Research Article

An Efficient Finite Element Method and Error Analysis for Schrödinger Equation with Inverse Square Singular Potential

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We provide in this study an effective finite element method of the Schrödinger equation with inverse square singular potential on circular domain. By introducing proper polar condition and weighted Sobolev space, we overcome the difficulty of singularity caused by polar coordinates’ transformation and singular potential, and the weak form and the corresponding discrete scheme based on the dimension reduction scheme are established. Then, using the approximation properties of the interpolation operator, we prove the error estimates of approximation solutions. Finally, we give a large number of numerical examples, and the numerical results show the effectiveness of the algorithm and the correctness of the theoretical results.

1. Introduction

Schrödinger equation with the inverse square or centrifugal potential plays an important role in quantum mechanics, quantum cosmology, nuclear physics, molecular physics, and so on [1–8]. The potential has the same differential order as the Laplacian operator near the origin, which usually leads to strong singularities and cannot be treated as a lower-order perturbation term [9–14]. Li et al. [15] proposed an efficient finite element method to discuss the numerical solution of time-fractional Schrödinger equations. Thus, we need to develop some new numerical methods to solve Schrödinger equation with inverse square singular potential.

In recent years, more and more attention has been paid to the numerical methods of the Schrödinger equations with similar singular potential [1, 16–21]. However, many numerical methods are based on low-order finite element methods. If we solve these problems directly in two-dimensional domain, it will cost a lot of computing time and memory capacity to obtain high-precision numerical solutions [22–24]. In practice, we usually need to solve the Schrödinger equation with inverse square singular potential on circular domain. As far as we know, there are few reports on an effective numerical method for the Schrödinger equation with inverse square potential in circular domain. Thus, the purpose of this paper is to propose an effective finite element method of the Schrödinger equation with inverse square singular potential on circular domain. By introducing proper polar condition and weighted Sobolev space, we overcome the difficulty of singularity caused by polar coordinates transformation and singular potential and establish the weak form and corresponding discrete scheme based on the dimension reduction format. Then, using the approximation properties of interpolation operator, we prove the error estimates of approximation solutions. Finally, we give a large number of numerical examples, and the numerical results show the effectiveness of the algorithm and the correctness of the theoretical results.

The rest of this paper is organized as follows. In Section 2, we derive an equivalent scheme based on variable separation. In Section 3, we prove the existence and uniqueness of the solution. In Section 4, we prove the error estimation of approximation solutions. In Section 5, we describe the details for an efficient implementation of the algorithm. In
Section 6, we provide some numerical experiments to show the accuracy and efficiency of our algorithm. Finally, in Section 7, we give some concluding remarks.

2. An Equivalent Scheme Based on Variable Separation

We are interested in studying the following Schrödinger equation with inverse square singular potential:

\[ -\Delta \psi(x, y) + \frac{\beta(r)}{r} \psi(x, y) = f(x, y), \quad \text{in } D, \]  

(1)  \[ \psi(x, y) = 0, \quad \text{on } \partial D, \]  

(2)  

where \( 0 < \beta_s \leq \beta(r) \leq \beta^* \) and \( D = \{ x \in \mathbb{R}^2 : 0 \leq r < R \} \) with \( r = \sqrt{x^2 + y^2} \). Let \( x = r \cos \theta, y = r \sin \theta, U(r, \theta) = \psi(x, y), \) and \( F(r, \theta) = f(x, y) \). Then, the Laplace operator in polar coordinates is as follows:

\[ \mathcal{L} U = \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial U}{\partial r} \right) + \frac{1}{r^2} U_{\theta\theta}. \]  

(3)  

We can rewrite (1) and (2) as follows:

\[ -r \mathcal{L} U(r, \theta) + \frac{\beta(r)}{r} U(r, \theta) = rF(r, \theta), \quad (r, \theta) \in (0, R) \times [0, 2\pi], \]  

(4)  \[ U(R, \theta) = 0. \]  

(5)  

Since \( U(r, \theta) \) and \( F(r, \theta) \) are \( 2\pi \) periodic in \( \theta \), then we have

\[ U(r, \theta) = \sum_{|m| = 0}^{\infty} u_m(r) e^{im\theta}, \]  

(6)  \[ F(r, \theta) = \sum_{|m| = 0}^{\infty} f_m(r) e^{im\theta}, \]  

where \( u_m \) and \( f_m \) are the Fourier coefficients of \( U(r, \theta) \) and \( F(r, \theta) \), respectively. We can derive from (3) and (6) that

\[ r \mathcal{L} U(r, \theta) = \sum_{|m| = 0}^{\infty} \left[ \frac{\partial}{\partial r} \left( r \frac{\partial u_m(r)}{\partial r} \right) - \frac{m^2}{r} u_m(r) \right] e^{im\theta}, \]  

(7)  

\[ \frac{U(r, \theta)}{r} = \sum_{|m| = 0}^{\infty} \frac{u_m(r)}{r} e^{im\theta}. \]  

(8)  

To make (7) and (8) meaningful, we need introduce the following essential pole conditions:

\[ m^2 u_m(0) = 0, \quad u_m(0) = 0. \]  

(9)  

The pole condition (9) can be further reduced to

\[ u_m(0) = 0. \]  

(10)  

Using the orthogonal properties of Fourier basis functions and polar condition (10), we can reduce (4) and (5) to a series of equivalent one-dimensional Schrödinger equations as follows:

\[ -r \mathcal{L} u_m(r) + \frac{\beta(r)}{r} u_m(r) = r f_m(r), \quad r \in (0, R), \]  

(11)  \[ u_m(0) = u_m(R) = 0, \]  

(12)  

where

\[ \mathcal{L} u_m(r) = \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial u_m(r)}{\partial r} \right) - \frac{m^2}{r^2} u_m(r). \]  

(13)  

3. Existence and Uniqueness of the Solution

For convenience, we use the expression \( a \leq b \) to mean that \( a \leq Cb \), where \( C \) is a positive constant. In order to derive the weak form and corresponding discrete scheme of equations (11) and (12), we need to introduce the usual weighted Sobolev space:

\[ L_\omega^2(0, R) = \left\{ u : \int_0^R \omega u^2 \, dr < \infty \right\}, \]  

(14)  

with the corresponding inner product and norm,

\[ (u, v)_\omega = \int_0^R \omega uv \, dr, \]  

(15)  \[ \|u\|_\omega = \left( \int_0^R \omega u^2 \, dr \right)^{1/2}, \]  

and the nonuniformly weighted Sobolev space:

\[ H_{0, \omega}^1(0, R) = \left\{ u_m : \partial^k_r u_m \in L_\omega^2(0, R), \quad k = 0, 1, u_m(0) = u_m(R) = 0 \right\}, \]  

(16)  

with the corresponding inner product and norm,

\[ (u_m, v_m)_{L, \omega} = \int_0^R \partial \partial^k_r u_m \partial \partial^k_r v_m + \frac{1}{r} u_m v_m \, dr, \]  

(17)  \[ \|u_m\|_{L, \omega} = \left( \int_0^R \partial \partial^k_r u_m \partial \partial^k_r v_m + \frac{1}{r} u_m v_m \, dr \right)^{1/2}, \]  

where \( \omega = r \) is a weight function. Then, the weak form of equations (11) and (12) is to find \( u_m \in H_{0, \omega}^1(0, R) \), such that

\[ a_m(u_m, v_m) = F_m(v_m), \quad \forall v_m \in H_{0, \omega}^1(0, R), \]  

(18)  

where

\[ a_m(u_m, v_m) = \int_0^R \partial \partial^k_r u_m \partial \partial^k_r v_m + \frac{m^2}{r^2} u_m v_m \, dr, \]  

(19)  \[ F_m(v_m) = \int_0^R r f_m v_m \, dr. \]  

(20)  

Define approximation space \( X_h = P_h \cap H_{0, \omega}^1(0, R) \), where \( P_h \) is a piecewise linear interpolation polynomial space. Then, the corresponding discrete scheme of (18) is to find \( u_{mh} \in X_h \), such that

\[ a_m(u_{mh}, v_{mh}) = F_m(v_{mh}), \quad \forall v_{mh} \in X_h. \]  

(20)
Lemma 1. \( a_m(u_m, v_m) \) is a continuous and coercive bilinear functional on \( \mathcal{H}_h K \times \mathcal{H}_h K \), i.e.,
\[
\begin{align*}
|a_m(u_m, v_m)| &\leq \left\| u_m \right\|_{1,\omega} \left\| v_m \right\|_{1,\omega}, \\
\forall u_m, v_m \in \mathcal{H}_h K
\end{align*}
\]
(21)

Proof. We derive from the Cauchy–Schwarz inequality that
\[
|a_m(u_m, v_m)| = \left| \int_0^R \overline{r} \partial_r u_m \partial_r v_m + \frac{m^2 + \beta(r)}{r} u_m v_m \, dr \right|
\leq \int_0^R \overline{r} \partial_r |u_m \partial_r v_m| + \frac{m^2 + \beta^*(r)}{r} |u_m v_m| \, dr
\leq \int_0^R \overline{r} \partial_r |u_m \partial_r v_m| + \frac{1}{r} |u_m v_m| \, dr
\leq \left( \int_0^R \overline{r} \partial_r u_m \right)^{1/2} \left( \int_0^R \overline{r} \partial_r v_m \right)^{1/2}
+ \left( \int_0^R \frac{1}{r} |u_m|^2 \, dr \right)^{1/2} \left( \int_0^R \frac{1}{r} |v_m|^2 \, dr \right)^{1/2}
\leq \left\| u_m \right\|_{1,\omega} \left\| v_m \right\|_{1,\omega},
\]
(22)

Lemma 2. If \( f_m \in L^2(0, R) \), then \( F_m(v_m) \) is a bounded linear functional on \( \mathcal{H}_h K \times \mathcal{H}_h K \), i.e.,
\[
\left| F_m(v_m) \right| \leq \left\| u_m \right\|_{1,\omega}
\]
(23)

Proof. From Cauchy–Schwarz inequality, we have
\[
\left| F_m(v_m) \right| = \left| \int_0^R f_m v_m \, dr \right| \leq \left( \int_0^R \overline{r} (f_m)^2 \, dr \right)^{1/2} \left( \int_0^R \overline{r} (v_m)^2 \, dr \right)^{1/2}
\leq \left\| f_m \right\| \left( \int_0^R \overline{r} (\partial_r u_m)^2 + \frac{R^2}{r} (v_m)^2 \, dr \right)^{1/2} \leq \left\| u_m \right\|_{1,\omega},
\]
(24)

This finishes our proof.

Theorem 1. If \( f_m \in L^2(0, R) \), then problems (18) and (20) have unique solutions \( u_m \) and \( u_{m_b} \), respectively.

Proof. From Lemma 1, we have
\[
\left| a_m(u_m, v_m) \right| \leq \left\| u_m \right\|_{1,\omega} \left\| v_m \right\|_{1,\omega},
\]
(25)

for \( \forall u_m, v_m \in \mathcal{H}_h K \). That is, \( a_m(u_m, v_m) \) is a bounded and positive definite bilinear functional defined on \( \mathcal{H}_h K \times \mathcal{H}_h K \). In addition, from Lemma 2, we have
\[
\left| F_m(v_m) \right| \leq \left\| u_m \right\|_{1,\omega},
\]
(26)

which means \( F_m(v_m) \) is a bounded linear functional defined on \( \mathcal{H}_h K \). Then, from Lax–Milgram lemma, we know that equations (18) and (20) have unique solutions \( u_m \) and \( u_{m_b} \), respectively.

4. Error Estimation of Approximation Solutions

In this section, we will present the error estimates of approximate solutions. Define the piecewise linear interpolation operator \( \mathcal{H}_h K \): \( \mathcal{H}_h K \times \mathcal{H}_h K \rightarrow X_h \) by
\[
\mathcal{H}_h K u_m(r) = p_m(r), \quad r \in I_i,
\]
(27)

where \( p_m(r) \) is the linear interpolation polynomial of \( u_m \) on interval \( I_i = [r_{i-1}, r_i] \). Let
\[
u_m(r) = u_m(r), \quad r \in I_i.
\]
(28)

Then, from error formula of linear interpolating remainder term, we have
\[
u_m(r) - p_m(r) = \frac{\partial^2 u_m(\xi)}{2!} (r - r_{i-1})(r - r_i),
\]
(29)

where \( \xi \in I_i \) is a function depending on \( r \).

Theorem 2. Let \( G_m(r) = \frac{\partial^2 u_m(\xi)}{2!} \). Suppose that \( u_m \) is smooth enough such that \( \left| \partial^k G_m(r) \right| \leq M (k = 0, 1) \), where \( M \) is a large enough constant \( (0 \leq m \leq M) \) in Fourier transformation. Then, it holds
\[
\int_0^R \left| \overline{r} \partial_r (\mathcal{H}_h u_m(r) - u_m(r)) \right|^2 \, dr \leq h^2,
\]
(30)

where \( h = \max_{1 \leq i \leq n} |h_i| \), \( h_i = r_i - r_{i-1} \).

Proof. Since
\[
u_m(r) - \mathcal{H}_h u_m(r) = u_m(r) - p_m(r)
= G_m(r)(r - r_{i-1})(r - r_i),
\]
(31)

then we derive that
\[ \partial_r (u_m (r) - \mathcal{F}_h u_m (r)) = \partial_r G_m (r) (r - r_{i-1}) (r - r_i) + G_m (r) \partial_r ((r - r_{i-1}) (r - r_i)). \]

(32)

Then, we obtain
\[
\left| \partial_r (u_m (r) - \mathcal{F}_h u_m (r)) \right|^2 \leq \frac{1}{4} [r - r_{i-1}) (r - r_i)]^2 \\
+ [r - r_i - (r - r_{i-1})] (r - r_{i-1})]^2 \\
\leq \frac{1}{4} h_i^2 + (2h_i)^2 \\
\leq h_i^2.
\]

Thus, we derive that
\[
\int_0^R \left| \partial_r (\mathcal{F}_h u_m (r) - u_m (r)) \right|^2 dr \\
= \sum_{i=1}^{N} \int_{r_{i-1}}^{r_i} \left| \partial_r (\mathcal{F}_h u_m (r) - u_m (r)) \right|^2 dr \\
\leq \frac{1}{2} h_i^2 \\
\leq h^2.
\]

The proof of Theorem 2 is complete.

**Lemma 3.** For any \( u_m (r) \in \mathbb{R}^1_{0,0} (0, R) \), the following inequality holds:
\[
\int_0^R \frac{1}{r} u_m^2 (r) dr \leq R \int_0^R (\partial_r u_m (r))^2 dr.
\]

(35)

**Proof.** Since \( u_m (r) \in \mathbb{R}^1_{0,0} (0, R) \), then we have
\[
\frac{1}{r} u_m^2 (r) = \frac{1}{r} \left( \int_0^r \partial_r u_m (t) dt \right)^2 \leq \frac{1}{r} \int_0^r 1^2 dt \int_0^r (\partial_r u_m (t))^2 dt \\
= \int_0^r (\partial_r u_m (t))^2 dt \leq \int_0^R (\partial_r u_m (r))^2 dr.
\]

(36)

Thus, we derive that
\[
\int_0^R \frac{1}{r} u_m^2 (r) dr \leq R \int_0^R (\partial_r u_m (r))^2 dr.
\]

\[
\| u_m - u_m (r) \|_{1,0} \leq h.
\]

(38)

**Proof.** We derive from (18) and (20) that
\[
a_m (u_m, v_m) = F_m (v_m), \quad \forall v_m \in X_h, \\
a_m (u_m, \psi_m) = F_m (v_m), \quad \forall \psi_m \in X_h.
\]

(39)

Then, we have
\[
a_m (u_m - u_m, \psi_m) = 0, \quad \forall \psi_m \in X_h.
\]

(40)

We derive from Lemma 1 and (40) that
\[
\| u_m - u_m \|_{1,0} \leq a_m \| u_m - u_m, u_m + \psi_m \|_{1,0} \\
\quad \leq \| u_m - u_m \|_{1,0} \| u_m - \mathcal{F}_h u_m \|_{1,0} \\
= \int_0^R \left[ \partial_r (u_m - \mathcal{F}_h u_m) \right]^2 + \frac{1}{r} (u_m - \mathcal{F}_h u_m)^2 dr.
\]

(41)

Then, we obtain
\[
\| u_m - u_m \|_{1,0} \leq \| u_m - \mathcal{F}_h u_m \|_{1,0}, \quad \forall \psi_m \in X_h.
\]

(42)

Then, we have
\[
\| u_m - u_m \|_{1,0} \leq \inf_{v_m \in X_h} \| u_m - v_m \|_{1,0} \leq \| u_m - \mathcal{F}_h u_m \|_{1,0} \\
= \int_0^R \left[ \partial_r (u_m - \mathcal{F}_h u_m) \right]^2 + \frac{1}{r} (u_m - \mathcal{F}_h u_m)^2 dr.
\]

(43)

We derive from Lemma 3 that
\[
\| u_m - u_m \|_{1,0} \leq \int_0^R \left[ \partial_r (u_m - \mathcal{F}_h u_m) \right]^2 + \frac{1}{r} (u_m - \mathcal{F}_h u_m)^2 dr \\
\leq \int_0^R \left[ \partial_r (u_m - \mathcal{F}_h u_m) \right]^2 dr \leq \int_0^R \left[ \partial_r (u_m - \mathcal{F}_h u_m) \right]^2 dr.
\]

(44)

Combining with Theorem 2, we can obtain the desired result.

5. Implementation of the Algorithm
To solve the discrete scheme (20), we need to construct a set of basis functions of approximation space. Let
\[
\psi_i (r) = \begin{cases} \frac{r - r_{i-1}}{h_i}, & r_{i-1} \leq r \leq r_i, \\
\frac{r - r_{i+1}}{h_{i+1}}, & r_i \leq r \leq r_{i+1}, \\
0, & \text{others,} \end{cases}
\]

(45)

where \( i = 1, \ldots, N - 1 \). It is clear that
We will perform some numerical tests in order to show the accuracy and convergence of our algorithm. We present the figures and their error figures of exact solution and approximation solution in Tables 1 for different $M$ and $h$. In order to further show the accuracy and convergence of our algorithm, we present the figures and their error figures of exact solution and approximation solution in Figures 1 and 2, respectively.

We observe from Table 1 that the error $e(\psi(x, y), \psi_{Mh}(x, y))$ achieves about 10^{-4} with $h \leq (1/32)$ and $M = 6$. In addition, we can see from Figures 1 and 2 that the numerical solution converges to exact solution with the decrease of $h$.

**Example 2.** We take $\beta(r) = (2/3), R = 1,$ and $u = (x^2 + y^2 - 1)\sin(x^2 + y^2)$. It is obvious that $\psi(x, y)$ satisfies the boundary condition (2). Similarly, $f(x, y)$ can be obtained by substituting $\psi(x, y)$ into equation (1). We list the errors between exact solution and approximation solutions in Table 2 for different $M$ and $h$. In order to further show the accuracy and convergence of our algorithm, we present the figures and their error figures of exact solution and approximation solution in Figures 3 and 4, respectively.

We observe from Table 2 that the error $e(\psi(x, y), \psi_{Mh}(x, y))$ achieves about 10^{-4} with $h \leq (1/32)$ and $M = 6$. In addition, we can see from Figures 3 and 4 that the numerical solution converges to exact solution with the decrease of $h$.

**Example 3.** We take $\beta = 1/2, R = 1,$ and $\psi(x, y) = (x^2 + y^2 - 1)e^{x+y}$. We list the errors between exact solution and approximation solutions in Table 3 for different $M$ and $h$. We also present the figures and their error figures of exact solution and approximation solution in Figures 5 and 6, respectively.
Table 1: The error $e(\psi(x, y), \psi_{Mh}(x, y))$ for different $M$ and $h$.

| $h$  | $M = 6$ | $M = 8$ | $M = 10$ | $M = 12$ |
|------|---------|---------|---------|---------|
| 1/8  | 0.0517  | 0.0517  | 0.0754  | 0.0754  |
| 1/16 | $4.4437e-04$ | $4.4437e-04$ | $4.4437e-04$ | $4.4437e-04$ |
| 1/32 | $1.1380e-04$ | $1.1380e-04$ | $1.1380e-04$ | $1.1380e-04$ |
| 1/64 | $2.8623e-05$ | $2.8623e-05$ | $2.8623e-05$ | $2.8623e-05$ |

Figure 1: Figures of the exact solution (a) and the numerical solution (b) with $h = 1/64, m = 12$.

Table 2: The error $e(\psi(x, y), \psi_{Mh}(x, y))$ for different $M$ and $h$.

| $h$  | $M = 6$ | $M = 8$ | $M = 10$ | $M = 12$ |
|------|---------|---------|---------|---------|
| 1/8  | 0.0027  | 0.0978  | 0.0978  | 0.0978  |
| 1/16 | $6.5774e-04$ | $6.5774e-04$ | $6.5774e-04$ | $6.5774e-04$ |
| 1/32 | $1.6360e-04$ | $1.6360e-04$ | $1.6360e-04$ | $1.6360e-04$ |
| 1/64 | $4.0798e-05$ | $4.0798e-05$ | $4.0798e-05$ | $4.0798e-05$ |

Figure 2: The error figures of exact solution and numerical solution with $h = 1/32, m = 10$ (a) and $h = 1/64, m = 12$ (b).

Figure 3: Figures of the exact solution (a) and the numerical solution (b) with $h = 1/64, m = 12$. 
Figure 4: The error figures of numerical solution and exact solution with $h = 1/32, m = 10$ (a) and $h = 1/64, m = 12$ (b).

Table 3: The error $e(\psi(x, y), \psi_{Mh}(x, y))$ for different $M$ and $h$.

| $h$    | $M = 6$   | $M = 8$   | $M = 10$  | $M = 12$  |
|--------|-----------|-----------|-----------|-----------|
| $1/16$ | 0.0022    | 0.0022    | 0.0022    | 0.0050    |
| $1/32$ | 5.4324e-04| 5.4324e-04| 5.4324e-04| 5.4324e-04|
| $1/64$ | 1.3583e-04| 1.3583e-04| 1.3583e-04| 1.3583e-04|
| $1/128$| 4.1754e-05| 3.3967e-05| 3.3944e-05| 3.3944e-05|

Figure 5: Figures of the exact solution (a) and the numerical solution (b) with $h = 1/128, m = 12$.

Figure 6: The error figures of numerical solution and exact solution with $h = 1/64, m = 10$ (a) and $h = 1/128, m = 12$ (b).
We observe from Table 3 that the error $\epsilon(\psi(x, y), \psi_{M_h}(x, y))$ achieves about $10^{-4}$ with $h \leq (1/64)$ and $M = 6$. In addition, we can see from Figures 5 and 6 that the numerical solution converges to exact solution with the decrease of $h$.

7. Conclusions

We present in this paper an efficient finite element method for the Schrödinger equation with the inverse square potential on the circular domain. By using polar coordinate transformation and Fourier basis function expansion, we reduce the original problem into a series of equivalent one-dimensional problems. By introducing polar conditions, we overcome not only the difficulty brought by the singular potential but also the degree of freedom which is greatly reduced by dimension reduction. Thus, we only spend less computing time and memory capacity to obtain high-precision numerical solutions. Numerical results show that our algorithm is very effective. We mainly focus on, in this paper, the Schrödinger equation with the inverse square potential on the circular domain. In fact, we can extend our method to the Schrödinger equation with more complex potentials.

Data Availability

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

Conflicts of Interest

The authors declare that they have no conflicts of interest.

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