^2_\Omega \); then \( |v|_{2,r,\Omega} = 0 \) and \( \sum_{i=1}^M f_i(v) = 0 \) by (3.26). Thus \( v \in P_1(\Omega) \), and \( v = 0 \) by (3.24). Therefore, \( v = 0 \) contradicts the following identities: \( \|v\|_{2,r,\Omega} = \lim_{n \to \infty} \|v_n\|_{2,r,\Omega} = 1 \). Thus (3.25) is true for \( m = 2 \).

(ii) Suppose that \( \Omega \) satisfies the condition (b). Without loss of generality, we may suppose that \( \Omega_{r_2}(r_1, \theta) \) is simply connected for any \( (r_1, \theta) \in \Omega_{r_1, \theta} \). By Lemma 3.3, we have

\[
\int_{\Omega_{r_2}(r_1, \theta)} \left( \frac{\partial u_n}{\partial \theta} \right)^2 r_1^2 \sin \theta dr_2 \leq C \int_{\Omega_{r_2}(r_1, \theta)} \left[ \left( \frac{\partial v_n}{\partial \theta} \right)^2 r_1^2 + \left( \frac{\partial^2 v_n}{\partial r \partial \theta} \right)^2 \right] r_1^2 \sin \theta dr_2
\]

\forall (r_1, \theta) \in \Omega_{r_1, \theta}, \text{ where } C \text{ depends on } d \text{ but is independent of } (r_1, \theta). \text{ Thus we can get (3.25) by the argument of (i).} \]

Remark 3.6. Assume that \( \Omega \) satisfies the conditions in Theorem 3.5. Define

\[
|\Omega| = \int_{\Omega} r_1^2 r_2^2 \sin \theta dr_1 dr_2 d\theta, \quad f(v) = \frac{1}{|\Omega|} \int_{\Omega} vr_1^2 r_2^2 \sin \theta dr_1 dr_2 d\theta.
\]
By Hölder’s inequality, we have $|f(v)| \leq |\Omega|^{-2}\|v\|_{0, r, \Omega}$. Thus $f \in (H_0^1(\Omega))^\prime$. Now (3.26) implies
\[ (3.29) \quad \|v - f(v)\|_{1, r, \Omega} \leq |\Omega|^{-2}\|v\|_{0, r, \Omega} \quad \forall v \in H_0^1(\Omega). \]

**Remark 3.7.** Assume $R > 0$ and $\Omega = [0, R] \times [0, R] \times [0, \pi]$. Define
\[ H_{0, r}^1(\Omega) = \{ v \in H_0^1(\Omega) \mid v|_{r_1 = R} = v|_{r_2 = R} = 0 \}. \]
Then we have $H_{0, r}^1(\Omega) \hookrightarrow H_0^1(\Omega)$ in the sense of isomorphism, and, by Poincarré’s inequality,
\[ (3.30) \quad \|v\|_{1, r, \Omega} = \frac{\sqrt{\pi}}{4\pi}\|v\|_{1, \hat{\Omega}} \leq C(\Omega)|v|_{1, \hat{\Omega}} = \sqrt{8\pi\sigma(\Omega)}|v|_{1, r, \Omega}. \]

Equations (3.29) and (3.30) are the so-called Friedrichs-type inequality and Poincarré-type inequality, respectively.

**Theorem 3.8.** Let $\Omega \subset X$ be the domain in Theorem 3.5 and $T : H_0^1(\Omega) \rightarrow H_0^1(\Omega)$ be a linear and continuous mapping satisfying
\[ (3.31) \quad Tp = p \quad \forall p \in P_{k-1}(\Omega). \]
Then there exists a constant $C(\Omega)$ such that
\[ (3.32) \quad \|u - Tu\|_{m, r, \Omega} \leq C(\Omega)|u|_{k, r, \Omega} \quad \forall u \in H_0^1(\Omega), \]
where $0 \leq m \leq 2$, $1 \leq k \leq 2$, $m \leq k$.

**Proof.** (3.32) can be proved by virtue of Theorem 3.5 and the argument of Theorem 3.1.4 in [9, p. 121]. \[ \square \]

**4. Local regularization operator.** Because we cannot say that the solutions of (2.13) and (5.1) are continuous, difficulties appear in proving the convergency of the finite element scheme. The technique of local regularization (Clément’s interpolation [11]) will be used. Thus we are in the position of describing the construction of the three-dimensional local regularization operator.

Set $R > 0$ be large enough, and define
\begin{align*}
\Omega &= [0, R] \times [0, R] \times [0, \pi], \\
\partial \Omega &= \{(r_1, r_2, \theta) \in \Omega \mid r_1 = R \text{ or } r_2 = R\}, \\
\Gamma_1 &= \{(r_1, r_2, \theta) \in \partial \Omega \mid r_1 = 0\}, \\
\Gamma_2 &= \{(r_1, r_2, \theta) \in \partial \Omega \mid r_2 = 0\}, \\
\Gamma_3 &= \{(r_1, r_2, \theta) \in \partial \Omega \mid \theta = 0\}, \\
\Gamma_4 &= \{(r_1, r_2, \theta) \in \partial \Omega \mid \theta = \pi\}.
\end{align*}
Suppose that $T_h$ is a regular subdivision of $\Omega$. Each element in $T_h$ is a cuboid. (We can also obtain similar results for regular hexahedrons, but the analysis is very tedious.) $h$ is the maximal diameter of all elements. The regularity of $K$ means that there exists a constant $\sigma$ independent of $K$ such that $\forall K \in T_h, h_K \leq \sigma |e|$: here $h_K$ is the diameter of $K$, $e$ is any edge of $K$. Denote all nodes of $\Omega$ by $A_1, A_2, \ldots, A_l$, and define $\Delta_i = \cup_{K \in T_h, A_i \in K} K$ as the macro element associated with the node $A_i$. 
\[ Q_k(K) = \left\{ p \mid p = \sum_{l,m,n=0}^{k} \alpha_{lmn} r_1^{l} r_2^{m} \theta^n, (r_1, r_2, \theta) \in K \right\}. \]

Since the behaviors of the weights (see (3.18)) on an inner element differ from those on a boundary element, different kinds of elements or macro elements must be affine equivalent to different reference elements or macro elements, respectively. Each macro element must be one of the following four cases:
1. An element in $\mathcal{T}_h$. Let $l_{10} = [0, 1]$, $l_{11} = [1, 2]$; its affine equivalent reference macro element must be one of $l_{ij} \times l_{jk} \times l_{ik}$, $0 \leq i, j, k \leq 1$.

2. The combination of two elements with a common face. Let $l_{20} = [0, 2]$, $l_{21} = [1, 3]$; its affine equivalent reference macro element must be one of $l_{2i} \times l_{1j} \times l_{1k}$, $0 \leq i, j, k \leq 1$.

3. The combination of four elements with a common edge. Its affine equivalent reference macro element must be one of $l_{i1} \times l_{2j} \times l_{2k}$, $0 \leq i, j, k \leq 1$.

4. The combination of eight elements with a common vertex. Its affine equivalent reference macro element must be one of $l_{2i} \times l_{2j} \times l_{2k}$, $0 \leq i, j, k \leq 1$.

Each reference element is a cube with unit volume and is included in some reference macro element. Clearly, the total number of reference elements and reference macro elements is finite.

Suppose $h_\Delta < \sigma h_K$, for any $K \subset \Delta$, where $h_\Delta$ is the diameter of $\Delta$. For any $K \in \mathcal{T}_h$, $F_K : K \to K$ is the affine transform from some reference element $\hat{K}$ to $K$. For any macro element $\Delta$, assume that $\hat{\Delta} = \cup_{K \subset \Delta} F_K^{-1}(K)$ is a macro reference element defined in cases 1, 2, 3, or 4. Define $F_\Delta : F_\Delta|_K = F_K$ and $F_\Delta^{-1} : F_\Delta^{-1}|_K = F_K^{-1}$, with $F_K(\hat{K}) = K$.

If $v$ is a function defined on $\Delta$ and $\hat{v}$ is defined on $\hat{\Delta}$, denote $\hat{v} := v \circ F_\Delta$ and $\hat{u} := \hat{v} \circ F_\Delta^{-1}$, respectively. Without ambiguity, we also use piecewise-defined norms on macro elements:

$$|\hat{v}|^2_{m,r,\Delta} = \sum_{K \subset \Delta} |v \circ F_K|^2_{m,r,K}, \quad |u|^2_{m,r,\Delta} = \sum_{K \subset \Delta} |\hat{u} \circ F_K^{-1}|^2_{m,r,K}. \tag{4.1}$$

In view of (4.1), it is easy to prove $v \in H^m(\Delta) \iff \hat{v} \in H^m(\hat{\Delta})$, $m = 0, 1, 2$.

We define the $H^0$-projection $P_\Delta : H^0(\hat{\Delta}) \to P_h(\hat{\Delta})$ as follows: $\forall v \in H^0(\hat{\Delta})$,

$$\langle P_\Delta v, p \rangle = \langle v, p \rangle \quad \forall p \in P_h(\hat{\Delta}). \tag{4.2}$$

Since the weights vanish on some boundary elements $K \cap (\cup_{i=1}^4 \Gamma_i) \neq \emptyset$, we need to deal with their transformations under the affine transforms by detailed analysis. To do so, we first need the following estimate for the transformation of $\sin \theta$. Define

$$\Lambda(\theta, h) = \begin{cases} 1, & \pi/2 - h \leq \theta \leq \pi/2, \\ \sin \theta, & \theta \geq \pi/2, \\ \sin(\theta + h), & \theta \leq \pi/2 - h. \end{cases} \tag{4.3}$$

**Lemma 4.1.** Let $\sigma > 0$ be a constant, $h_1, h_2 \leq h \leq \sigma \min\{h_1, h_2\}$, $\theta \geq h_1$, and $\theta + h_1 + h_2 + h/\sigma \leq \pi$. When $h$ is sufficiently small, there exists a constant $C$ independent of $h$ and $\theta$ such that

$$\Lambda(\theta, h_1) \cdot \max \left\{ \frac{1}{\sin \theta}, \frac{1}{\sin(\theta + h_1)}, \frac{1}{\sin(\theta + h_1 + h_2)} \right\} \leq C. \tag{4.4}$$

**Proof.** Let $M = \max\{1/\sin \theta, 1/\sin(\theta + h_1), 1/\sin(\theta + h_1 + h_2)\}$. We consider (4.4) in three cases:

1. When $\pi/2 - h_1 - h_2 \leq \theta \leq \pi/2$, $\Lambda \cdot M \leq M$, since $h$ is small enough, (4.4) is true obviously.

2. When $\theta \geq \pi/2$, it is clear that

$$\Lambda M \leq \frac{\sin \theta}{\sin(\theta + h_1 + h_2)} = \frac{\sin(\pi - \theta)}{\sin(\pi - \theta - h_1 - h_2)}.$$
The proof is complete.

where

\[ \zeta \]

we have

\[ (4.5) \]

\[ \|
\]

On any finite-dimensional space, all norms are equivalent, and so we have

\[ K \]

\[ K \]

\[ \begin{bmatrix} 0 \\ 1 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \]

\[ \Theta \]

When \( \theta \leq \pi/2 - h_1 - h_2 \), \( \Lambda M \) satisfies

\[ \| P_u \|_1 \]

\[ K \]

\[ K \]

\[ \hat{\Delta} = [0,1] \times [0,2] \times [0,2], \quad \hat{K}_1 = [0,1] \times [0,1] \times [0,1], \]

\[ \hat{K}_2 = [0,1] \times [0,1] \times [1,2], \quad \hat{K}_3 = [0,1] \times [2,1] \times [0,1], \quad \hat{K}_4 = [0,1] \times [1,2] \times [1,2]. \]

The reference macro element and reference elements are defined as

\[ \hat{\Delta} = \bigcup_{i=1}^{4} K_i \]

and analyze

\[ \| \cdot \|_{i,r,\Delta} \]

\[ \| \cdot \|_{i,r,\Delta} \]

\[ \| \cdot \|_{0,r,\Delta} \]

\[ \| \cdot \|_{0,r,\Delta} \]

Hence the projection \( \mathcal{P}_\Delta \) is stable on \( \| \cdot \|_{i,r,\Delta} \), \( i = 1, 2 \). By (4.2) and Theorem 3.8, we have

\[ \| u - \mathcal{P}_\Delta u \|_{i,r,\Delta}^2 \leq h_3^2 h_2^2 h_3 \int_{K_i} |\hat{\zeta} - \mathcal{P}_\Delta \hat{\zeta}|^2 \xi^2 \eta^2 \sin(h_3 \zeta) d\xi d\eta d\zeta \]

\[ \leq \max\{2, 1/\sin \zeta\} h_3^2 h_2^2 h_3^2 \|\hat{\zeta} - \mathcal{P}_\Delta \hat{\zeta}\|_{0,r,\hat{K}_i}^2 \]

\[ \leq C h_3^2 |\hat{\zeta}|_{m,r,\Delta}^2, \quad m = 1, 2, \]

where \( \zeta_0 \in (0,1) \) satisfies \( \zeta_0 \leq 2 \sin \zeta_0 \). Similarly, we have

\[ \| u - \mathcal{P}_\Delta u \|_{0,r,\hat{K}_4}^2 \leq h_3^2 h_2^2 (h_2 + h_3^2) \int_{K_4} |\hat{\zeta} - \mathcal{P}_\Delta \hat{\zeta}|^2 d\xi d\eta d\zeta \]

\[ \leq C h_3^2 |\hat{\zeta}|_{m,r,\Delta}^2, \quad m = 1, 2; \]
analysis similar to (4.13), we have defined as
\[ r \]

\[ h \]

Then for \( \text{Set} \) (4.10)

\[ C(4.11) \]

and (4.8), we have

\[ \text{Set} \]

(4.14)

Combining (4.12)–(4.15), we obtain (4.5) by Lemma 4.1.

Similarly, for \( \hat{K} \) we have

\[ \hat{K}_1 = [1, 2] \times [1, 3] \times [1, 3], \quad \hat{K}_2 = [1, 2] \times [2, 3] \times [1, 2], \quad \hat{K}_3 = [1, 2] \times [1, 2] \times [2, 3], \quad \hat{K}_4 = [1, 2] \times [2, 3] \times [2, 3]. \]

Then for \( m = 1, 2 \), by affine transforms, there exists a generic constant \( C \) independent of \( h \), such that

\[ \|u - \mathcal{P}_h u\|_{0,r,K_1}^2 \leq C h \|u\|_{0,r,K_1}^2 \]

\[ \leq C h \|u\|_{0,r,K_1}^2 \]

\[ \leq C h \|u\|_{0,r,K_1}^2 \]

Similarly, for \( i = 2, 3, 4 \) we have

\[ \|u - \mathcal{P}_h u\|_{0,r,K_2}^2 \]

\[ \leq C h \|u\|_{0,r,K_2}^2 \]

\[ \leq C h \|u\|_{0,r,K_2}^2 \]

Set \( h \) small enough such that \( h < \sin(2h) \); by affine transforms and detailed analysis similar to (4.13), we have

\[ \|u - \mathcal{P}_h u\|_{0,r,K_3}^2 \leq C h \|u\|_{0,r,K_3}^2 \]

\[ \leq C h \|u\|_{0,r,K_3}^2 \]

Combining (4.12)–(4.15), we obtain (4.5) by Lemma 4.1. We can prove (4.5) for other macro elements similarly. \( \square \)
5. Finite element approximations. The equivalent weak form of (3.6) is the following: Find \((\lambda, u) \in \mathcal{V} \times \mathcal{H}_0^1(\Omega)\) and \(u \neq 0\) such that

\[
\begin{align*}
\lambda - K + E, K \text{ is the constant in (2.10), and} \quad a_r(u, v) &= \int_{\Omega} \left[ r^2 r_2 \left( \frac{\partial u}{\partial r_1} \frac{\partial v}{\partial r_1} + \frac{\partial u}{\partial r_2} \frac{\partial v}{\partial r_2} \right) + (r_1^2 + r_2^2) \frac{\partial u}{\partial \theta} \frac{\partial v}{\partial \theta} \right. \\
&\quad + \left. \left( \frac{2r_1^2 r_2^2}{\sqrt{r_1^2 + r_2^2} - 2r_1 r_2 \cos \theta} - 4r_1^2 r_2 - 4r_1 r_2^2 \right) uv \right] \sin \theta dr_1 dr_2 d\theta.
\end{align*}
\]

Since \(a(\cdot, \cdot)\) is continuous and coercive on \(\mathcal{V}\), we know that \(a_r(\cdot, \cdot)\) is continuous and coercive on \(\mathcal{V}\) by the proof of Lemma 3.1. We define \(\| \cdot \|_{1,r} = a_r(\cdot, \cdot)\) for the sake of simplicity in notation.

We consider the Lagrangian finite element approximation to (5.1). For any \(K \in \mathcal{T}_h\), denote the set of nodes in \(K\) as

\[\mathcal{V}(K) = \{8 \text{ vertices and } (k + 1)^3 - 8 \text{ k-section points of } K\}.\]

\[\cup_{K \in \mathcal{T}_h} \mathcal{V}(K)\] is the set of nodes of \(\mathcal{T}_h\). Define the finite element space as

\[V_h = \{ v(r_1, r_2, \theta) \in C^0(\Omega) \mid v|_{\partial \Omega} = 0, v|_K \in Q_k(K) \forall K \in \mathcal{T}_h\}.\]

The discrete approximation of (5.1) is the following: Find \((\lambda_h, u_h) \in \mathcal{V} \times V_h\) and \(u_h \neq 0\) such that

\[
\begin{align*}
a_r(u_h, v_h) &= \lambda_h (u_h, v_h) \quad \forall v_h \in V_h.
\end{align*}
\]

Obviously, \(V_h \subset C^0(\Omega) \cap \mathcal{H}_0^1(\Omega)\), and so (5.2) is the Galerkin approximation of (5.1). We drop the subscript “B” in (2.13) (or (5.1)) and suppose that \(0 < \lambda_1 \leq \lambda_2 \leq \cdots\) are the eigenvalues of (5.1), \(0 < \lambda_{h1} \leq \lambda_{h2} \leq \cdots \leq \lambda_{h_N_k}\) are the eigenvalues of (5.2), \(N_k = \text{dim}(V_h)\). Denote the eigenspaces associated with \(\lambda_i\) and \(\lambda_{hj}\) as \(V_i\) and \(V_{hj}\), respectively, \(1 \leq i \leq \cdots, 1 \leq j \leq N_k\). By the minmax theorem [10], \(\lambda_i \leq \lambda_{h_i}, 1 \leq i \leq N_k\).

Let \(\hat{\Delta}\) be a reference macro element and \(\hat{K} \subset \hat{\Delta}\) be a reference element. Define

\[\mathcal{V}(\hat{K}) = \{ \varphi_i^\hat{K} \mid 1 \leq i \leq (k + 1)^3 \}\]

associated with a basis \(\{ \varphi_i^\hat{K} \mid 1 \leq i \leq (k + 1)^3 \}\) of \(Q_k(\hat{K})\). Assume

\[\varphi_i(a_i^\hat{K}) = \delta_{ij}, \quad 1 \leq i, j \leq (k + 1)^3,\]

where \(\delta_{ij} = 1\) if \(i = j\), \(\delta_{ij} = 0\) if \(i \neq j\). For any \(\hat{v} \in H_0^0(\hat{K})\), we define the finite element interpolation operator by means of the local regularization as follows:

\[
\pi_{\hat{K}} \hat{v} = \sum_{i=1}^{(k+1)^3} (P_{\hat{K}} \hat{v}) (a_i^\hat{K}) \varphi_i^\hat{K}.
\]

Suppose \(v \in H_0^0(\Omega)\). For any \(K = F_{\hat{K}}(\hat{K}) \in \mathcal{T}_h\), define the finite element interpolation operator on \(\Delta, K,\) and \(\Omega\) as follows: \(\pi_{\hat{K}} v|_K = \pi_{\hat{K}} v, \pi_{\hat{K}} v = (\pi_{\hat{K}} v) \circ F_{\hat{K}}^{-1}\), \(\pi v|_K = \pi_{\hat{K}} v,\)
where \( \hat{K} \subset \hat{\Delta} \) is some reference element. On any space of finite dimension, all norms are equivalent. There exists a constant \( C \) such that
\[
\| \pi_{\hat{K}} \hat{v} \|_{m,r,\hat{K}} \leq C \| \delta v \|_{0,\infty,\hat{\Delta}} \leq C \| P_{\hat{\Delta}} \hat{v} \|_{0,r,\hat{K}} \leq \| \hat{u} \|_{0,r,\Delta}.
\]
Thus the operator \( \pi_{\hat{K}} : H_0^1(\hat{\Delta}) \to H_0^m(\hat{K}) \) is linear and continuous, \( m = 0, 1 \).

Theorem 5.1. There exists a constant \( C \) independent of \( h \) such that for any \( v \in H_2^r(\Omega) \),
\[
\| v - \pi v \|_{m,r,\Omega} \leq Ch^2 |v|_{2,r,\Omega}, \quad m = 0, 1.
\]

Proof. Suppose that \( \hat{\Delta} \) is a reference macro element and \( \hat{K} \subset \hat{\Delta} \) is a reference element. By the definition of the operators \( \pi_{\hat{K}}, \pi_{\hat{\Delta}}, \) and \( P_{\hat{\Delta}} \), we have
\[
\pi_{\hat{\Delta}} p = p \quad \forall p \in P_k(\hat{\Delta}).
\]
By (5.4), (5.6), and Theorem 3.8, for any \( \hat{v} \in H_2^r(\hat{\Delta}) \) we have
\[
\| \hat{v} - \pi_{\hat{\Delta}} \hat{v} \|_{m,r,\hat{\Delta}} \leq C|\hat{v}|_{2,r,\hat{\Delta}}, \quad m = 0, 1.
\]
For any macro element \( \Delta \), by affine transforms, (5.7), and the argument in the proof of Theorem 4.2, we know that there exists a constant \( C \) independent of \( h \) such that
\[
\| v - \pi v \|_{m,r,\Delta} \leq Ch^2 |v|_{2,r,\Delta}, \quad m = 0, 1.
\]
Summing up each side of (5.8) over all macro elements, we get (5.5).

Theorem 5.2. For any \( 1 \leq i \leq N_h \), suppose \( (\lambda_i, u_i) \) is an eigenpair of (5.1) with \( \| u_i \|_{0,r,\Omega} = 1 \). There exist a constant \( C \) independent of \( h \) and an eigenfunction \( u_{hi} \in V_{hi} \) with \( \| u_{hi} \|_{0,r,\Omega} = 1 \) such that
\[
|\lambda_i - \lambda_{hi}| < Ch^2, \quad m = 0, 1.
\]

Proof. By the theory of abstract spectrum approximation (p. 699 of [10]), we know that, for any \( 1 \leq i \leq N_h \), there exists a constant \( C \) independent of \( h \) such that
\[
|\lambda_i - \lambda_{hi}| < C\varepsilon(\lambda_i)^2,
\]
where
\[
\varepsilon(\lambda_i) = \sup_{v \in V_i, \| v \|_{1,r,\Omega} = 1} \inf_{v_h \in V_h} \| v - v_h \|_{1,r,\Omega}.
\]
Let \( \{ u_{ij}, 1 \leq j \leq N_i \} \) be a basis of \( V_i, \| u_{ij} \|_{1,r,\Omega} = 1, N_i = \dim V_i \). By Theorem 5.1, we have
\[
\varepsilon(\lambda_i) \leq \sum_{j=1}^{N_i} \| u_{ij} - \pi u_{ij} \|_{1,r,\Omega} \leq C h \sum_{j=1}^{N_i} |u_{ij}|_{2,r,\Omega} \leq Ch.
\]
Thus (5.9) is true.

We can prove (5.10) by Theorem 5.2 and the argument of Theorem 6.2 in [32, p. 235], but we do not give the tedious description here. \[\square\]
Remark 5.3. In real computation, we have introduced a variational equation equivalent to (5.1). Define \( \mu = \cos \theta \); then \( \Omega = [0, R] \times [0, R] \times [-1, 1] \), and the corresponding bilinear form, inner products, and norms are

\[
(u, v)_0 = \int_{\Omega} u v r_1^2 r_2^2 dr_1 dr_2 d\mu, \quad \|u\|_{0, r, \Omega}^2 = \int_{\Omega} u^2 r_1^2 r_2^2 dr_1 dr_2 d\mu.
\]

\[
(u, v)_1 = (u, v)_0 + \int_{\Omega} \left[ r_1^2 r_2^2 \left( \frac{\partial u}{\partial r_1} \frac{\partial v}{\partial r_1} + \frac{\partial u}{\partial r_2} \frac{\partial v}{\partial r_2} \right) + (r_1^2 + r_2^2)(1 - \mu^2) \frac{\partial u}{\partial \mu} \frac{\partial v}{\partial \mu} \right] dr_1 dr_2 d\mu,
\]

\[
|u|_{1, r, \Omega}^2 = \int_{\Omega} r_1^2 r_2^2 \left( \frac{\partial u}{\partial r_1} \right)^2 + r_1^2 r_2^2 \left( \frac{\partial u}{\partial r_2} \right)^2 + (r_1^2 + r_2^2)(1 - \mu^2) \left( \frac{\partial u}{\partial \mu} \right)^2 dr_1 dr_2 d\mu,
\]

\[
\|u\|_{1, r, \Omega}^2 = \|u\|_{0, r, \Omega}^2 + |u|_{1, r, \Omega}^2, \quad H_0^1(\Omega) = \{ v | \|v\|_{i, r, \Omega} < +\infty \}, \quad i = 0, 1,
\]

\[
a_r(u, v) = \int_{\Omega} \left[ r_1^2 r_2^2 \left( \frac{\partial u}{\partial r_1} + \frac{\partial u}{\partial r_2} \right) + (r_1^2 + r_2^2)(1 - \mu^2) \frac{\partial u}{\partial \mu} \right] dr_1 dr_2 d\mu + \frac{2r_1^2 r_2^2}{\sqrt{r_1^2 + r_2^2 - 2r_1 r_2 \mu}} - 4r_1^2 r_2 - 4r_1 r_2^2 \right) uv dr_1 dr_2 d\mu.
\]

We define \( H_0^1(\Omega) \) as in Remark 3.7. A variational equation equivalent to (5.1) is the following: Find \( (\lambda, u) \in R^1 \times H_0^1(\Omega) \) and \( u \neq 0 \) such that

\[
(5.14) \quad a_r(u, v) = \lambda \langle u, v \rangle_0 \quad \forall v \in H_0^1(\Omega).
\]

The partitions \( \mathcal{T}_h \) for \( \Omega = [0, R] \times [0, R] \times [-1, 1] \) are similar to those in section 4. \( \forall K \in \mathcal{T}_h \) define

\[
Q_k(K) = \left\{ p | p = \sum_{t,m,n=0}^k \alpha_{t,m,n} r_1^t r_2^m \mu^n, (r_1, r_2, \mu) \in K \right\}.
\]

The finite element approximation to (5.14) is: Find \( (\lambda_h, u_h) \in R^1 \times V_h \) and \( u_h \neq 0 \) such that

\[
(5.15) \quad a_r(u_h, v_h) = \lambda_h \langle u_h, v_h \rangle_0 \quad \forall v \in V_h,
\]

where

\[
V_h = \{ v(r_1, r_2, \mu) \in C(\Omega) | v|_K \in Q_k(K) \ \forall K \in \mathcal{T}_h; \ v|_{\partial\Omega} = 0 \}
\]

is the finite element space.

Comparing (5.15) with (5.2) in real computation, we have found that (5.15) gives more precise results with the same number of unknowns. The analysis for (5.15) will be the subject of our future research.

6. Numerical results. Since \( V_h \) is a finite-dimensional space, define \( N = \dim(V_h) \). We can choose a basis \( \{ \Phi_1, \ldots, \Phi_N \} \) of \( V_h \) such that

\[
\text{supp} \Phi_1 = \bigcup_{K \in \mathcal{T}_h} \mathcal{D}_{a_1} \in \mathcal{S}_h K,
\]
where \( a_i \) is a node of \( T_h \). Let \( u_h = \sum_{i=1}^{N} \alpha_i \Phi_i \) and \( v_h = \Phi_i, 1 \leq i \leq N \), in (5.2) and (5.15). Then we obtain an equivalent generalized eigenvalue problem:

(6.1) \[
A X = \lambda h M X,
\]

where \( X = (\alpha_1, \ldots, \alpha_N)^T \), \( A = (a(\Phi_i, \Phi_j))_{N \times N} \), \( M = ((\Phi_i, \Phi_j))_{N \times N} \).

We use the inverse iteration method [5] to solve the generalized eigenvalue problem (6.1). This method is convenient for computing the smallest (real) eigenvalue of an (unsymmetric) generalized eigenvalue problem with large and sparse matrices. In each step of iteration, the main computational cost is the solution of the following system of equations for \( Y \):

(6.2) \[
AY = F.
\]

However, in fact we need only solve (6.2) in the first step if using \( LU \)-factorization of \( A \), since we can store the inverse matrix of \( A \) for all following steps.

The computational cost of (6.2) is of order \( O(N^3) \) for a dense matrix. Since the finite element matrices are banded, and their band widths are bounded by some positive integer \( M \ll N \), the cost of (6.2) is not more than \( 2MN^2 \). Thus the first iteration of our eigenvalue solver needs \( O(N^2) \) floating point operations, but each of the following iterations needs only \( O(N) \) floating point operations. For the solution of large sparse generalized eigenvalue problems, improvements of this method have been developed rapidly. They devote themselves to reducing the cost of the first iteration; i.e., they solve (6.2) by efficient iterative methods instead of \( LU \)-factorization. Each iterative step of their eigenvalue solvers (such as preconditioned inverse iteration [26]) needs only \( O(N) \) operations. For more detailed analyses, we refer to Neymeyr’s excellent work [26], or to the journal articles [27], [28], [29] and references therein. We consider the improvement of our eigenvalue solver as future work.

We carried out our computation on a personal computer: Intel PIII750 with 1G SDRAM. The experiment shows that 1. the energy errors decrease with \( R \) or the number of nodes increasing; 2. with the considered state becoming more highly exited, \( R \) should be larger, and more nodes far from the nucleus are needed; 3. very large \( R \) makes no remarkable improvement in the precision.

The main error concerns the potential \( V = -\frac{2}{r_1} - \frac{2}{r_2} + \frac{1}{r_{12}} \). For the triplet, the wave function is antisymmetric with respect to the two electrons, so they cannot be very close to each other. That is to say, when \( r_{12} \) is very small, the wave function \( u \) tends to zero. When we calculate \( \int_{\Omega} \frac{u^2}{r_{12}} d\tau_1 d\tau_2 d\mu \) with a Gaussian integration formula [33], the error for the triplet is much smaller than that for the singlet with the same number of Gaussian points. Furthermore, from the figures below, we can see that the wave function \( |u| \) of the ground state is much larger than that of excited states in the domain where \( r_{12} \) is small and in the neighborhood of the nucleus containing the singularities. Thus we have used more and more Gaussian points and grid points along the \( \mu \)-direction, when the state varies from the triplet, the singlet to the ground state.

All matrix elements are computed by the standard Gaussian integration formula. With the number of Gaussian points increasing, the computing time becomes longer. Let \( N_e \) be the number of elements associated with some partition of \( \Omega \), \( N_g \) be the number of Gaussian points along one direction, and \( T_e \) be the CPU time to compute a pair of element matrices by the one-point Gaussian formula. The CPU time to obtain the global stiffness matrix and mass matrix is

(6.3) \[
T \approx N_e \times T_e \times N_g^3.
\]
Table 6.1
Computational efforts for the S-states.

<table>
<thead>
<tr>
<th>State</th>
<th>Number of DOF</th>
<th>Number of GPs</th>
<th>CPU time $T$ (hours)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$1s^1S$</td>
<td>57472</td>
<td>$27 \times 27 \times 27$</td>
<td>44.3</td>
</tr>
<tr>
<td>$1s^2S$</td>
<td>65320</td>
<td>$21 \times 21 \times 21$</td>
<td>20.6</td>
</tr>
<tr>
<td>$1s^2S$</td>
<td>68243</td>
<td>$9 \times 9 \times 9$</td>
<td>1.62</td>
</tr>
</tbody>
</table>

Table 6.2
FEM results for the helium atom (all values in a.u.).

<table>
<thead>
<tr>
<th>State</th>
<th>$1s^1S$</th>
<th>$1s^2S$</th>
<th>$1s^3S$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Highly precise results [12],[23]</td>
<td>$-2.903724377034119 \ldots$</td>
<td>$-2.1459740460544 \ldots$</td>
<td>$-2.1752293782367 \ldots$</td>
</tr>
<tr>
<td>Results given by (5.15)</td>
<td>$-2.903724106$</td>
<td>$-2.145974042$</td>
<td>$-2.1752293277$</td>
</tr>
<tr>
<td>Results given by (5.2)</td>
<td>$-2.903715597$</td>
<td>$-2.1459703835$</td>
<td>$-2.1752288326$</td>
</tr>
<tr>
<td>FEM [31]</td>
<td>$-2.90326$</td>
<td>$-2.145960$</td>
<td>$-2.1752214$</td>
</tr>
</tbody>
</table>

The number of degrees of freedom (DOF), number of Gaussian points (GPs), and the computational time $T$ are listed in Table 6.1.

We place grid points symmetrically along $r_1$ and $r_2$ for all states. The grid points are (for $r_1, r_2, \mu$)

1. $1s^1S$:
   - $0.0, 0.05, 0.1, 0.15, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 1.0, 1.2, 1.6, 2.0,
     2.6, 3.2, 4.2, 6.0, 9.0, 15.0;
   - $-1.0, -0.6, -0.2, 0.2, 0.6, 1.0$;

2. $1s^2S$:
   - $0.0, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 1.0, 1.2, 1.4, 1.6, 1.8, 2.0,
     2.2, 2.4, 2.6, 3.0, 3.4, 3.8, 4.2, 4.8, 5.6, 8.0, 11.5, 15.0, 20.0;
   - $-1.0, -0.5, 0.5, 1.0$;

3. $1s^3S$:
   - $0.0, 0.05, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1.0, 1.2, 1.4, 1.6,
     1.8, 2.0, 2.2, 2.4, 2.6, 2.8, 3.0, 3.2, 3.4, 3.6, 4.0, 4.5, 5.5, 7.0, 10.0,
     13.0, 16.0, 20.0, 25.0;
   - $-1.0, 0.0, 1.0$.

The relative error of our approximate eigenvalue for the ground (1s1s-) state is $10^{-7}$a.u., and those for the 1s2s-states are $10^{-8}$a.u. by (5.15). The precisions of existing finite element eigenvalues are generally $10^{-4} - 10^{-6}$a.u. (see Table 6.2).

From the graphs of approximate wave functions (see Figures 6.1–6.2), we can get the following properties. 1. Although we add no physical assumptions to our computations a priori, such as the symmetry (for the singlets) and the antisymmetry (for the triplet), our approximate wave functions coincide with these properties very well. 2. Wave functions oscillate heavily in the neighborhood of the nucleus where the singularity of the Coulomb potential is very strange. This is well known by physicists and chemists. 3. In a sufficiently small neighborhood of the nucleus, absolute values $|u_k|$ of wave functions are very small. This implies that electrons seldom visit there. 4. With the distance between each electron and the nucleus increasing, wave functions decrease quickly. Thus it is reasonable to solve the Schrödinger equation in bounded
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Fig. 6.1. Wave function of the 1s1s $^1S$-state.

Fig. 6.2. Wave functions of the 1s2s $^1S$-state (left) and the 1s2s $^3S$-state (right).

domains.

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