

Spectral Analysis for Fractional Hydrogen Atom Equation

Erdal Bas, Funda Metin

Department of Mathematics, Faculty of Science, Elazığ, Turkey

Email: erdalmat@yahoo.com, fnd-44@hotmail.com

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Abstract

In this paper, spectral analysis of fractional Sturm Liouville problem defined on $(0, 1]$, having the singularity of type $-\frac{2}{r} + \frac{l(l+1)}{r^2}$ at zero and researched the fundamental properties of the eigenfunctions and eigenvalues for the operator. We show that the eigenvalues and eigenfunctions of the problem are real and orthogonal, respectively.

Keywords

Sturm-Liouville, Fractional, Hydrogen Atom, Singular, Spectral

1. Introduction

Fractional calculus have been available and applicable to various fields of science, the investigation of the theory of fractional differential equations has only been started recently. At the same time, fractional differential equations have great interest due to their numerous applications in many fields of science, such as physics, mechanics, chemistry, finance, electromagnetics, acoustics, viscoelasticity, electrochemistry, economy, etc. So far, there have been several fundamental works on the fractional derivative and fractional differential equations, written by Miller and Ross [1] Podlubny [2] Kilbas, Srivastava and Trujillo [3].

In recent years, fractional Sturm-Liouville problems have been studied and these studies, which the eigenvalues and eigenfunctions associated to these operators and also their properties, have been published by M. Klimek and O. P. Argawal [4] [7]. Furthermore, there are a lot of studies in this topic [4]-[13].

Sturm-Liouville problems have been studied for over two hundred years. The great progress has been made related to spectral theory. And this topic has an increasing interest for years from different points of view [14]-[23].

2. Preliminaries

Firstly, we consider singular Sturm-Liouville equation

$$\frac{d^2 R}{dr^2} + \frac{2}{r} \frac{dR}{dr} - \frac{l(l+1)}{r^2} R + \left(E + \frac{2}{r} \right) R = 0 \quad (0 < r < \infty).$$

In quantum mechanics the study of the energy levels of the hydrogen atom leads to this equation [5]. Where R is the distance of the mass center to the origin. l is positive integer, a is a real number E is energy constant and r is the distance between the nucleus with the electron.

Substitution $R = y/r$ reduces above equation to the form

$$\frac{d^2 y}{dr^2} + \left\{ E + \frac{2}{r} - \frac{l(l+1)}{r^2} \right\} y = 0.$$

In most cases we took the reference potential to be

$$V(r) = \frac{2}{r} - \frac{l(l+1)}{r^2}.$$

When $V(r)$ is defined by last differential equation it contains a centripetal and Coulomb part, the usual singularities of the nuclear problem. We consider the following fractional singular Sturm-Liouville problem for hydrogen atom equation

$$L_\alpha y_\lambda(r) + \lambda w_\alpha(r) y_\lambda(r) = 0$$

$$y_\lambda(0) = 0,$$

$$d_1 y(1) + d_2 I_{1,-}^{1-\alpha} p(1) {}^c D_{0,+}^\alpha y(1) = 0,$$

where the fractional order $\alpha \in (0, 1]$ and L_α is defined as

$$L_\alpha = D_{1,-}^\alpha p(r) {}^c D_{0,+}^\alpha + \left(-\frac{2}{r} + \frac{l(l+1)}{r^2} + q_0(r) \right),$$

where $D_{1,-}^\alpha$ and ${}^c D_{0,+}^\alpha$ refers to the Riemann-Liouville and Caputo fractional derivative defined below by definition 2, respectively. The main theoretical result of the paper is prove spectral properties fractional singular Sturm-Liouville problem for hydrogen atom equation.

Definition 1. [2] Let $0 < \alpha \leq 1$. The left-sided and respectively right-sided Riemann-Liouville integrals of order α are given by the formulas

$$(I_{a,+}^\alpha f)(r) = \frac{1}{\Gamma(\alpha)} \int_a^r (r-s)^{\alpha-1} f(s) ds \quad r > a, \tag{1}$$

$$(I_{b,-}^\alpha f)(r) = \frac{1}{\Gamma(\alpha)} \int_r^b (s-r)^{\alpha-1} f(s) ds \quad r < b, \tag{2}$$

where Γ denotes the gamma function.

Definition 2. [2] Let $0 < \alpha \leq 1$. The left-sided and respectively right-sided Riemann-Liouville derivatives of order α are defined as

$$(D_{a,+}^\alpha f)(r) = D(I_{a,+}^{1-\alpha} f)(r) \quad r > a, \tag{3}$$

$$(D_{b,-}^\alpha f)(r) = -D(I_{b,-}^{1-\alpha} f)(r) \quad r < b. \tag{4}$$

Analogous formulas yield the left and right-sided Caputo derivatives of order α :

$$({}^c D_{a,+}^\alpha f)(r) = (I_{a,+}^{1-\alpha} Df)(r) \quad r > a, \tag{5}$$

$$({}^c D_{b,-}^\alpha f)(r) = (I_{b,-}^{1-\alpha} (-D)f)(r) \quad r < b, \tag{6}$$

Property 3. [7] The fractional differential operators defined in (3)-(6) satisfy the following identities:

$$\int_a^b f(r) D_{b,-}^\alpha g(r) dr = \int_a^b g(r) {}^C D_{a,+}^\alpha f(r) dr - f(r) I_{b,-}^{1-\alpha} g(r) \Big|_a^b$$

$$\int_a^b f(r) D_{b,-}^\alpha g(r) {}^C D_{a,+}^\alpha k(r) dr = \int_a^b g(r) {}^C D_{a,+}^\alpha f(r) {}^C D_{a,+}^\alpha k(r) dr - f(r) I_{b,-}^{1-\alpha} g(r) {}^C D_{a,+}^\alpha k(r) \Big|_a^b, \tag{7}$$

$$\int_a^b f(r) D_{a,+}^\alpha g(r) dr = \int_a^b g(r) {}^C D_{b,-}^\alpha f(r) dr + f(r) I_{a,+}^{1-\alpha} g(r) \Big|_a^b. \tag{8}$$

Property 4. [7] Assume $\alpha \in (0,1), \beta > \alpha$ and $f \in C[a,b]$. Then the following relations

$$\begin{aligned} D_{a,+}^\alpha I_{a,+}^\alpha f(r) &= f(r), \\ D_{b,-}^\alpha I_{b,-}^\alpha f(r) &= f(r), \\ D_{a,+}^\alpha I_{a,+}^\beta f(r) &= I_{a,+}^{\beta-\alpha} f(r), \\ D_{b,-}^\alpha I_{b,-}^\beta f(r) &= I_{b,-}^{\beta-\alpha} f(r), \\ {}^C D_{a,+}^\alpha I_{a,+}^\alpha f(r) &= f(r), \\ {}^C D_{b,-}^\alpha I_{b,-}^\alpha f(r) &= f(r), \end{aligned} \tag{9}$$

hold for any $r \in [a,b]$. Furthermore, the integral operators defined in (1), (2) satisfy the following semi-group properties.

$$I_{a,+}^\alpha I_{a,+}^\beta = I_{a,+}^{\alpha+\beta}, \quad I_{b,-}^\alpha I_{b,-}^\beta = I_{b,-}^{\alpha+\beta}.$$

Now, let's take up a fractional Sturm-Liouville problem for hydrogen atom equation.

3. A Singular Fractional Sturm-Liouville Problem for Hydrogen Atom Equation

Let's denote a singular fractional Sturm-Liouville problem for hydrogen atom equation with the differential part containing the left and right-sided derivatives. Let's use the form of the integration by parts formulas (7) and (8) for this new approximation. Main properties of eigenfunctions and eigenvalues in the theory of classical Sturm-Liouville problems are related to the integration by parts formula for the appear and the essential pairs are the left Riemann-Liouville derivative with the right Caputo derivative and the right Riemann-Liouville derivative with the left Caputo one.

Definition 5. For $\alpha \in (0,1]$. Fractional hydrogen atom operator is written as

$$L_\alpha = D_{1,-}^\alpha p(r) {}^C D_{0,+}^\alpha + \left(-\frac{2}{r} + \frac{l(l+1)}{r^2} + q_0(r) \right) \tag{10}$$

consider the fractional hydrogen atom equation

$$L_\alpha y_\lambda(r) + \lambda w_\alpha(r) y_\lambda(r) = 0, \tag{11}$$

where $p(r) \neq 0, w_\alpha(r) > 0, \forall r \in (0,1]$ and p, q are real valued continuous functions in interval $(0, 1]$. The boundary conditions for the operator L are the following:

$$y_\lambda(0) = 0, \tag{12}$$

$$d_1 y(1) + d_2 I_{1,-}^{1-\alpha} p(1) {}^C D_{0,+}^\alpha y(1) = 0, \tag{13}$$

where $d_1^2 + d_2^2 \neq 0$. The fractional boundary-value problem (11)-(13) is fractional Sturm-Liouville problem for hydrogen atom operator.

Theorem 6. Fractional hydrogen operator is self-adjoint on $(0, 1]$.

Proof. Let us consider the following equation

$$\begin{aligned} \langle L_\alpha \varphi \phi \rangle &= \int_0^1 L_\alpha \varphi \phi dr = \int_0^1 \phi(r) \left[D_{1,-}^\alpha p(r) {}^C D_{0,+}^\alpha \varphi(r) + \left(-\frac{2}{r} + \frac{l(l+1)}{r^2} + q_0(r) \right) \varphi(r) \right] dr \\ &= \int_0^1 \phi(r) D_{1,-}^\alpha p(r) {}^C D_{0,+}^\alpha \varphi(r) dr + \int_0^1 \left(-\frac{2}{r} + \frac{l(l+1)}{r^2} + q_0(r) \right) \varphi(r) \phi(r) dr. \end{aligned}$$

Considering property 3 to the first integral in the last equation, we obtain the identity

$$\begin{aligned} \langle L_\alpha \varphi \phi \rangle &= \int_0^1 p(r) {}^C D_{0,+}^\alpha \phi(r) {}^C D_{0,+}^\alpha \varphi(r) dr + \frac{d_1}{d_2} \varphi(1) \phi(1) \\ &\quad + \int_0^1 \left(-\frac{2}{r} + \frac{l(l+1)}{r^2} + q_0(r) \right) \varphi(r) \phi(r) dr \end{aligned} \tag{14}$$

Similarly, we obtain

$$\begin{aligned} \langle \varphi, L_\alpha \phi \rangle &= \int_0^1 p(r) {}^C D_{0,+}^\alpha \varphi(r) {}^C D_{0,+}^\alpha \phi(r) dr + \frac{d_1}{d_2} \varphi(1) \phi(1) \\ &\quad + \int_0^1 \left(-\frac{2}{r} + \frac{l(l+1)}{r^2} + q_0(r) \right) \phi(r) \varphi(r) dr. \end{aligned} \tag{15}$$

The right hand sides of the Equations (14) and (15) are equal hence we may see that the left sides are equal that is

$$\langle L_\alpha \varphi, \phi \rangle = \langle \varphi, L_\alpha \phi \rangle$$

Therefore, $L_\alpha = L_\alpha^*$ The proof is completed.

Theorem 7. The eigenvalues of fractional hydrogen atom operator (11)-(13) are real.

Proof. Let us observe that following relation results from property (3)

$$\begin{aligned} \int_0^1 f(r) L_\alpha g(r) dr &= \int_0^1 p(r) {}^C D_{0,+}^\alpha f(r) {}^C D_{0,+}^\alpha g(r) dr - f(r) I_{1,-}^{1-\alpha} p(r) {}^C D_{0,+}^\alpha g(r) \Big|_0^1 \\ &\quad + \int_0^1 \left(-\frac{2}{r} + \frac{l(l+1)}{r^2} + q_0(r) \right) g(r) f(r) dr. \end{aligned} \tag{16}$$

Suppose that λ is the eigenvalue for (11)-(13) corresponding to eigenfunction y the following equalities are satisfy y and its complex conjugate \bar{y}

$$L_\alpha y(r) + \lambda w_\alpha(r) y(r) = 0, \tag{17}$$

$$y(0) = 0, \tag{18}$$

$$d_1 y(1) + d_2 I_{1,-}^{1-\alpha} p(1) {}^C D_{0,+}^\alpha y(1) = 0, \tag{19}$$

$$L_\alpha \bar{y}(r) + \bar{\lambda} w_\alpha(r) \bar{y}(r) = 0, \tag{20}$$

$$\bar{y}(0) = 0, \tag{21}$$

$$d_1 \bar{y}(1) + d_2 I_{1,-}^{1-\alpha} p(1) {}^C D_{0,+}^\alpha \bar{y}(1) = 0, \tag{22}$$

where $d_1^2 + d_2^2 \neq 0$ We multiply Equation (17) by function \bar{y} and (20) by function y respectively and subtract:

$$(\lambda - \bar{\lambda}) w_\alpha(r) y(r) \bar{y}(r) = y(r) L_\alpha \bar{y}(r) - \bar{y}(r) L_\alpha y(r).$$

Now, we integrate over interval (0, 1] and applying relation (16) we note that the right-hand side of the integrated equality contains only boundary terms:

$$\begin{aligned}
 & (\lambda - \bar{\lambda}) \int_0^1 w_\alpha(r) y(r) \bar{y}(r) dr = \int_0^1 y(r) L_\alpha \bar{y}(r) dr - \int_0^1 \bar{y}(r) L_\alpha y(r) dr \\
 & = \int_0^1 y(r) \left[D_{1,-}^\alpha p(r) {}^C D_{0,+}^\alpha \bar{y}(r) + \left(-\frac{2}{r} + \frac{l(l+1)}{r^2} + q_0(r) \right) \bar{y}(r) \right] dr \\
 & \quad - \int_0^1 \bar{y}(r) \left[D_{1,-}^\alpha p(r) {}^C D_{0,+}^\alpha y(r) + \left(-\frac{2}{r} + \frac{l(l+1)}{r^2} + q_0(r) \right) y(r) \right] dr \\
 & = \int_0^1 y(r) D_{1,-}^\alpha p(r) {}^C D_{0,+}^\alpha \bar{y}(r) dr + \int_0^1 \left(-\frac{2}{r} + \frac{l(l+1)}{r^2} + q_0(r) \right) \bar{y}(r) y(r) dr \\
 & \quad - \int_0^1 \bar{y}(r) D_{1,-}^\alpha p(r) {}^C D_{0,+}^\alpha y(r) dr - \int_0^1 \left(-\frac{2}{r} + \frac{l(l+1)}{r^2} + q_0(r) \right) \bar{y}(r) y(r) dr \\
 & = \int_0^1 p(r) {}^C D_{0,+}^\alpha y(r) {}^C D_{0,+}^\alpha \bar{y}(r) dr - y(r) I_{1,-}^{1-\alpha} p(r) {}^C D_{0,+}^\alpha \bar{y}(r) \Big|_0^1 \\
 & \quad + \int_0^1 \left(-\frac{2}{r} + \frac{l(l+1)}{r^2} + q_0(r) \right) y(r) \bar{y}(r) dr - \int_0^1 p(r) {}^C D_{0,+}^\alpha \bar{y}(r) {}^C D_{0,+}^\alpha y(r) dr \\
 & \quad + \bar{y}(r) I_{1,-}^{1-\alpha} p(r) {}^C D_{0,+}^\alpha y(r) \Big|_0^1 - \int_0^1 \left(-\frac{2}{r} + \frac{l(l+1)}{r^2} + q_0(r) \right) y(r) \bar{y}(r) dr \\
 & (\lambda - \bar{\lambda}) \int_0^1 w_\alpha(r) |y(r)|^2 dr = -y(r) I_{1,-}^{1-\alpha} p(r) {}^C D_{0,+}^\alpha \bar{y}(r) \Big|_1 + y(r) I_{1,-}^{1-\alpha} p(r) {}^C D_{0,+}^\alpha y(r) \Big|_0 \\
 & \quad + \bar{y}(r) I_{1,-}^{1-\alpha} p(r) {}^C D_{0,+}^\alpha y(r) \Big|_1 - \bar{y}(r) I_{1,-}^{1-\alpha} p(r) {}^C D_{0,+}^\alpha \bar{y}(r) \Big|_0,
 \end{aligned}$$

by virtue of the boundary conditions (18), (19), (21), (22), we find

$$(\lambda - \bar{\lambda}) \int_0^1 w_\alpha(r) |y(r)|^2 dr = 0$$

and because y is a non-trivial solution and $w_\alpha(r) > 0$, it easily seen that $\lambda = \bar{\lambda}$.

Theorem 8. The eigenfunctions corresponding to distinct eigenvalues of fractional hydrogen atom operator (11)-(13) are orthogonal weight function w_α on $(0, 1]$ that is

$$\int_0^1 w_\alpha(r) y_{\lambda_1}(r) y_{\lambda_2}(r) dr = 0 \quad \lambda_1 \neq \lambda_2$$

Proof. We have by assumptions fractional Sturm-Liouville for hydrogen atom operator fulfilled by two different eigenvalues (λ_1, λ_2) and the respective eigenfunctions $(y_{\lambda_1}, y_{\lambda_2})$, in that case

$$L_\alpha y_{\lambda_1}(r) + \lambda_1 w_\alpha(r) y_{\lambda_1}(r) = 0, \tag{23}$$

$$y_{\lambda_1}(0) = 0, \tag{24}$$

$$d_1 y_{\lambda_1}(1) + d_2 I_{1,-}^{1-\alpha} p(1) {}^C D_{0,+}^\alpha y_{\lambda_1}(1) = 0, \tag{25}$$

$$L_\alpha y_{\lambda_2}(r) + \lambda_2 w_\alpha(r) y_{\lambda_2}(r) = 0, \tag{26}$$

$$y_{\lambda_2}(0) = 0, \tag{27}$$

$$d_1 y_{\lambda_2}(1) + d_2 I_{1,-}^{1-\alpha} p(1) {}^C D_{0,+}^\alpha y_{\lambda_2}(1) = 0, \tag{28}$$

we multiply Equation (23) by function y_{λ_2} and (26) by function y_{λ_1} respectively and subtract:

$$(\lambda_1 - \lambda_2) w_\alpha(r) y_{\lambda_1} y_{\lambda_2} = y_{\lambda_1} L_\alpha y_{\lambda_2} - y_{\lambda_2} L_\alpha y_{\lambda_1}$$

Integrating over interval $(0, 1]$ and applying relation (16) we note that the right-hand side of the integrated equality contains only boundary terms:

$$\begin{aligned}
& (\lambda_1 - \lambda_2) \int_0^1 w_\alpha(r) y_{\lambda_1}(r) y_{\lambda_2}(r) dr \\
&= \int_0^1 y_{\lambda_1}(r) L_\alpha y_{\lambda_2}(r) dr - \int_0^1 y_{\lambda_2}(r) L_\alpha y_{\lambda_1}(r) dr \\
&= \int_0^1 y_{\lambda_1}(r) \left[D_{1,-}^\alpha p(r) {}^C D_{0,+}^\alpha y_{\lambda_2}(r) + \left(-\frac{2}{r} + \frac{l(l+1)}{r^2} + q_0(r) \right) y_{\lambda_2}(r) \right] dr \\
&\quad - \int_0^1 y_{\lambda_2}(r) \left[D_{1,-}^\alpha p(r) {}^C D_{0,+}^\alpha y_{\lambda_1}(r) + \left(-\frac{2}{r} + \frac{l(l+1)}{r^2} + q_0(r) \right) y_{\lambda_1}(r) \right] dr \\
&= \int_0^1 p(r) {}^C D_{0,+}^\alpha y_{\lambda_1}(r) {}^C D_{0,+}^\alpha y_{\lambda_2}(r) dr - y_{\lambda_1}(r) I_{1,-}^{1-\alpha} p(r) {}^C D_{0,+}^\alpha y_{\lambda_2}(r) \Big|_0^1 \\
&\quad + \int_0^1 \left(-\frac{2}{r} + \frac{l(l+1)}{r^2} + q_0(r) \right) y_{\lambda_1}(r) y_{\lambda_2}(r) dr \\
&\quad - \int_0^1 p(r) {}^C D_{0,+}^\alpha y_{\lambda_2}(r) {}^C D_{0,+}^\alpha y_{\lambda_1}(r) dr + y_{\lambda_2}(r) I_{1,-}^{1-\alpha} p(r) {}^C D_{0,+}^\alpha y_{\lambda_1}(r) \Big|_0^1 \\
&\quad - \int_0^1 \left(-\frac{2}{r} + \frac{l(l+1)}{r^2} + q_0(r) \right) y_{\lambda_1}(r) y_{\lambda_2}(r) dr \\
&= (\lambda_1 - \lambda_2) \int_0^1 w_\alpha(r) y_{\lambda_1}(r) y_{\lambda_2}(r) dr \\
&= -y_{\lambda_1}(r) I_{1,-}^{1-\alpha} p(r) {}^C D_{0,+}^\alpha y_{\lambda_2}(r) \Big|_0^1 + y_{\lambda_2}(r) I_{1,-}^{1-\alpha} p(r) {}^C D_{0,+}^\alpha y_{\lambda_1}(r) \Big|_0^1.
\end{aligned}$$

Using the boundary conditions (24), (25), (27), (28), we find that

$$(\lambda_1 - \lambda_2) \int_0^1 w_\alpha(r) y_{\lambda_1}(r) y_{\lambda_2}(r) dr = 0,$$

where $\lambda_1 \neq \lambda_2$. The proof is completed.

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