EVOLUTION OF BOUND AND SCATTERING STATES IN FRACTIONAL HEAVISIDE STEP-DIRAC DELTA FUNCTION POTENTIALS

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Fractional calculus is used to introduce intermediate potential wells between the attractive Dirac delta function and the negative potential step. Schrodinger equation is solved numerically to obtain solutions for bound states and scattering states. The ground states and their eigen energies evolve until they coincide with bound state for the Dirac delta potential as the intermediate potential evolves into the Dirac delta function potential. For scattering states, the transmission coefficients were obtained and shown to agree with the value of the potential step and then increases to one as the intermediate potential takes the shape of the Dirac delta potential. The disagreement between the transmission coefficients for Dirac delta function and the corresponding intermediate potential was explained by examining the continuity of the derivative of the wave function across the intermediate potentials.

Key words: fractional calculus; potential wells; scattering; bound states

1. Introduction

Fractional calculus has been applied to study the evolution of different phenomena in physics [1]-[7]. For example Engheta [1] introduced fractional order electric multipoles that can serve as intermediate sources between integer order point multipoles. Rousan *et al* [2] used similar approach to study the evolution of the gravitational fields from a point mass to semi-infinite linear mass distribution. Different groups [4]-[7] studied electrical circuits and developed fractional differential equations that can combine multiple circuits simultaneously.

On the other hand, the potential well has been used as a model to solve quantum physical problems in nuclear, atomic, condensed matter physics and others. The well-known example in condensed matter is the Kronig- Penny Model which explains the existence of energy bands in solid materials [8]. The effect of the potential wells and potential barriers get much interest in the scattering theory

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[9]. Solving the time independent Schrodinger equation for such potentials provides information about the quantum states of the particles, and hence more understanding of the realistic potential it models.

Recently, fractional calculus was introduced to quantum mechanics by the pioneer work of Laskin who presented the term fractional Schrödinger equation [10]. Principally, the time derivative can be generalized to non- integer order leading to time fractional Schrodinger equation [11] or by varying the space derivative to non-integer order leading to space fractional Schrodinger equation [12]-[13] or by varying both leading to Space–time fractional Schrödinger equation [14]-[16]. Different potential wells were proposed using the fractional Schrödinger equation such as the Dirac delta function wells [17]-[20]. Therefore, the fractional derivative concept can be aimed to generate the evolution of quantum states and their eigen energies as the derivative admits non-integer values.

In this work we will apply the fractional calculus to vary the nature of potentials rather than the time or the space derivatives. We will start from a negative potential step where no bound states exist and vary this potential to approach the attractive Dirac delta function potential where only one bound state exists. This approach will generate the evolution of the bound states and their energies and it will give us new perspective about the behavior of the scattering states.

2. Fractional Heaviside step-Dirac delta function Potentials

The mathematical form of the attractive Dirac delta function potential can be expressed as follows:

$$U(x) = -U_0 x_0 \delta(x) \tag{1}$$

where $x_0 = 1$, is introduced for the purpose of dimensionality since the delta function has the unit of (1/x). This potential allows only one bound state given by [21]:

$$\psi(x) = \frac{\sqrt{mU_0 x_0}}{\hbar} \text{Exp}(\frac{-mU_0 x_0 |x|}{\hbar^2}) \tag{2}$$

with the corresponding energy of

$$E = -\frac{m(U_0 x_0)^2}{2\hbar^2} \tag{3}$$

On the other hand, the negative Heaviside step potential, which is basically a potential drop, is given by:

$$U(x) = -U_0 H(x) \tag{4}$$

This potential does not allow any bound state.
Recalling that the derivative of the Heaviside step function gives the Dirac delta function, therefore, we anticipate that the fractional derivative of the step potential which is equivalent to the fractional integral of the Dirac delta function would yield an intermediate potential. This potential can be expressed mathematically as

follows:

$$U_\alpha(x) = \frac{d^\alpha}{d(x-a)^\alpha}[-U_0 H(x)] = -U_0 x_0^\alpha \frac{d^{\alpha-1}}{d(x-a)^{\alpha-1}} \delta(x) =$$
$$-U_0 x_0^\alpha \frac{x^{-\alpha}}{\Gamma(1-\alpha)} \quad , \quad x > 0 \quad\quad (5)$$

where $a < 0 < x$, and $0 < \alpha < 1$, it is evident that for $\alpha = 0, U_\alpha(x)$ reduces to the step potential and for $\alpha = 1, U_\alpha(x)$ reduces to Dirac potential.

In the above expression, we have used the fact that the fractional derivative of a constant is given by [22]:

$$\frac{d^\alpha}{d(x-a)^\alpha}(C) = C\frac{x^{-\alpha}}{\Gamma(1-\alpha)} \quad\quad (6)$$

Here $a < x$, as a result of that the fractional derivative of zero is zero. Therefore,

$$U_\alpha(x) = 0, \ x \leq 0 \quad\quad (7)$$

Based on this, Schrodinger equation can be expressed as follows:

$$\frac{-\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) - U_0 x_0^\alpha \frac{x^{-\alpha}}{\Gamma(1-\alpha)}H(x)\psi(x) = E\psi(x) \quad\quad (8)$$

This equation cannot be solved analytically for an arbitrary value of α, therefore, we will solve it numerically using shooting method in Mathematica 8. The boundary conditions for bound states necessitate that the wave function and its derivative must vanish at both ends away from the potential.

For scattering states, it is important to check the continuity of the derivative of the wave function at x = 0 where there is a discontinuity in the potential. Typically, the continuity is checked by directly integrating Schrodinger equation over an infinitesimal distance around the boundary points. For our case this can be done as follows:

$$\int_{-\epsilon}^{+\epsilon}\frac{d^2}{dx^2}\psi(x)dx = \frac{2m}{\hbar^2}\int_{-\epsilon}^{+\epsilon}(U(x) - E)\psi(x)\,dx \quad\quad (9)$$

where ϵ goes to zero. The left hand side gives the change in the first derivative of the wave function around zero. The second term in the right hand side always gives zero since the wave function must be finite. For a finite potential such as the potential drop, the first term in the right hand side is also zero and therefore, the derivative of the wave function is continuous.

For the Dirac potential, the integration is straightforward using Dirac delta function properties and gives:

$$\Delta[\frac{d}{dx}\psi(x)] = -\frac{2mU_0}{\hbar^2}\psi(0) \qu\quad (10)$$

Therefore, the derivative suffers from a discontinuity at the boundary. Finally, for the intermediate potential we get:

$$\Delta\left[\frac{d}{dx}\psi(x)\right] = \frac{2m}{\hbar^2}\int_{-\epsilon}^{+\epsilon}U_\alpha(x)\psi(x)\,dx = -\frac{2m}{\hbar^2}\int_0^{+\epsilon}U_0 x_0^\alpha \frac{x^{-\alpha}}{\Gamma(1-\alpha)}\,\psi(x)\,dx \quad\quad (11)$$

Since the potential does not change sign and the wave function must be

continuous then based on the mean value theorem for integrals $\psi(x)$ can be taken outside the integration and replaced by $\psi(\xi)$ where $\xi \in (0, \epsilon)$ [23] then we get:

$$\Delta \left[\frac{d}{dx} \psi(x) \right] = \frac{-2m\psi(\xi)}{\hbar^2} U_0 x_0^\alpha \frac{\epsilon^{1-\alpha}}{(1-\alpha)\Gamma(1-\alpha)} \tag{12}$$

It is clear that when ϵ goes to zero the right hand side must vanish for any $0 < \alpha < 1$ and hence the derivative of the wave function is continuous for all intermediate potentials. It is worth mentioning here that only at the limit when $\alpha = 1$, the derivative suffers discontinuity since the intermediate potential in this case is the Dirac delta potential.

3. Results and Discussion

For the sake of simplicity, we will assume that $U_0 = 1$, and $2m/\hbar^2 = 1$, therefore, the energy is given in the units of $2m/\hbar^2$. This is equivalent to scale x by the factor $(\hbar^2/2m)^{0.5}$ which is also one.

Fig. 1 shows the fractional potentials for different values of α. It shows as α goes to one, the potential dies off quickly and reduces to the shape of the Dirac delta function. For example, when $\alpha = 0.99$, the depth of the potential drops from infinite value to -0.1 just by moving to $x = 0.1$. On the other hand, when α goes to zero the potential rapidly saturates to -1 and almost does not change even for relatively large values of x. For instance, when $\alpha = 0.01$, the potential reaches -1 just by moving to $x = 0.01$. For the intermediate values of α, we see that the fractional potential gradually grows from the shape of the step function to the shape of the Dirac delta function as α varies from 0 to 1.

We have solved Schrodinger equation for different values of α. Our result for the normalized ground state wave functions is shown in **Figure** 2. As α goes to one, the wave functions become steeper and its maxima shift to the left towards zero and its shape becomes more symmetric. This tendency is expected since the fractional potential itself sharpens and becomes more symmetric as α goes to one. This overall behavior describes the evolution of the wave function into the bound state of the Dirac delta potential. This resemblance is very close when $\alpha = 0.99$ at which the peak height is 0.703 where the peak height for the bound state of the Dirac delta potential is 0.707. In terms of symmetry, as α goes to one, the probability of finding a particle trapped in this potential increases gradually for < 0 , and decreases on the other side until it reaches 50.50% at $\alpha = 0.99$ and this is very close to 50% at either side of x which is the case for the bound state of the Dirac delta potential.

Moreover, when α goes to zero, the ground state wave function expands and its center shifts to the right away from zero. This will reduce the probability for position enormously for $x < 0$. For example at $\alpha = 0.01$, the probability

decreases to less than 0.04% on the negative side of x and that is in some way little closer to the scattering state behavior which is characteristic for the step function potential.

Fig. 3 shows (red dots) the energy of the ground state versus α. As α goes to one the energy increases until it coincides with the energy of the bound state for the Dirac delta function which is -0.25, and that shows one more time the evolution process of the wave function.

In contrast, as α goes to zero the energy goes to -1 which basically is the depth of the potential drop and that is expected since the fractional potential progressively takes the shape of a negative step function. Furthermore, we have fitted these data (**Fig.** 3 blue line) with the following relation:

$$E_\alpha = -0.25 + 0.72U_\alpha(10) = -0.25 - \frac{0.72 \times 10^{-\alpha}}{\Gamma(1-\alpha)} \tag{13}$$

In this relation the first term is the bound state energy for Dirac delta function, and the second is the variation term proportional to the potential energy at $x = 10$, where the wave function mostly vanishes. Even though this formula is very simple, it fits the data very well. When $\alpha = 1$, it gives $E_\alpha = -0.25$, as it should be and when $\alpha = 0$, it gives $E_\alpha = -0.97$ where it is supposed to give -1. This deviation can be explained in the view of the fact that the wave function vanishes at a distance greater than 10 as α approaches zero.

Finally, we will investigate the scattering states where the energy can take any positive value. We picked $E = 0.5$ for our study since it is comparable to the depth of the potential drop.

For the negative potential step, the transmission coefficient for a beam of particles coming from left is given by:

$$T = \frac{4\sqrt{E(E+U_0)}}{\left(\sqrt{E}+\sqrt{E+U_0}\right)^2} = 0.928 \tag{14}$$

And the transmission coefficient for the case of the Dirac delta function is given by [21]:

$$T = \left(1 + \frac{mU_0^2 x_0^2}{2\hbar^2 E}\right)^{-1} = 0.667 \tag{15}$$

Fig. 4, shows the transmission coefficients for the case of the fractional potentials. It is obvious that when α goes to zero the transmission probability agrees with the case for the potential drop. For instance when $\alpha = 0.001, T = 0.928$. However, when α goes to one the transmission coefficient goes to one in disagreement with the case for Dirac potential. The reason for this is that even though the fractional potential takes the shape of the Dirac potential when α goes one, the fractional potential does not cause a discontinuity in the derivative of the wave function. That is in contrast to the case of the Dirac potential as shown previously. Therefore, care must be taken whenever Dirac potential is employed for approximation purposes.

When α is close to zero, the fractional potential well is basically a potential drop as shown before and the transmission probability coincides with its expected value. As α increases the width of the well decreases and that causes the transmission probability to oscillate. Such behavior has been noticed in the rectangular potential well [21]. The oscillatory behavior persists as far as the width of the well is finite, that is $\alpha \neq 1$. As α approaches one, the well becomes very narrow and that raises the transmission coefficient to one. Only at the limit when $\alpha = 1$, the width of the well is truly zero and the well in this case is the Dirac potential well and therefore the transmission probability falls down to 0.667.

4. Conclusion

In this work we have applied the idea of evolution using fractional calculus on transforming the Heaviside step potential through intermediate steps into Dirac delta potential. The evolution of the correlated wave functions and their corresponding energies were studied by solving the time independent Schrodinger equation numerically for bound and scattering states. The transformation of the ground state wave functions for the intermediate potentials into the bound state of the Dirac delta function was demonstrated. The gradual change in the transmission coefficient was observed for the intermediate potentials from the value of the step potential to one. We explained the disagreement between the transmission coefficient for the Dirac potential and the corresponding intermediate potential by studying the derivative of the wave function. We showed that the derivative of wave function for the intermediate potential is always continuous in contrast to the discontinuity in the case of the Dirac potential. Therefore, care must be taken whenever Dirac delta function is used for approximation purposes.
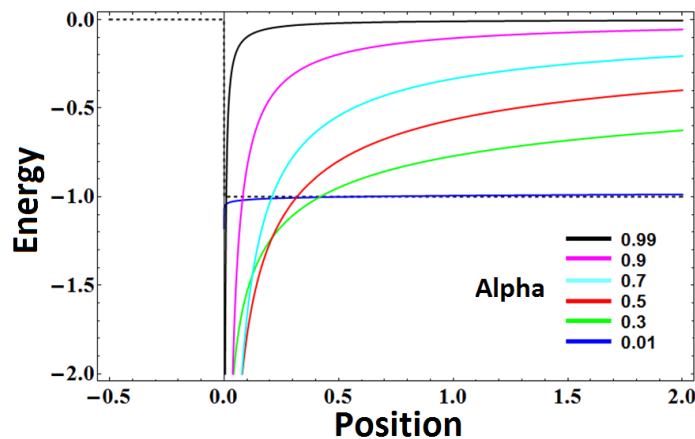

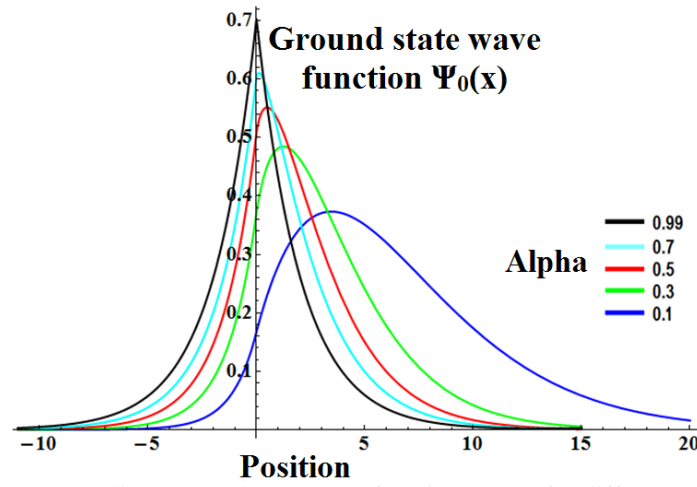Fig. 1: The Fractional Heaviside step-Dirac delta function Potentials for different values of α

Fig. 2: The normalized ground state wave functions $\Psi_0(x)$ for different values of α
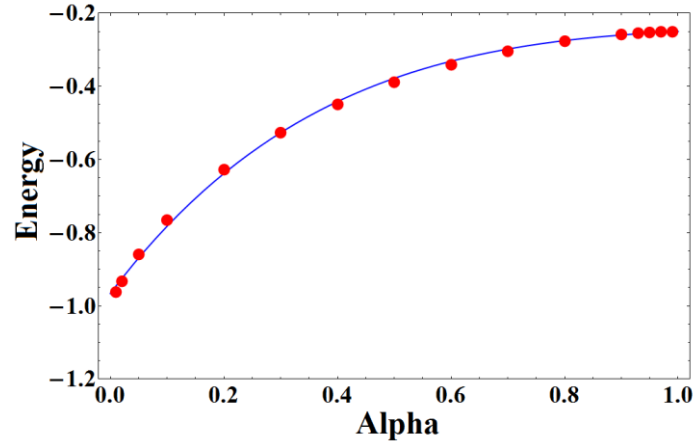

Fig. 3: The ground states eigen energies for different values of α (in red dots) and the fitting curve (in blue).
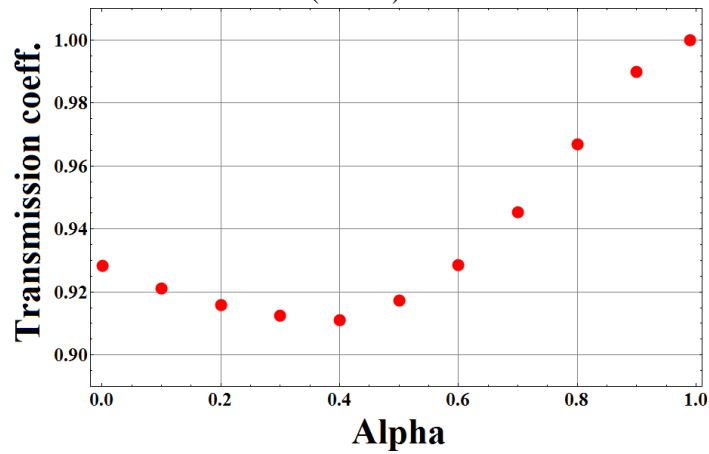

Fig. 4: The transmission coefficients for different values of α

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[1] *N. Engheta*, On Fractional Calculus and Fractional Multipoles in Electromagnetism. IEEE Trans. Antennas Propagat., **44**, No 4 (1996), 554-566.

[2] *Akram A. Rousan, E. Malkawi, E. Rabei and H. Widyan*, Applications of Fractional Calculus to Gravity. Fractional Calculus & Applied Analysis. **5**, No. 2 (2002), 155-168.

[3] *A. A. Rousan, N.Y. Ayoub and Kh. Khasawinah*, Fractional simple harmonic oscillator. Intern. J. Appl. Math. **19** (2006), 263–276.

[4] *A.A. Rousan, N.Y. Ayoub, F.Y. Alzoubi, H. Khateeb, M. Al-Qadi, M.K. Hasan (Qaseer), B.A. Albiss,* A fractional LC-RC circuit. Fract. Calc. Appl. Anal. **9**, No 1 (2006), 33–41.

[5] *Gómez-Aguilar José Francisco, Rosales-García Juan, Guía-Calderón Manuel, Razo-Hernández José Roberto*, Fractional RC and LC Electrical Circuits, Ingeniería, Investigación y Tecnología, **15**, No 2 (2014), 311-319.

[6] *A. Obeidat, M. Gharaibeh, M. Al-Ali, A. Rousan*, Evolution of a current in a resistor. Fract. Calc. App. Anal. **14,** No 2 (2011),), 247–259.

[7] *Alsaedi, A., et al.,* Fractional electrical circuits, Advances in Mechanical Engineering, **7** No 12 (2015),1-7

[8] *C. Kittle*, Introduction to Solid State Physics, John Wiley & Sons, Inc., New York, 7th Ed., (1996),173.

[9] *E. Merzbacher*, Quantum Mechanics, John wiley & Sons, Inc. New York, 3rd Ed. (1998), 278.

[10] *N. Laskin*, Fractional quantum mechanics and L´evy path integrals, Physics Letters A, **268,** No.4–6 (2000), 298–305.

[11] *M. Naber*, Time fractional Schr¨odinger equation, Journal of Mathematical Physics, **45**, No. 8 (2004), 3339–3352.

[12] *N. Laskin*, Fractional quantum mechanics, Physical Review E, **62**, No. 3 (2000),3135–3145.

[13] *N. Laskin*, Fractional Schr¨odinger equation, Physical Review E **66**, No. 5 (2002),7.

[14] *R. K. Saxena, R. Saxena, and S. L. Kalla,* Solution of spacetime fractional Schr¨odinger equation occurring in quantum mechanics, Fractional Calculus & Applied Analysis **13**, No. 2 (2010), 177–190.

[15] *S. Wang and M. Xu*, Generalized fractional Schr¨odinger equation with space-time fractional derivatives, Journal of Mathematical Physics **48**,No. 4 (2007), 10

[16] *X. Y. Jiang,* Time-space fractional Schr¨odinger like equation with a nonlocal term, European Physical Journal: Special Topics, **193**, No. 1 (2011), 61–70.

[17] *S Kondej and J Vaz,* Fractional Schrodinger operator with delta potential localized on circle J. Math. Phys. **53** (2012) 33503.

[18] *E. C. Oliveira, F. S. Costa, and J. Vaz Jr.,* The fractional Schr¨odinger equation for delta potentials, Journal of Mathematical Physics, vol. **51**, No. 12 (2010), 16.

[19] *S. Muslih*, Solutions of a particle with fractional [delta]-potential in a fractional dimensional space, International Journal of Theoretical Physics **49** (9) (2010) 2095–2104.

[20] *Y. Luchko*, Fractional Schrödinger equation for a particle moving in a potential well J. Math. Phys. **54** (2013), 012111.

[21] *D. J. Griffiths*, Introduction to Quantum Mechanics, Pearson Prentice Hall, Upper Saddle River, 2nd Ed., 2005, Ch 2, P 68, 82.

[22] *Oldham, K.B., and J. Spanier*, The Fractional Calculus. Academic Press, New York (1974),Ch4,P 61

[23] *R. G. Bartle*, A Modern Theory of Integration, American Mathematical Soc., Rhode Island (2001),Vol. 32, P 193