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An efficient finite element method and error analysis for eigenvalue problem of Schrödinger equation with an inverse square potential on spherical domain

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Abstract

We provide an effective finite element method to solve the Schrödinger eigenvalue problem with an inverse potential on a spherical domain. To overcome the difficulties caused by the singularities of coefficients, we introduce spherical coordinate transformation and transfer the singularities from the interior of the domain to its boundary. Then by using orthogonal properties of spherical harmonic functions and variable separation technique we transform the original problem into a series of one-dimensional eigenvalue problems. We further introduce some suitable Sobolev spaces and derive the weak form and an efficient discrete scheme. Combining with the spectral theory of Babuška and Osborn for self-adjoint positive definite eigenvalue problems, we obtain error estimates of approximation eigenvalues and eigenvectors. Finally, we provide some numerical examples to show the efficiency and accuracy of the algorithm.

MSC: 65N15; 65N30

Keywords: Eigenvalue problem; Singularity; Dimension reduction scheme; Finite element method; Error estimation

1 Introduction

The Schrödinger eigenvalue problem with the inverse-square (IS) or centrifugal potential is widely used in nuclear physics, quantum physics, nonlinear optics, and so on [1–6]. The potential in many electronic equations produces singularity and can describe the attraction or repulsion between objects, which usually leads to strong singularities of the eigenfunctions, and this cannot be simply regarded as a perturbation term [7–11]. Therefore new tools and techniques, different from linear elliptic operators with bounded coefficients, are urgently needed for such an eigenvalue problem with the IS potential, both in analysis and in numerics. Ghanbari et al. [12–15] and Khater et al. [16–20] discussed some effective numerical methods to remove the singularity of nonlocal operators. In addition, some other works [21–26] mainly focus on studying exact solitary wave solutions.

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In the last decade, increasing attention is paid to the numerical approximation of Schrödinger operators with similar singular potentials [1, 27–30]. If we solve the Schrödinger eigenvalue problem directly in a three-dimensional domain, it will take a lot of computing time and memory capacity to obtain high-precision numerical solutions [11, 31, 32]. In practice, we usually need to solve the Schrödinger eigenvalue problem on a three-dimensional spherical domain. As far as we know, there is little work discussing the eigenvalue problem with IS potential on a spherical domain.

The purpose of this work is developing an effective finite element method for the eigenvalue problem of the Schrödinger equation with an IS potential on spherical domain. To overcome the difficulties caused by the singularities of coefficients, we introduce spherical coordinate transformation and transfer the singularities from the interior of the domain to the boundary of the domain. Then by using orthogonal properties of spherical harmonic functions and variable separation technique we reduce the original problem to a series of one-dimensional eigenvalue problems. We further introduce some suitable Sobolev spaces and derive an effective discrete scheme. Combined with the theory of self-adjoint eigenvalues, we obtain error estimates of approximation eigenvalues and eigenvectors. Finally, we give several numerical examples to verify the convergence and accuracy of the algorithm.

The rest of the paper is organized as follows. In Sect. 2, we obtain a dimensional reduction scheme for the Schrödinger eigenvalue problem with IS potential. In Sect. 3, we construct a weak form and numerical discretization scheme. In Sect. 4, we obtain error estimates of approximation eigenvalues and eigenfunctions. In Sect. 5, we study the implementation details of the algorithm. In Sect. 6, we test the accuracy and convergence of the numerical algorithm. Finally, in Sect. 7, we provide some concluding remarks.

2 Dimension reduction scheme

In this paper, we consider the following eigenvalue problem with Dirichlet boundary conditions:

$$-\Delta u + \frac{c^2}{x^2 + y^2 + z^2} u = \lambda u \quad \text{in } \Omega, \tag{1}$$

$$u = 0 \quad \text{on } \partial\Omega, \tag{2}$$

where c is a bounded constant, and $\Omega = \{(x, y, z) \in \mathbb{R}^3 : 0 \leq a < r < b\}$ with $r = \sqrt{x^2 + y^2 + z^2}$. Let $x = r \sin \theta \cos \phi$, $y = r \sin \theta \sin \phi$, $z = r \cos \theta$, $\psi(r, \theta, \phi) = u(x, y, z)$. We take the Laplacian in spherical coordinates

$$\mathcal{L}\psi = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial \psi}{\partial r} \right) + \frac{1}{r^2} \Delta_S \psi, \tag{3}$$

where

$$\Delta_S = \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2}. \tag{4}$$

Then (1)–(2) can be rewritten as the eigenvalue problem of the Schrödinger equation in spherical coordinates:

$$-\mathcal{L}\psi + \frac{c^2}{r^2}\psi = \lambda\psi, \quad (r, \theta, \phi) \in (a, b) \times [0, \pi] \times [0, 2\pi], \tag{5}$$

$$(1) \quad \psi(b, \theta, \phi) = 0, \quad (\theta, \phi) \in [0, \pi] \times [0, 2\pi] \text{ for } a = 0, \tag{6}$$

$$(2) \quad \psi(a, \theta, \phi) = \psi(b, \theta, \phi) = 0, \quad (\theta, \phi) \in [0, \pi] \times [0, 2\pi] \text{ for } a > 0. \tag{7}$$

We recall that an important property of the spherical harmonics $\{Y_m^l\}$ (as normalized in [33]) is that they are eigenfunctions of the Laplace–Beltrami operator Δ_S . More precisely,

$$\Delta_S Y_l^m = -l(l+1)Y_l^m, \quad l \geq 0, |m| \leq l, \tag{8}$$

and from the definition of $L^2(S)$ we find

$$\int_S Y_l^m Y_{l'}^{m'} dS = \delta_{ll'} \delta_{mm'}. \tag{9}$$

Using spherical harmonic expansion, we obtain that

$$\psi(r, \theta, \phi) = \sum_{l=0}^{\infty} \sum_{|m|=0}^l \psi_l^m Y_l^m. \tag{10}$$

First of all, we take into account the case $a = 0$. Define the differential operator $\tilde{L}_l \psi_l^m = \frac{1}{r^2}(\partial_r(r^2 \partial_r \psi_l^m) - l(l+1)\psi_l^m)$. By substituting expression (10) into (5) and (6) we can obtain a series of equivalent one-dimensional eigenvalue problems:

$$-\tilde{L}_l \psi_l^m + \frac{c^2}{r^2} \psi_l^m = \lambda_l \psi_l^m, \quad r \in (0, b), \tag{11}$$

$$\psi_l^m(b) = 0. \tag{12}$$

Let $r = \frac{t+1}{2}b$, $u_l^m(t) = \psi_l^m(\frac{t+1}{2}b)$, and $\mathcal{L}_l u_l^m = \frac{1}{(t+1)^2} \partial_t((t+1)^2 \partial_t u_l^m) - \frac{l(l+1)}{(t+1)^2} u_l^m$. Then (11)–(12) can be rewritten as

$$-\mathcal{L}_l u_l^m + \frac{c^2}{(t+1)^2} u_l^m = \frac{b^2}{4} \lambda_l u_l^m, \quad t \in (-1, 1), \tag{13}$$

$$u_l^m(1) = 0. \tag{14}$$

Analogously, for the case $a > 0$, inserting expression (10) into (5) and (7), we can derive the following one-dimensional eigenvalue problem:

$$-\tilde{L}_l \psi_l^m + \frac{c^2}{r^2} \psi_l^m = \lambda_l \psi_l^m, \quad r \in (0, b), \tag{15}$$

$$\psi_l^m(a) = \psi_l^m(b) = 0. \tag{16}$$

Let $r = \frac{b-a}{2}t + \frac{b+a}{2}$, $u_l^m(t) = \psi_l^m(r)$, and $L_l u_l^m = \frac{4}{(b-a)^2 r^2} \partial_t(r^2 \partial_t u_l^m) - \frac{l(l+1)}{r^2} u_l^m$. From (15)–(16) we derive that

$$-\mathcal{L}_l u_l^m + \frac{c^2}{r^2} u_l^m = \lambda_l u_l^m, \quad t \in (-1, 1), \tag{17}$$

$$u_l^m(-1) = u_l^m(1) = 0. \tag{18}$$

3 Weak form and discrete scheme

When $a = 0$, we can define the space

$$H_{0,l}^1(I) := \left\{ u_l^m : \int_I (t+1)^2 |\partial_t u_l^m|^2 + [l(l+1) + c^2] u_l^m{}^2 dt < \infty, u_l^m(1) = 0 \right\}.$$

The inner product and norm can be defined as follows:

$$(u_l^m, v_l^m)_{1,l} = \int_I (t+1)^2 \partial_t u_l^m \partial_t v_l^m + [l(l+1) + c^2] u_l^m v_l^m dt,$$

$$\|u_l^m\|_{1,l} = (u_l^m, u_l^m)_{1,l}^{\frac{1}{2}}.$$

Thus the weak form of (13)–(14) is: Find $(\lambda_l, u_l^m) \in \mathbb{R} \times H_{0,l}^1(I)$ such that

$$a_l(u_l^m, v_l^m) = \lambda_l b_l(u_l^m, v_l^m), \quad \forall v_l^m \in H_{0,l}^1(I), \tag{19}$$

where

$$a_l(u_l^m, v_l^m) = \int_I (t+1)^2 \partial_t u_l^m \partial_t v_l^m + [l(l+1) + c^2] u_l^m v_l^m dt,$$

$$b_l(u_l^m, v_l^m) = \frac{b^2}{4} \int_I (t+1)^2 u_l^m v_l^m dt.$$

We denote by $\tilde{V}_h(I) = \tilde{P}_{1h} \cap H_{0,l}^1(I)$ the approximation space, where \tilde{P}_{1h} is a piecewise linear interpolation polynomial space. Thus the corresponding numerical scheme of (19) is: Find $(\lambda_{lh}, u_{lh}^m) \in \mathbb{R} \times \tilde{V}_h(I)$ such that

$$a_l(u_{lh}^m, v_{lh}^m) = \lambda_{lh} b_l(u_{lh}^m, v_{lh}^m), \quad \forall v_{lh}^m \in \tilde{V}_h(I). \tag{20}$$

When $a > 0$, the usual space can be denoted as

$$H_0^1(I) := \{u_l^m : u_l^m, \partial_t u_l^m \in L^2(I), u_l^m(-1) = u_l^m(1) = 0\}.$$

We define the inner product and norm as

$$(u_l^m, v_l^m)_{1,l} = \int_I (\partial_t u_l^m \partial_t v_l^m + u_l^m v_l^m) dt, \quad \|u_l^m\|_{1,l} = (u_l^m, u_l^m)_{1,l}^{\frac{1}{2}}.$$

Thus the weak form of (17)–(18) is: Find $(\lambda_l, u_l^m) \in \mathbb{R} \times H_0^1(I)$ such that

$$a_l(u_l^m, v_l^m) = \lambda_l b_l(u_l^m, v_l^m), \quad \forall v_l^m \in H_0^1(I), \tag{21}$$

where

$$a_l(u_l^m, v_l^m) = \int_I \frac{4}{(b-a)^2} r^2 \partial_t u_l^m \partial_t v_l^m + [l(l+1) + c^2] u_l^m v_l^m dt,$$

$$b_l(u_l^m, v_l^m) = \int_I r^2 u_l^m v_l^m dt.$$

We denote by $V_h = P_{1h} \cap H_0^1(I)$ the approximation space, where P_{1h} is a piecewise linear interpolation polynomial space. Then the corresponding numerical scheme of (21) is: Find $(\lambda_{lh}, u_{lh}^m) \in \mathbb{R} \times S_h(I)$ such that

$$a_l(u_{lh}^m, v_{lh}^m) = \lambda_{lh} b_l(u_{lh}^m, v_{lh}^m), \quad \forall v_{lh}^m \in V_h. \tag{22}$$

4 Error estimation of approximation solutions

In this section, we prove error estimates of approximate eigenvalues and eigenfunctions. Without loss of generality, we only consider the case $a > 0$.

Use the technique of [34], we deduce the following results.

Theorem 1 $a_l(u_l^m, v_l^m)$ is positive definite and continuous on $H_0^1(I) \times H_0^1(I)$, that is,

$$|a_l(u_l^m, v_l^m)| \lesssim \|u_l^m\|_{1,I} \|v_l^m\|_{1,I},$$

$$a_l(u_l^m, u_l^m) \gtrsim \|u_l^m\|_{1,I}^2.$$

Proof Using the Cauchy–Schwarz inequality, we find

$$\begin{aligned} |a_l(u_l^m, v_l^m)| &= \left| \int_I \frac{4}{(b-a)^2} r^2 \partial_t u_l^m \partial_t v_l^m + [l(l+1) + c^2] u_l^m v_l^m dt \right| \\ &\leq \int_I \frac{4}{(b-a)^2} b^2 |\partial_t u_l^m \partial_t v_l^m| + [l(l+1) + c^2] |u_l^m v_l^m| dt \\ &\lesssim \int_I |\partial_t u_l^m \partial_t v_l^m| + |u_l^m v_l^m| dt \\ &\leq \left(\int_I |\partial_t u_l^m|^2 dt \right)^{\frac{1}{2}} \left(\int_I |\partial_t v_l^m|^2 dt \right)^{\frac{1}{2}} + \left(\int_I |u_l^m|^2 dt \right)^{\frac{1}{2}} \left(\int_I |v_l^m|^2 dt \right)^{\frac{1}{2}} \\ &\leq \left[\int_I |\partial_t u_l^m|^2 + |u_l^m|^2 dt \right]^{\frac{1}{2}} \left[\int_I |\partial_t v_l^m|^2 + |v_l^m|^2 dt \right]^{\frac{1}{2}} \\ &= \|u_l^m\|_{1,I} \|v_l^m\|_{1,I}. \end{aligned}$$

From the Poincaré inequality we derive that

$$a_l(u_l^m, u_l^m) = \int_I \frac{4}{(b-a)^2} r^2 (\partial_t u_l^m)^2 + [l(l+1) + c^2] (u_l^m)^2 dt$$

$$\geq \int_I \frac{4}{(b-a)^2} a^2 (\partial_t u_l^m)^2 dt \gtrsim |u_l^m|_{1,I}^2 \gtrsim \|u_l^m\|_{1,I}^2. \quad \square$$

Similarly, we have the following conclusions.

Theorem 2 $b_l(u_l^m, v_l^m)$ is also positive definite and continuous on $L^2(I) \times L^2(I)$, that is,

$$|b_l(u_l^m, v_l^m)| \lesssim \|u_l^m\|_{0,I} \|v_l^m\|_{0,I}, \tag{23}$$

$$b_l(u_l^m, u_l^m) \gtrsim \|u_l^m\|_{0,I}^2. \tag{24}$$

Let $V(\lambda_l)$ and $V(\lambda_{lh})$ be the eigenfunction spaces corresponding to the eigenvalues λ_l and λ_{lh} , respectively. Let

$$\varepsilon_h = \sup_{u_l^m \in V(\lambda_l), \|u_l^m\|_{a_l}=1} \inf_{v_{lh}^m \in V_h} \|u_l^m - v_{lh}^m\|_{a_l},$$

where $\|u_l^m\|_{a_l} = \sqrt{a_l(u_l^m, u_l^m)}$. From Theorems 1 and 2 we know that $a_l(u_l^m, v_l^m)$ (resp., $b_l(u_l^m, v_l^m)$) is a symmetric, continuous, and coercive bilinear form on $H_0^1(I) \times H_0^1(I)$ (resp., $L^2(I) \times L^2(I)$).

By the spectral theory of eigenvalue problems [34] we have the following theorem.

Theorem 3 Let (λ_l, u_l^m) and (λ_{lh}, u_{lh}^m) be respectively the eigenpairs of (21) and (22). Then the following inequalities hold:

$$\|u_l^m - u_{lh}^m\|_{a_l} \lesssim \varepsilon_h, \tag{25}$$

$$\lambda_{lh} - \lambda_l \lesssim \varepsilon_h^2. \tag{26}$$

Define the piecewise linear interpolation operator $I_h : H_0^1(I) \rightarrow V_h$ by

$$I_h u_l^m(t) = p_{li}(t), \quad t \in I_i,$$

where $p_{li}(t)$ denotes the linear interpolation polynomial of u_l^m on the interval $I_i = [t_{i-1}, t_i]$. Let

$$u_{li}^m(t) = u_l^m(t), \quad t \in I_i.$$

Then from an error formula of linear interpolating remainder term we derive that

$$u_{li}^m(t) - p_{li}(t) = \frac{(u_{li}^m)^{(2)}(\xi_i(t))}{2!} (t - t_{i-1})(t - t_i),$$

where $\xi_i(t) \in I_i$ is a function depending on t .

For u_l^m , we have the following error results.

Theorem 4 Let $K_{li}(t) = \frac{(u_{li}^m)^{(2)}(\xi_i(t))}{2!}$, $u_l^m \in H_0^1(I)$. Suppose that u_l^m is smooth enough such that $|\partial_t^k K_{li}(t)| \leq M$ ($k = 0, 1$), where M is a positive constant. Then

$$|I_h u_l^m - u_l^m|_{1,I} \lesssim h, \tag{27}$$

where $h = \max_{1 \leq i \leq n} \{h_i\}$, $h_i = t_i - t_{i-1}$.

Proof Since

$$u_{li}^m(t) - p_{li}(t) = K_{li}(t)(t - t_{i-1})(t - t_i),$$

we have

$$\partial_t(u_{li}^m(t) - p_{li}(t)) = \partial_t K_{li}(t)(t - t_{i-1})(t - t_i) + K_{li}(t)\partial_t((t - t_{i-1})(t - t_i)).$$

Thus we obtain

$$\begin{aligned} |\partial_t(u_{li}^m(t) - p_{li}(t))|^2 &\lesssim |(t - t_{i-1})(t - t_i)|^2 + |\partial_t((t - t_{i-1})(t - t_i))|^2 \\ &= |(t - t_{i-1})(t - t_i)|^2 + |(t - t_i) + (t - t_{i-1})|^2 \\ &\leq \left(\frac{h_i}{2}\right)^4 + (2h_i)^2 \lesssim h_i^2. \end{aligned}$$

From the Poincaré inequality we derive that

$$\begin{aligned} \|I_h u_l^m - u_l^m\|_{1,I}^2 &\lesssim |I_h u_l^m - u_l^m|_{1,I}^2 \\ &= \sum_{i=1}^n |I_h u_l^m - u_l^m|_{1,I_i}^2 = \sum_{i=1}^n |p_{li} - u_{li}^m|_{1,I_i}^2 \\ &= \sum_{i=1}^n \int_{I_i} |\partial_t(u_{li}^m(t) - p_{li}(t))|^2 dt \\ &\lesssim \sum_{i=1}^n h_i^3 \lesssim h^2. \end{aligned}$$

This ends the proof. □

We can get the following standard error estimation results.

Theorem 5 *Let (λ_l, u_l^m) and (λ_{lh}, u_{lh}^m) be the eigenpairs of (21) and (22), respectively. If $u_l^m \in H_0^1(I)$ satisfy the condition of Theorem 4, then the following inequalities hold:*

$$\|u_l^m - u_{lh}^m\|_{a_l} \lesssim h, \quad \lambda_{lh} - \lambda_l \lesssim h^2. \tag{28}$$

Proof Since

$$\begin{aligned} \varepsilon_h &= \sup_{u_l^m \in V(\lambda_l), \|u_l^m\|_{a_l}=1} \inf_{v_{lh}^m \in V_h} \|u_l^m - v_{lh}^m\|_{a_l} \\ &\leq \sup_{u_l^m \in V(\lambda_l), \|u_l^m\|_{a_l}=1} \|u_l^m - I_h u_{lh}^m\|_{a_l} \\ &\lesssim \sup_{u_l^m \in V(\lambda_l), \|u_l^m\|_{a_l}=1} \|u_l^m - I_h u_{lh}^m\|_{1,I}, \end{aligned}$$

from the Poincaré inequality and Theorem 4 we derive that

$$\begin{aligned} \varepsilon_h &\lesssim \sup_{u_l^m \in V(\lambda), \|u_l^m\|_{a_l} = 1} \|u_l^m - I_h u_{lh}^m\|_{1,I} \\ &\lesssim \sup_{u_l^m \in V(\lambda), \|u_l^m\|_{a_l} = 1} |u_l^m - I_h u_{lh}^m|_{1,I} \\ &\lesssim h. \end{aligned}$$

Combining this with Theorem 3, we obtain (28). □

5 Implementation of the numerical scheme

In this section, we present the algorithm to solve problems (20) and (22). First, we define some basis functions. Let

$$\begin{aligned} \psi_0(t) &= \begin{cases} -\frac{t-t_1}{h_1}, & t_0 \leq t \leq t_1, \\ 0, & \text{otherwise,} \end{cases} \\ \psi_i(t) &= \begin{cases} \frac{t-t_{i-1}}{h_i}, & t_{i-1} \leq t \leq t_i, \\ -\frac{t-t_{i+1}}{h_{i+1}}, & t_i \leq t \leq t_{i+1}, \\ 0, & \text{otherwise,} \end{cases} \end{aligned}$$

where $i = 1, \dots, N - 1$. We find that

$$\begin{aligned} \tilde{V}_h &= \text{span}\{\psi_0(t), \dots, \psi_{N-1}(t)\}, \\ V_h &= \text{span}\{\psi_1(t), \dots, \psi_{N-1}(t)\}. \end{aligned}$$

Case 1. $a = 0$. Set

$$\begin{aligned} a_{ij} &= \int_I (t + 1)^2 (\psi_j)' (\psi_i)' dt, & b_{ij} &= \int_I \psi_j \psi_i dt, \\ c_{ij} &= \int_I (t + 1)^2 \psi_j \psi_i dt. \end{aligned}$$

Let

$$u_{lh}^m = \sum_{i=0}^{N-1} u_i \psi_i. \tag{29}$$

Substituting expression (29) into (20) and noticing the v_{lh}^m , we can observe the linear system

$$[\mathbb{A} + (l^2 + l + c^2)\mathbb{B}]\mathbb{U} = \frac{b^2}{4} \lambda_{lh} \mathbb{C}\mathbb{U}, \tag{30}$$

where

$$\mathbb{A} = (a_{ij}), \quad \mathbb{B} = (b_{ij}), \quad \mathbb{C} = (c_{ij}), \quad \mathbb{U} = (u_0, \dots, u_{N-1})^T.$$

From the properties of the basis functions we know that the stiff matrices and mass matrix in (30) are all tridiagonal sparse matrices.

Case 2. $a > 0$. Let

$$u_{lh}^m = \sum_{i=1}^{N-1} u_i \psi_i. \tag{31}$$

Substituting expression (31) into (22) and taking v_{lh}^m in V_h , we obtain the linear system

$$\mathcal{A}\mathcal{U} = \lambda_{lh}\mathcal{B}\mathcal{U}, \tag{32}$$

where

$$\begin{aligned} \mathcal{A} &= (a_{ij,l}), & \mathcal{B} &= (b_{ij,l}), & a_{ij,l} &= a_l(\psi_j, \psi_i), & b_{ij,l} &= b_l(\psi_j, \psi_i), \\ \mathcal{U} &= (u_1, \dots, u_{N-1})^T. \end{aligned}$$

Similarly, from the properties of the basis functions we know that the stiff matrices and mass matrix in (32) are all tridiagonal sparse matrices.

Remark 1 Our numerical method can transform three-dimensional problems into a series of eigenvalue problems. By constructing appropriate basis functions these one-dimensional value problems will be discretized into a sparse stiffness matrix and mass matrix, which can be efficiently solved.

6 Numerical experiments

In this section, we present several numerical examples to check the convergence and accuracy of the numerical algorithm.

Example 1 We take $c = 0, a = 0, b = 1$, and $l = 0, 1, 2$ as our example. In Tables 1–3, we provide the first four eigenvalues with different l and h of Example 1.

Example 2 We take $c = \frac{1}{3}, a = 0, b = 1$, and $l = 0, 1, 2$ as our example. In Tables 1–3, we give the first four eigenvalues with different l and h of Example 2.

We know from Tables 1–6 that the approximation eigenvalues achieve at least three-digit accuracy with $h \leq \frac{1}{512}$ for $l = 0, 1, 2$. To further show the convergence of approximation eigenvalues, we let the numerical solution of $h = \frac{1}{1024}$ be the reference solution. The error of the approximate eigenvalues with different h are provided in Figs. 1–6.

We observe from Figs. 1–6 that the numerical eigenvalues are convergent.

Table 1 $a = 0$, the four eigenvalues with $l = 0$ and h

h	λ_{0h}^1	λ_{0h}^2	λ_{0h}^3	λ_{0h}^4
1/64	9.869857717467	39.497938355087	88.947662545164	158.330138143300
1/128	9.869667769569	39.483298848912	88.856747023505	158.017765253015
1/256	9.869620245684	39.479637982214	88.834016573723	157.939692761527
1/512	9.869608362394	39.478722703012	88.828333857921	157.920175919198
1/1024	9.869605391441	39.478493879297	88.826913172297	157.915296787651

Table 2 $a = 0$, the four eigenvalues with $l = 1$ and h

h	λ_{1h}^1	λ_{1h}^2	λ_{1h}^3	λ_{1h}^4
1/64	20.192597755854	59.718503283484	119.092115617980	198.448082264746
1/128	20.191196002143	59.689264430485	118.947930249028	198.005334602179
1/256	20.190845426967	59.681953168655	118.911884395986	197.894689220523
1/512	20.190757774611	59.680125256653	118.902872969163	197.867030522764
1/1024	20.190735860985	59.679668272588	118.900620114823	197.860116014585

Table 3 $a = 0$, the four eigenvalues with $l = 2$ and h

h	λ_{2h}^1	λ_{2h}^2	λ_{2h}^3	λ_{2h}^4
1/64	33.221527912004	82.779965293070	152.120849702143	241.466504738343
1/128	33.218478774072	82.734418406613	151.921374315241	240.893774149263
1/256	33.217716151749	82.723028162111	151.871499583334	240.750621394948
1/512	33.217525475045	82.720180381294	151.859030542575	240.714835156415
1/1024	33.217477804567	82.719468422366	151.855913260174	240.705888719943

Table 4 $a = 0$, the four eigenvalues with $l = 0$ and h

h	λ_{0h}^1	λ_{0h}^2	λ_{0h}^3	λ_{0h}^4
1/64	10.784422087149	41.409061237094	91.862254368608	162.255452978584
1/128	10.783897714384	41.391953774531	91.763361765200	161.924692186926
1/256	10.783722018000	41.387479496580	91.738161486718	161.841125052992
1/512	10.783658754253	41.386276025201	91.731657235236	161.819852309708
1/1024	10.783634535429	41.385938328125	91.729942732668	161.814368929169

Table 5 $a = 0$, the four eigenvalues with $l = 1$ and h

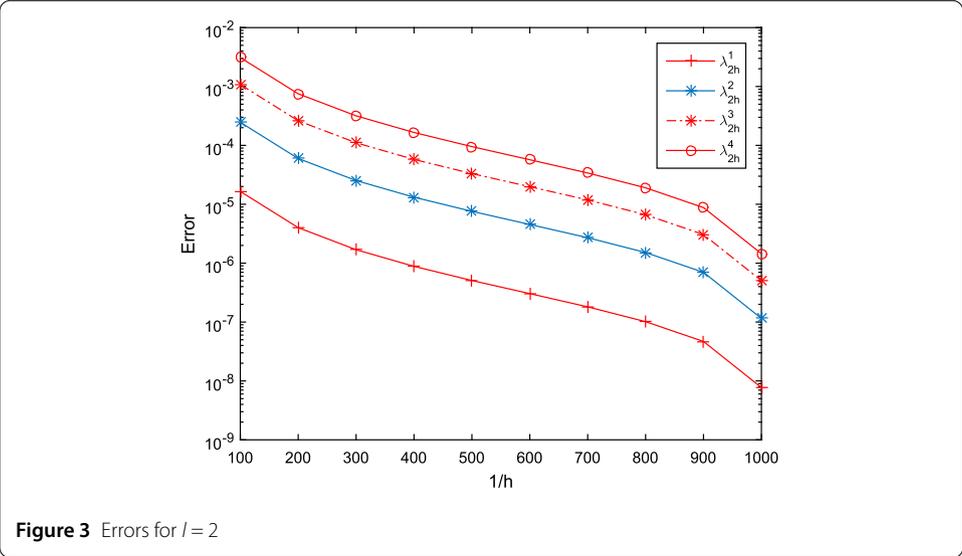
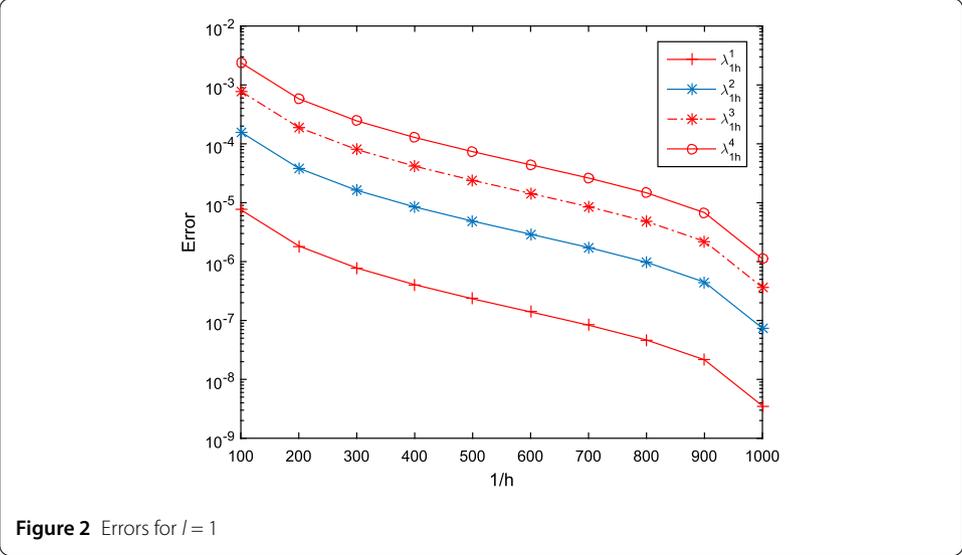
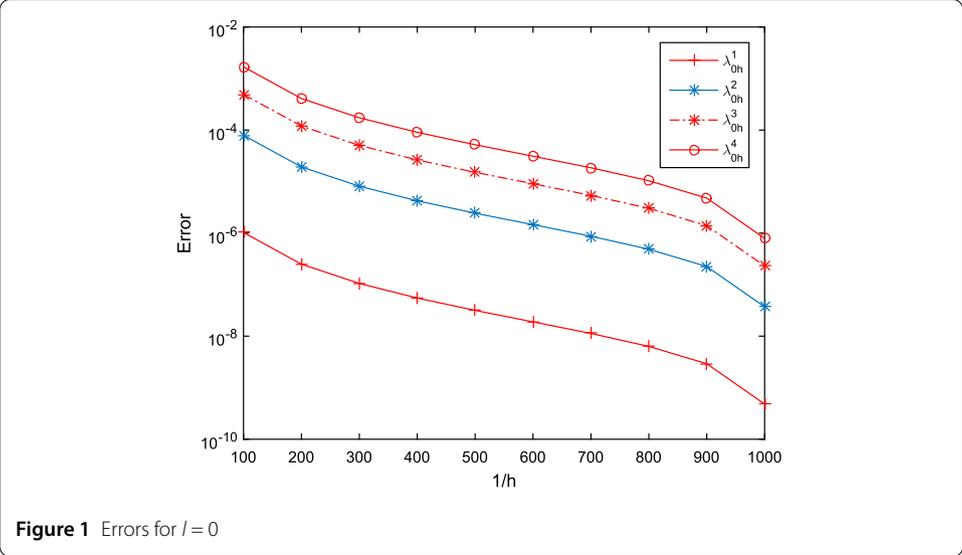
h	λ_{1h}^1	λ_{1h}^2	λ_{1h}^3	λ_{1h}^4
1/64	20.622531429872	60.512755868097	120.249994940413	199.970863052496
1/128	20.621082705047	60.482989673348	120.103951531653	199.523657856357
1/256	20.620720381598	60.475546521030	120.067441003649	199.411897858243
1/512	20.620629791855	60.473685633053	120.058313398197	199.383960493605
1/1024	20.620607143877	60.473220404839	120.056031498617	199.376976318024

Table 6 The first four eigenvalues for $l = 2$ and different h with $a = 0$

h	λ_{2h}^1	λ_{2h}^2	λ_{2h}^3	λ_{2h}^4
1/64	33.539386696208	83.321688069218	152.883872499399	242.450993494860
1/128	33.536292906786	83.275738174388	152.683074749736	241.875210146000
1/256	33.535519115145	83.264247113685	152.632869196580	241.731293670130
1/512	33.535325645709	83.261374124815	152.620317436233	241.695316468978
1/1024	33.535277277012	83.260655863631	152.617179473073	241.686322289850

Example 3 We take $c = \frac{1}{2}$, $a = 1$, $b = 2$, and $l = 0, 1, 2$ as our example. The first four eigenvalues for different l and h are listed in Tables 7–9.

We know from Tables 7–9 that the numerical eigenvalues can achieve six-digit accuracy at least for $h \leq \frac{1}{512}$ for $l = 0, 1, 2$. Similarly, we select the solutions with $h = \frac{1}{1024}$ as the reference solutions. In Figs. 7–8, we plot the error of the approximate eigenvalues. We observe from Figs. 7–8 that the numerical eigenvalues are also convergent.



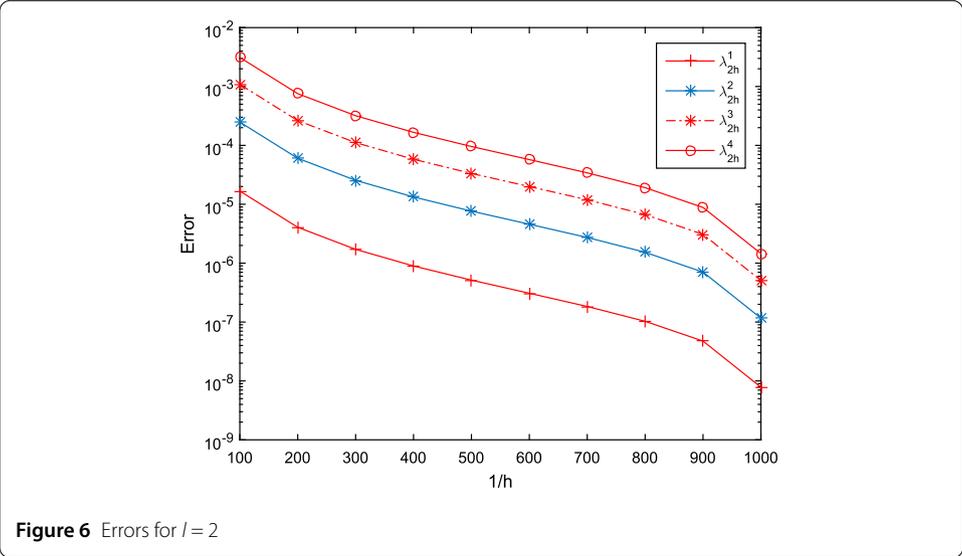
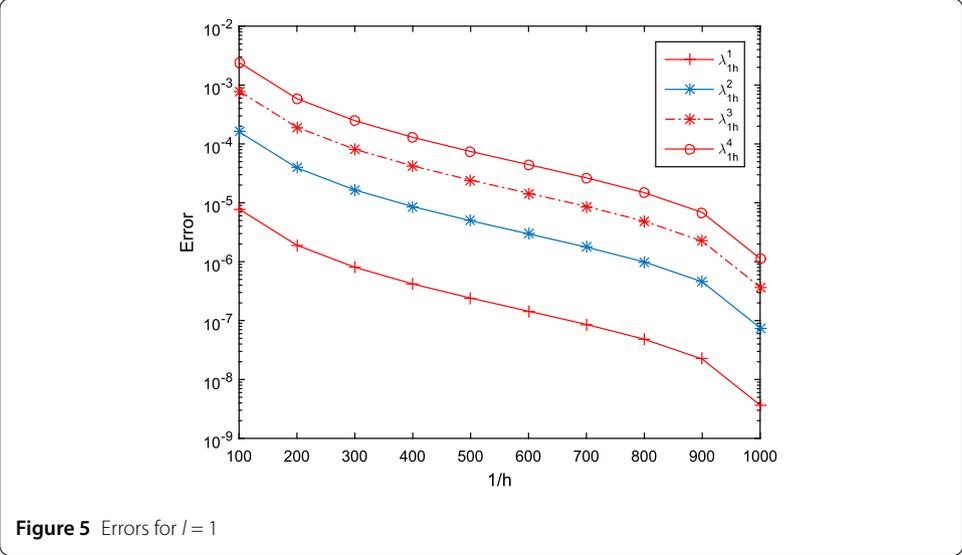
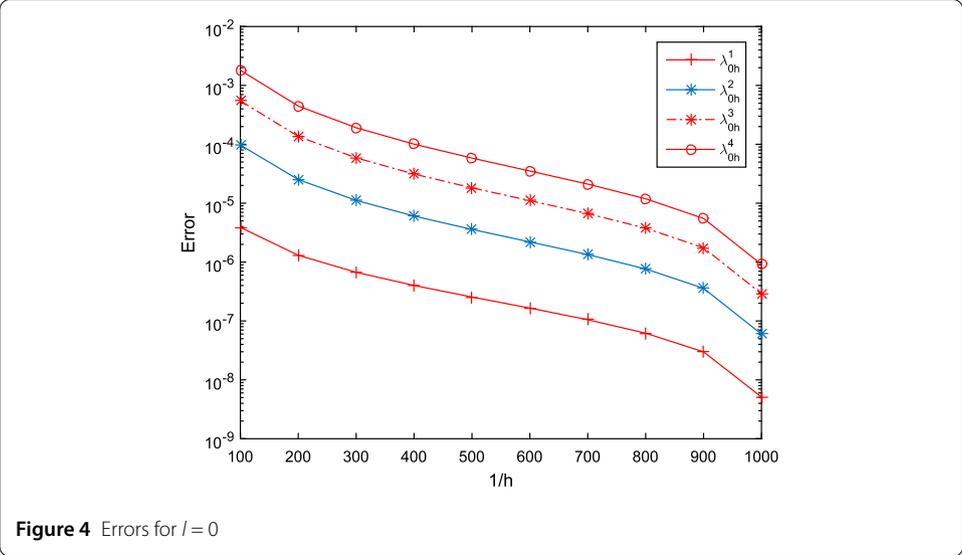


Table 7 $a > 0$, the four eigenvalues with $l = 0$ and h

h	λ_{0h}^1	λ_{0h}^2	λ_{0h}^3	λ_{0h}^4
1/64	9.988012930043	39.633375167001	89.112712061030	158.549222565147
1/128	9.986375926619	39.608980395076	88.990846603507	158.165675283969
1/256	9.985966717519	39.602883767284	88.960402033368	158.069907148956
1/512	9.985864417864	39.601359739506	88.952792255536	158.045972559582
1/1024	9.985838843186	39.600978740678	88.950889896467	158.039989377952

Table 8 $a > 0$, the four eigenvalues with $l = 1$ and h

h	λ_{1h}^1	λ_{1h}^2	λ_{1h}^3	λ_{1h}^4
1/64	10.915762724023	40.613236009777	90.103550633775	159.544012021946
1/128	10.914153283961	40.588873995812	89.981719322438	159.160499469372
1/256	10.913750964537	40.582785551208	89.951283273667	159.064739988704
1/512	10.913650387204	40.581263568823	89.943675625219	159.040807561191
1/1024	10.913625243058	40.580883081317	89.941773798436	159.034824919945

Table 9 $a > 0$, the four eigenvalues with $l = 2$ and h

h	λ_{2h}^1	λ_{2h}^2	λ_{2h}^3	λ_{2h}^4
1/64	12.7606082907083	42.5751685615016	92.0871194476254	161.5348743615320
1/128	12.7590444146313	42.5508636384775	91.9653485323629	161.1514235895622
1/256	12.7586534825387	42.5447894481584	91.9349275389073	161.0556794745995
1/512	12.7585557518340	42.5432710282045	91.9273236515782	161.0317508835969
1/1024	12.7585313192603	42.5428914311462	91.9254227648108	161.0257692010616

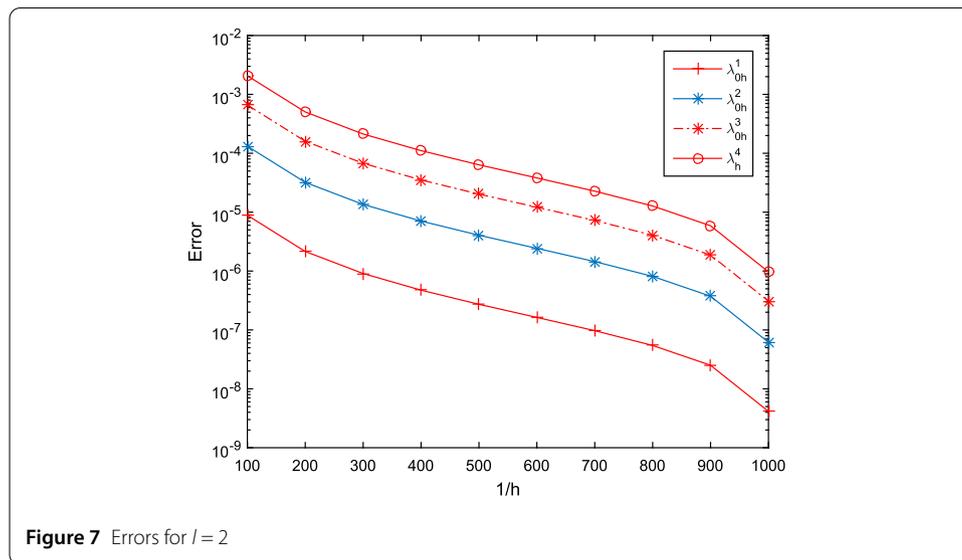
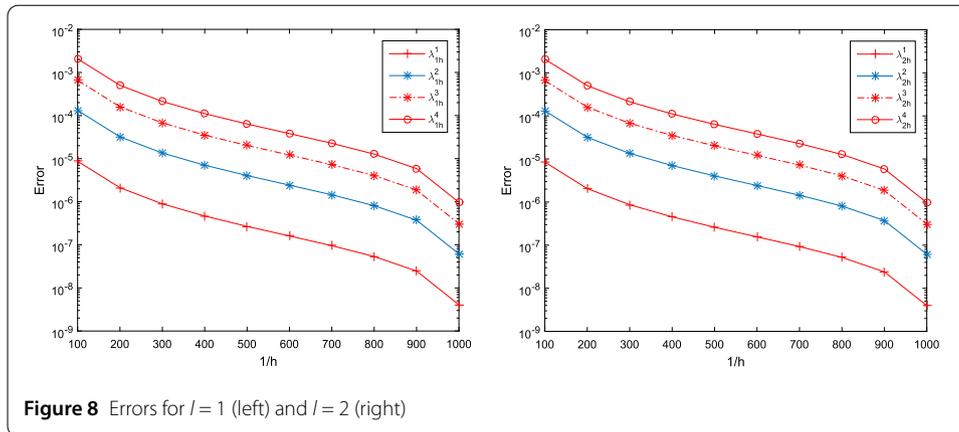


Figure 7 Errors for $l = 2$

7 Conclusions

In this work, an efficient finite element method is constructed to solve the Schrödinger eigenvalue problem with the IS potential on a spherical domain. By using spherical coordinate transformation and variable separation technique, we reduce the original problem into a series of equivalent and independent eigenvalue problems, which not only overcomes the difficulty brought by the singular coefficient, but also reduces the degrees of freedom greatly by dimension reduction. Thus we can spend less computing time and memory capacity to obtain high-precision numerical solutions. Numerical results show



that our algorithm is very effective. We believe that this method can be extended to more complex practical problems.

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Availability of data and materials

Data sharing not applicable to this paper as no datasets were generated or analyzed during the current study.

Ethics approval and consent to participate

Not applicable.

Competing interests

The authors declare that they have no competing interests.

Consent for publication

We agree.

Authors' contributions

YS and ZD carried out an efficient numerical approach to the eigenvalue problem of Schrödinger equation. JC helped to draft the manuscript. JZ is responsible for numerical experiments and proofs. All authors read and approved the final manuscript.

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