AN APPLICATION OF COMPARISON CRITERIA TO FRACTIONAL SPECTRAL PROBLEM HAVING COULOMB POTENTIAL

by

Erdal BAS [a*] ***and Funda METIN TURK*** [b]

[a] Department of Mathematics, Faculty of Science, Firat University, Elazig, Turkey
[b] Department of Mathematics, Faculty of Science, Bartın University, Bartın, Turkey

Original scientific paper
https://doi.org/10.2298/TSCI170612273B

In this study, the zeros of eigenfunctions of spectral theory are considered in fractional Sturm-Liouville problem. The 1st and 2nd comparison theorems for fractional Sturm-Liouville equation with boundary condition and their proofs are given. In this way, our new approximation will contribute to construct fractional Sturm-Liouville theory. Also, its an application is given in case of Coulomb potential and the results are presented by a symbolic graph.

Key words: *thermal conduction, angular momentum, Coulomb potential, energy equation, Sturm-Liouville, Schroedinger equation*

Introduction

Charles Francois Sturm was counted as the founder of Sturm-Liouville theory in the 1830s. Doubtless Sturm's the most important contribution is to introduce and center on Sturm-Liouville operators. Only, his most remarkable results are the oscillation and comparison theorems. The fundamental theory of Sturm-Liouville differential equations, is deeply influenced by the development of quantum mechanics. Sturm takes into consider the PDE for the diffusion of heat. The improvement of such a diffusion process in time derives a system of transformations whose effect on the zeros of a function has been much studied. Sturm-Liouville equation is in fact 1-D Schroedinger equation, which is a PDE but in the event of spherically symmetric potentials such as the Coulomb potential, it is reduced to the ODE, one for each pair of angular momentum quantum numbers. The importance of mathematics arises from the study of problems in the real world and a lot of physical applications like thermal conduction, vibrating of strings, interacting of atomic particles, quantum mechanics, mass-spring system, *etc.* [1]. The concept of Sturm-Liouville problems plays an important role in mathematics and physics. Sturm-Liouville boundary value problem is given:

$$-\frac{\mathrm{d}}{\mathrm{d}r}\left[p(r)\frac{\mathrm{d}y}{\mathrm{d}r}\right]+q(r)y=\lambda w(r)y,\quad r\in[a,b] \tag{1}$$

$$A_1 y(a)+A_2 y'(a)=0,\quad A_1^2+A_2^2>0 \tag{2}$$

$$B_1 y(b)+B_2 y'(b)=0,\quad B_1^2+B_2^2>0 \tag{3}$$

* Corresponding author, e-mail: erdalmat@yahoo.com

where $p(r)$, $w(r)>0$ and $p'(r), w(r)$, and $q(r)$ are continuous functions over the finite interval $[a,b]$.

Later on, many studies have been made on this subject. Regular-singular Sturm-Liouville problems are defined. Inverse problems have been proved by using various spectral datas. There are numerous studies about Sturm-Liouville problem, [2-6].

Together with coming up L'Hopital's fractional calculus idea in 1695, many advanced applications about this subject in various areas have been given for years. It has been demonstrated that many systems in different fields of physics, chemistry, biology, economics, control theory, optical systems, engineering can be modelled more accurately by means of fractional derivatives. Definitions and theory of fractional derivatives and integral, fractional differential equations, fractional PDE can be found in [7-11]. Majority of the mathematical theory to the study of fractional calculus was improved in the 20th century [12-16]. For last centuries the theory of fractional derivatives has been improved mainly as pure theoretical fields of mathematics useful only for mathematicians. And especially in the recent years, important studies have been aimed at combining fractional derivative and integral subject with Sturm-Liouville subject have been obtained, [17, 18]. Fundamental spectral theory for regular-singular Sturm-Liouville problems is given. Furthermore the spectral theory for fractional Sturm-Liouville problems having Bessel and Coulomb type singularity is investigated, in 2013 [17, 19-24].

Now, let's mention about Coulomb potential; motion of electrons moving under the Coulomb potential is of significance in quantum theory. We use to find energy levels for hydrogen atom and single valence electron atoms. For hydrogen atom, the Coulomb potential is given by $U=-e^2/s$, s is the radius of the nucleus and e is electronic charge. As regards, using the time-dependent Schroedinger equation:

$$i\tilde{h}\frac{\partial\omega}{\partial t}=-\frac{\tilde{h}^2}{2m}\frac{\partial^2\omega}{\partial r^2}+U(r,y,z)\omega,\quad \int_{R^3}|\omega|^2\,\mathrm{d}r\,\mathrm{d}y\,\mathrm{d}z=1$$

where ω is the wave function, $\tilde{h}$ – the Planck constant, and m – the mass of electron. In this equation, applying Fourier transform:

$$\tilde{\omega}=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}e^{-i\lambda t}\omega\mathrm{d}t$$

It shall transform energy equation dependent on the case:

$$\frac{\tilde{h}^2}{2m}\nabla^2\tilde{\omega}+\tilde{U}\tilde{\omega}=E\tilde{\omega}$$

Whence energy equation in the field with the Coulomb potential transforms:

$$\frac{\tilde{h}^2}{2m}\nabla^2\tilde{\omega}+\left(E+\frac{e^2}{s}\right)\tilde{\omega}=0$$

Replacing hydrogen atom to other potential area, the energy equation is:

$$-\frac{\tilde{h}^2}{2m}\nabla^2\tilde{\omega}+\left[E+\frac{e^2}{s}+q(r,y,z)\right]\tilde{\omega}=0$$

In a consequence of some transformations, we get Sturm-Liouville equation with Coulomb potential:

$$-y'' + \left[\frac{A}{r} + q(r)\right] y = \lambda y \tag{4}$$

where λ is a parameter corresponding to the energy [25].

In this study, the zeros of eigenfunctions of spectral theory are investigated, first and second comparison theorems for fractional Sturm-Liouville problems with their proofs are given. This note will provide an important contribution to develop fractional Sturm-Liouville theory.

In the following section, we get definitions and properties of fractional calculus [9-11, 21, 26].

Preliminaries

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

$$\left(I_{a+}^{\alpha} f\right)(r) = \frac{1}{\Gamma(\alpha)} \int_a^r (r-s)^{\alpha-1} f(s)\,\mathrm{d}s, \quad r > a \tag{5}$$

$$\left(I_{b-}^{\alpha} f\right)(r) = \frac{1}{\Gamma(\alpha)} \int_r^b (s-r)^{\alpha-1} f(s)\,\mathrm{d}s, \quad r < b \tag{6}$$

where Γ denotes the gamma function.

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

$$\left(\mathrm{D}_{a+}^{\alpha} f\right)(r) = \mathrm{D}\left(I_{a+}^{1-\alpha} f\right)(r) \quad r > a \tag{7}$$

$$\left(\mathrm{D}_{b-}^{\alpha} f\right)(r) = -\mathrm{D}\left(I_{b-}^{1-\alpha} f\right)(r) \quad r < b \tag{8}$$

Similar formulas are given for the left- and right-sided Caputo derivatives of order α:

$$({}^{C}\mathrm{D}_{a+}^{\alpha} f)(r) = \left(I_{a+}^{1-\alpha} \mathrm{D} f\right)(r) \quad r > a \tag{9}$$

$$\left({}^{C}\mathrm{D}_{b-}^{\alpha} f\right)(r) = \left[I_{b-}^{1-\alpha}(-\mathrm{D}) f\right](r) \quad r < b \tag{10}$$

Property 3. Let $0 < \alpha < 1$, the fractional differential operators defined in eqs. (5)-(10) satisfy the following identities:

$$\int_a^b f(r)\mathrm{D}_{b-}^{\alpha} g(r)\,\mathrm{d}r = \int_a^b g(r)\,{}^{C}\mathrm{D}_{a+}^{\alpha} f(r)\,\mathrm{d}r - f(r) I_{b-}^{1-\alpha} g(r)\Big|_a^b \tag{11}$$

$$\int_a^b f(r)\mathrm{D}_{a+}^{\alpha} g(r)\,\mathrm{d}r = \int_a^b g(r)\,{}^{C}\mathrm{D}_{b-}^{\alpha} f(r)\,\mathrm{d}r + f(r) I_{a+}^{1-\alpha} g(r)\Big|_a^b \tag{12}$$

$$\int_a^b f(r)\mathrm{D}_{b-}^{\alpha} g(r)\,{}^{C}\mathrm{D}_{a+}^{\alpha} k(r)\,\mathrm{d}r = \int_a^b g(r)\,{}^{C}\mathrm{D}_{a+}^{\alpha} f(r)\,{}^{C}\mathrm{D}_{a+}^{\alpha} k(r)\,\mathrm{d}r - f(r) I_{b-}^{1-\alpha} g(r)\,{}^{C}\mathrm{D}_{a+}^{\alpha} k(r)\Big|_a^b \tag{13}$$

Now, we prove fundamental theorems of Sturm according to the fractional Sturm-Liouville problem, also giving some applications.

Main results

Let us consider the following two fractional Sturm-Liouville boundary value problems:

$$\mathrm{D}_{b-}^{\alpha}p(r)^{C}\mathrm{D}_{a+}^{\alpha}u(r)+g(r)u(r)=0 \tag{14}$$

$$\mathrm{D}_{b-}^{\alpha}p(r)^{C}\mathrm{D}_{a+}^{\alpha}v(r)+h(r)v(r)=0 \tag{15}$$

where $p(r)>0, \forall r\in[a,b]$ and $p(r)$, $g(r)$, and $h(r)$ are real valued continuous functions in interval $[a,b]$ and $\alpha\in(0,1)$.

1st comparison theorem. Suppose that we are given two fractional Sturm-Liouville eqs. (14) and (15).

If $g(r)<h(r)$ over the entire interval $[a,b]$, then between every two zeros of any non-trivial solution of the first equation there is at least one zero of every solution of the second equation.

Proof. Let us multiply eq. (14) by function $v(r)$ and eq. (15) by function $u(r)$ and subtracting, we find:

$$v(r)\mathrm{D}_{b-}^{\alpha}p(r)^{C}\mathrm{D}_{a+}^{\alpha}u(r)+g(r)u(r)v(r)-u(r)\mathrm{D}_{b-}^{\alpha}p(r)^{C}\mathrm{D}_{a+}^{\alpha}v(r)-h(r)v(r)u(r)=0$$

$$v(r)\mathrm{D}_{b-}^{\alpha}p(r)^{C}\mathrm{D}_{a+}^{\alpha}u(r)-u(r)\mathrm{D}_{b-}^{\alpha}p(r)^{C}\mathrm{D}_{a+}^{\alpha}v(r)=\left[h(r)-g(r)\right]v(r)u(r) \tag{16}$$

Let r_1 and r_2 are two consecutive zeros of u. Integrating from r_1 to r_2, we can write the eq. (16):

$$\int_{r_1}^{r_2}v(r)\mathrm{D}_{b-}^{\alpha}p(r)^{C}\mathrm{D}_{a+}^{\alpha}u(r)\mathrm{d}r-\int_{r_1}^{r_2}u(r)\mathrm{D}_{b-}^{\alpha}p(r)^{C}\mathrm{D}_{a+}^{\alpha}v(r)\mathrm{d}r=\int_{r_1}^{r_2}\left[h(r)-g(r)\right]v(r)u(r)\mathrm{d}r$$

Applying property eq. (13) in last equation, we obtain:

$$\int_{r_1}^{r_2}p(r)\,{}^{C}\mathrm{D}_{\alpha+}^{\alpha}v(r){}^{C}\mathrm{D}_{\alpha+}^{\alpha}u(r)\,\mathrm{d}r-v(r)I_{b-}^{1-\alpha}p(r){}^{C}\mathrm{D}_{\alpha+}^{\alpha}u(r)\Big|_{r_1}^{r_2}-$$

$$-\int_{r_1}^{r_2}p(r)\,{}^{C}\mathrm{D}_{\alpha+}^{\alpha}u(r){}^{C}\mathrm{D}_{\alpha+}^{\alpha}v(r)\,\mathrm{d}r+u(r)I_{b-}^{1-\alpha}p(r){}^{C}\mathrm{D}_{\alpha+}^{\alpha}v(r)\Big|_{r_1}^{r_2}=$$

$$=-v(r)I_{b-}^{1-\alpha}p(r){}^{C}\mathrm{D}_{\alpha+}^{\alpha}u(r)\Big|_{r_2}+v(r)I_{b-}^{1-\alpha}p(r){}^{C}\mathrm{D}_{\alpha+}^{\alpha}u(r)\Big|_{r_1}+$$

$$+u(r)I_{b-}^{1-\alpha}p(r){}^{C}\mathrm{D}_{\alpha+}^{\alpha}v(r)\Big|_{r_2}-u(r)I_{b-}^{1-\alpha}p(r){}^{C}\mathrm{D}_{\alpha+}^{\alpha}v(r)\Big|_{r_1}=$$

$$=\int_{r_1}^{r_2}[h(r)-g(r)]v(r)u(r)\,\mathrm{d}r$$

Let us assume that v does not equal to zero anywhere in the interval (r_1,r_2). Without loss of generality, we can assume that $u(r)>0$ and $v(r)>0$ in the interval (r_1,r_2) and $u(r),v(r)$ are increasing functions. Therefore, the right hand side of the equality is positive. But left hand side of the equality is negative for sufficiently large value of $v(r)$ at r_2 point. Then we arrive at a contradiction and this completes the proof.

2nd comparison theorem. Let $u(r)$ be the solution of eq. (14) satisfying the initial conditions:

$$u(a)=1,\quad {}^{C}\mathrm{D}_{a+}^{\alpha}u(r)\Big|_{r=a}=0$$

and $v(r)$ is the solution of eq. (15) satisfying the same initial conditions. Assume $v(r)>0$, $u(r)>0$ and $u(r),v(r)$ are increasing functions. Moreover, suppose that $g(r)<h(r)$ over the entire interval $[a,b]$.

If $u(r)$ has m zeros in the interval $a < r \le b$, then $v(r)$ has not less than m zeros in the same interval and the k^{th} zero of $v(r)$ is less than the k^{th} zero of $u(r)$.

Proof. Let r_1 denote the zero of $u(r)$ closest to the point a. Now let us prove that $v(r)$ has at least one zero in the interval (a,r_1). Assume the contrary, without loss of generality, we may suppose that $v(r) > 0$ and $u(r) > 0$ in the interval (a,r_1), since $u(r_1) = 0$. Integrating the identity of eq. (16) from a to r_1 and apply relation of eq. (13) we obtain:

$$-v(r) I_{b-}^{1-\alpha} p(r)^C \mathrm{D}_{a+}^{\alpha} u(r)\Big|_{r_1} + v(r) I_{b-}^{1-\alpha} p(r)^C \mathrm{D}_{a+}^{\alpha} u(r)\Big|_{a}$$

$$-u(r) I_{b-}^{1-\alpha} p(r)^C \mathrm{D}_{a+}^{\alpha} v(r)\Big|_{a} = \int_a^{r_1} \left[h(r) - g(r) \right] v(r) u(r) \,\mathrm{d}r$$

Since assumption $v(r) > 0$, $u(r) > 0$ and $u(r)$, $v(r)$ are increasing functions in the interval (a,r_1), the left side in the previous equality is negative. But the right side is positive. This case is a contradiction. Hence, the theorem proves.

To make these comparison theorems clearer, we give the following example which includes only Riemann-Liouville fractional derivative.

Application 1. Let us consider two fractional Sturm-Liouville equations having Coulomb potential function:

$$\mathrm{D}^{1/2} y'(r) + \left(\lambda + \frac{1}{r} \right) y(r) = 0, \quad r \in (0,1) \tag{17}$$

$$y'(0) = 0, \quad y(1) = 0$$

and

$$\mathrm{D}^{1/2} y'(r) + \left(\lambda + \frac{1}{2r} \right) y(r) = 0, \quad r \in (0,1) \tag{18}$$

$$y'(0) = 0, \quad y(1) = 0$$

We estimate some zeros of eigenfunctions of fractional Sturm-Liouville problems of eqs. (17) and (18), by using Adomians decomposition method [17]. $\lambda_1 \cong 1.6609$, $\lambda_2 \cong 13.550$, $\lambda_3 \cong 20.514$, and $\mu_1 \cong 1.3705$, $\mu_2 \cong 11.1815$, $\mu_3 \cong 16.927$, respectively. We can see alternating of the zeros in fig. 1 as symbolic.

Application 2. Similary, the following two problems hold:

$$\mathrm{D}^{1/2} y'(r) + \left(\lambda - \frac{r}{2} \right) y(r) = 0, \quad r \in (0,1) \tag{19}$$

$$y'(0) = 0, \quad y(1) = 0$$

$$\mathrm{D}^{1/2} y'(r) + \left(\lambda - \frac{r}{4} \right) y(r) = 0, \quad r \in (0,1) \tag{20}$$

$$y'(0) = 0, \quad y(1) = 0$$

By performing necessary operations and computations, some zeros of eigenfunctions of fractional Sturm-Liouville problems of eqs. (19) and (20) are $\tau_1 \cong 40.3159$, $\tau_2 \cong 41.3390$, $\tau_3 \cong 42.4065$, $\tau_4 \cong 43.5211$, $\tau_5 \cong 44.6858$ and $\eta_1 \cong 39.8529$, $\eta_2 \cong 40.7157$, $\eta_3 \cong 41.6101$, $\eta_4 \cong 42.5378$, $\eta_5 \cong 43.9955$.

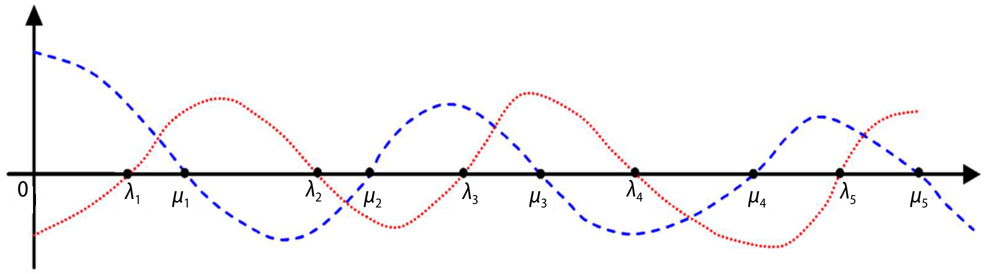

Figure 1. The alternating zeros of eigenfunctions (symbolic graph)

Conclusion

As known Sturm comparison theorems are crucial in classical spectral theory. Because, these theorems play an important role in the proof of oscillation theorem which is one of the most important theorems in spectral theory. In this regard, to move these important results to fractional calculus, we give the proof of classical Sturm comparison theorems in fractional case under certain conditions. This study will be an important step for the proof of the oscillation theorem in fractional case.

Acknowledgment

This paper includes a part of Ph.D thesis data of Funda Metin Turk.

References

[1] Akano, T. T., Fakinlede, O. A., Numerical Computation of Sturm-Liouville Problem with Robin Boundary Condition, *International Journal of Mathematical and Computational Sciences*, *9* (2015), 11, pp. 690-694
[2] Johnson, R. S., *An introduction to Sturm-Liouville theory*, University of Newcastle, Newcastle, UK, 2006
[3] Zettl, A., *Sturm-Liouville Theory*, Mathematical Surveys and Monographs, American Mathematical Society, Providence, R. I., USA, 2005
[4] Amrein, W. O., *et al*., *Sturm-Liouville Theory: Past and Present*, Birkhauser, Basel, Switzerland, 2005
[5] Levitan, B. M., Sargsjan, I. S., *Introduction to Spectral Theory: Self adjoint Ordinary Differential Operators*, American Math. Soc. Providence, R. I., USA, 1975
[6] Panakhov, E. S., On the Determination the Differential Operator Pecularity in Zero, *VINITI*, *4407-80* (1980), pp. 1-16
[7] Hilfer, R., *Applications of Fractional Calculus in Physics*, World Scientific, Singapore, 2000
[8] Carpinteri, A., Mainardi, F. , *Fractals and Fractional Calculus in Continum Mechanics* (Ed. A., Carpinteri, F. Mainardi), Telos: Springer-Verlag, Berlin, 1998
[9] Podlubny, I., *Fractional Differential Equations*, Academic Press, San Diego, Cal., USA, 1999
[10] Samko, S. G., *et al*., *Fractional Integrals and Derivatives: Theory and Applications*, Gordon and Breach, Philadelphia, Penn., USA, 1993
[11] Miller, K. S., Ross, B., *An Introduction to the Fractional Calculus and Fractional Differential Equations*, John Wiley and Sons, New York, USA, 1993
[12] Baleanu, D., *et al*., Asymptotic Integration of (1+Alpha)-Order Fractional Differential Equations, *Computers & Mathematics with Applications*, *62* (2011), 3, pp. 1492-1500
[13] Abolhassan, R., *et al*., Conditional Optimization Problems: Fractional Order Case, *Journal of Optimization Theory and Appl*., *156* (2013), 1, pp. 45-55
[14] Baleanu, D., Guo-Cheng, W., New Applications of the Variational Iteration Method-From Differential Equations to Q-Fractional Difference Equations, *Advances in Difference Eq.*, *21* (2013), Dec., pp. 1-16
[15] Said Grace, R., *et al*., On the Oscillation of Fractional Differential Equations, *Frac. Calc. App. Anal.*, *15* (2012), 2, pp. 222-231

[16] Klimek, M., *On Solutions of Linear Fractional Differential Equations of a Variational Type*, The Publishing Office of Czestochowa University of Technology, Czestochowa, Poland, 2009
[17] Al-Mdallal, Q. M., An Efficient Method for Solving Fractional Sturm-Liouville Problems, *Chaos, Solitons & Fractals*, *40* (2009), 1, pp. 183-189
[18] Klimek, M., Argawal, O. P., Fractional Sturm-Liouville Problem, *Computers and Mathematics with Applications*, *66* (2013), 5, pp.795-812
[19] Bas, E., Fundamental Spectral Theory of Fractional Singular Sturm-Liouville Operator, *Journal of Function Spaces and Applications*, *2013* (2013), ID 915830
[20] Erturk, V. S., Computing Eigenelements of Sturm-Liouville Problems of Fractional Order via Fractional Differential Transform Method, *Mathematical and Computational Applications*, *16* (2011), 3, pp. 712-720
[21] Klimek, M., Argawal, O. P., On a Regular Fractional Sturm-Liouville Problem with Derivatives of Order in (0,1), *Proceeding*, 13th Int. Cont. Conf., Tatry, Slovakia, 2012
[22] Bas, E., Metin, F., Fractional Singular Sturm-Liouville Operator for Coulomb Potential, *Advances in Differences Equations,* (2013), On-line first, https://doi:10.1186/1687-1847-300-2013
[23] Bas, E., Metin, F., Spectral Analysis for Fractional Hydrogen Atom Equation, *Advances in Pure Mathematics*, *5* (2015), Nov., pp. 767-773
[24] Bas, E., Ozarslan, R., Sturm-Liouville Problem via Coulomb Type in Difference Equations, *Filomat 31* (2017), 4, pp. 989-998
[25] Blohincev, D. I., *Foundations of Quantum Mechanics*, GITTL, Moscow, 1949
[26] Kilbas, A. A., *et al*., *Theory and Applications of Fractional Differential Equations*, Elsevier, Amsterdam, The Netherlands, 2006

Paper submitted: June 12, 2017
Paper revised: November 10, 2017
Paper accepted: November 20, 2017