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An iteration algorithm for the time-independent fractional Schrödinger equation with Coulomb potential

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Abstract. A numerical formula is derived which gives solutions of the fractional Schrödinger equation in time-independent form in the case of Coulomb potential using Riemann–Liouville definition of the fractional derivative and the quadrature methods. The formula is applied for electron in the nucleus field for multiple values of fractional parameter of the space-dependent fractional Schrödinger equation and for each value of the space-dependent fractional parameter, multiple values of energies are applied. Distances are found at which the probability takes its maximum value. Values of energy obtained in this study corresponding to the maximum value of probability are compared with the energy values resulted from the fractional Bohr's atom formula in the fractional quantum mechanics.

Keywords. Fractional Schrödinger equation; Liouville–Riemann definition; Coulomb potential; fractional parameter; fractional Bohr's atom formula.

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1. Introduction

The most important equation in quantum mechanics in its fractional formalism is the fractional Schrödinger equation and this fractional equation has two forms in the linear form. The first form of this equation is called the space-dependent or the space-fractional Schrödinger equation, which is the focus of this work, and the other is the time-dependent or the time-fractional Schrödinger equation. Both equations are derived from the general fractional Schrödinger equation which is given by

$$K_\beta^T \frac{\partial^\beta \Psi(\mathbf{r},t)}{\partial t^\beta} = \hat{H}_\alpha \Psi(\mathbf{r},t), \tag{1}$$

where α, β are respectively the fractional Schrödinger equation parameters in the space-dependent form and the time-dependent form ($1 < \alpha \leq 2$ and $0 < \beta \leq 1$), $\Psi(\mathbf{r},t)$ is the wave function of the system in the space formalism, K_β^T is a moderate parameter and $\hat{H}_\alpha$ is the fractional Hamiltonian operator. We get fractional Schrödinger equation in space form from the previous equation if we put $\beta = 1$. So the space-dependent fractional Schrödinger equation is given by the following equation [1–21]:

$$\hat{H}_\alpha \Psi(\mathbf{r},t) = i\frac{h}{2\pi}\frac{\partial \Psi(\mathbf{r},t)}{\partial t}. \tag{2}$$

Here h is the Planck constant, $i = (-1)^{1/2}$ and the fractional Hamiltonian operator is defined by the following formula:

$$\hat{H}_\alpha = \sigma_\alpha \left[-\left(\frac{h}{2\pi}\right)^2 \mathbf{\Delta}\right]^{\alpha/2} + V(\mathbf{r}), \tag{3}$$

where $V(\mathbf{r})$ is the interaction potential of the system, σ_α is a parameter and the space fractional operator is given by [1–7]

$$\left[-\left(\frac{h}{2\pi}\right)^2 \mathbf{\Delta}\right]^{\alpha/2} \Psi(\mathbf{r},t) = \frac{1}{h^3}\int \mathrm{d}^3\Pi \mathrm{e}^{i\frac{\Pi \mathbf{r}}{\hbar}} |\Pi|^\alpha \Theta(\Pi,t), \tag{4}$$

where $\Theta(\Pi,t)$ is the momentum representation's wave function corresponding to the space representation's

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wave function by Fourier transforms and Π is the linear momentum.

A few analytical and numerical solutions of some cases of the space-dependent fractional Schrödinger equation for some important potentials were proposed in [1–3,7,8,12]. There are many other applications of fractional Schrödinger equation in the space-dependent formalism of the equation such as expanding the equation to study solitons in the non-linear form by using the rational function method and the lump solutions with higher-order rational dispersion relations [5,6,22–28] in addition to the study of linear waves from the linear partial differential equations with lump solutions [29]. In this work, we represent a numerical solution for the fractional Schrödinger equation in the space-dependent form for the Coulomb's potential in one dimension. There are two studies about this case, the first is done by Laskin [1] about the fractional Bohr's atom and the other is related to this case and is done by Jianping Dong and Mingyu Xu [2]. We focus on the one-dimensional form of the space-fractional Schrödinger equation for Coulomb potential and this form, in general, is given by

$$i\frac{h}{2\pi}\frac{\partial\Psi(r,t)}{\partial t} = V(r)\Psi(r,t) - \sigma_\alpha\left(\frac{h}{2\pi}\nabla\right)^\alpha \Psi(r,t). \tag{5}$$

As it is known, the Coulomb's potential for the two electric charges in the MKSA unit system is given by

$$V(r) = \frac{1}{4\pi\varepsilon_0}\frac{q_1q_2}{r}, \tag{6}$$

where ε_0 is the permittivity of free space and q_1, q_2 are the first electric charge and the second electric charge respectively. The Coulomb potential is an important potential like many other potentials in fractional quantum mechanics.

2. The method

We write the space-dependent fractional Schrödinger equation for Coulomb's potential by merging eqs (5) and (6) as

$$i\frac{h}{2\pi}\frac{\partial\Psi(r,t)}{\partial t} = \frac{1}{4\pi\varepsilon_0}\frac{q_1q_2}{r}\Psi(r,t) - \sigma_\alpha(\hbar\nabla)^\alpha\Psi(r,t). \tag{7}$$

As Coulomb's potential does not depend on time, we write a solution for eq. (7) as follows:

$$\Psi(r,t) = R(r)\mathrm{e}^{-i\frac{2\pi Et}{h}} \tag{8}$$

which leads to the time-dependent form of the fractional Schrödinger equation and this form is given as follows:

$$\hat{H}_\alpha R(r) = E_\alpha R(r) \tag{9}$$

or by the following form for Coulomb's potential:

$$\sigma_\alpha(\hbar\nabla)^\alpha R(r) - \frac{q_1q_2}{4\pi\varepsilon_0}\frac{R(r)}{r} + E_\alpha R(r) = 0, \tag{10}$$

where $R(r)$ is the eigenvector of the space-fractional Hamiltonian operator and E_α is the eigenvalue of the same operator. When we use the mid-point formula and the right definition of Riemann–Liouville fractional derivatives [19–21], we find the following iteration formula for the wave function in the stationary state:

Table 1. Absolute values of wave function for α = 1.95.

r/a_0	R_1	R_2	R_3	R_4	R_5
3.0000E-05	4.6191E-11	4.4925E-11	4.4697E-11	4.4618E-11	4.4583E-11
7.0000E-05	6.4957E-08	6.3178E-08	6.2857E-08	6.2747E-08	6.2696E-08
1.5000E-04	4.0824E-05	3.9706E-05	3.9505E-05	3.9436E-05	3.9404E-05
3.1000E-04	1.2438E-02	1.2098E-02	1.2037E-02	1.2015E-02	1.2006E-02
6.3000E-04	1.9013E+00	1.8495E+00	1.8401E+00	1.8369E+00	1.8354E+00
1.2700E-03	1.4815E+02	1.4414E+02	1.4342E+02	1.4317E+02	1.4305E+02
2.5500E-03	5.9298E+03	5.7712E+03	5.7426E+03	5.7328E+03	5.7283E+03
5.1100E-03	1.2234E+05	1.1915E+05	1.1858E+05	1.1838E+05	1.1829E+05
1.0230E-02	1.3029E+06	1.2707E+06	1.2649E+06	1.2629E+06	1.2620E+06
2.0470E-02	7.1625E+06	7.0052E+06	6.9766E+06	6.9667E+06	6.9622E+06
4.0950E-02	2.0298E+07	1.9963E+07	1.9902E+07	1.9880E+07	1.9871E+07
8.1910E-02	2.9552E+07	2.9389E+07	2.9357E+07	2.9346E+07	2.9341E+07
1.6383E-01	2.1950E+07	2.2314E+07	2.2379E+07	2.2401E+07	2.2412E+07
3.2767E-01	8.2033E+06	8.7078E+06	8.8030E+06	8.8360E+06	8.8512E+06
6.5535E-01	1.5031E+06	1.7346E+06	1.7814E+06	1.7979E+06	1.8055E+06
1.3107	1.2895E+05	1.7404E+05	1.8434E+05	1.8808E+05	1.8982E+05

Table 2. Absolute values of wave function for $\alpha = 1.50$.

$r/a_0 \times 10^{-9}$	R_1	R_2	R_3	R_4	R_5
1.0000E-05	6.56E-09	5.70E-09	5.61E-09	5.58E-09	5.58E-09
3.0000E-05	8.35E-07	7.25E-07	7.13E-07	7.10E-07	7.09E-07
7.0000E-05	3.50E-05	3.04E-05	2.99E-05	2.98E-05	2.97E-05
1.5000E-04	0.00097	0.000843	0.000829	0.000826	0.000824
3.1000E-04	0.018383	0.015978	0.015714	0.015649	0.015625
6.3000E-04	0.242249	0.210671	0.207197	0.206338	0.206031
1.2700E-03	2.238065	1.948311	1.916381	1.908483	1.905658
2.5500E-03	14.54594	12.68868	12.4833	12.43248	12.41429
5.1100E-03	66.56175	58.30136	57.38138	57.1535	57.07195
1.0230E-02	214.1603	189.1235	186.293	185.5905	185.339
2.0470E-02	482.4997	433.0869	427.3103	425.8703	425.3541
4.0950E-02	754.5482	699.4645	692.4156	690.6378	689.9985
8.1910E-02	805.0785	794.9868	792.1698	791.4075	791.1283
1.6383E-01	567.6333	632.9712	639.0322	640.4698	640.9777
3.2767E-01	250.2497	349.891	362.4916	365.6379	366.7657
6.5535E-01	63.35275	131.9743	143.81	146.9107	148.0372
1.3107E+00	8.242929	32.89635	39.48124	41.35318	42.04919

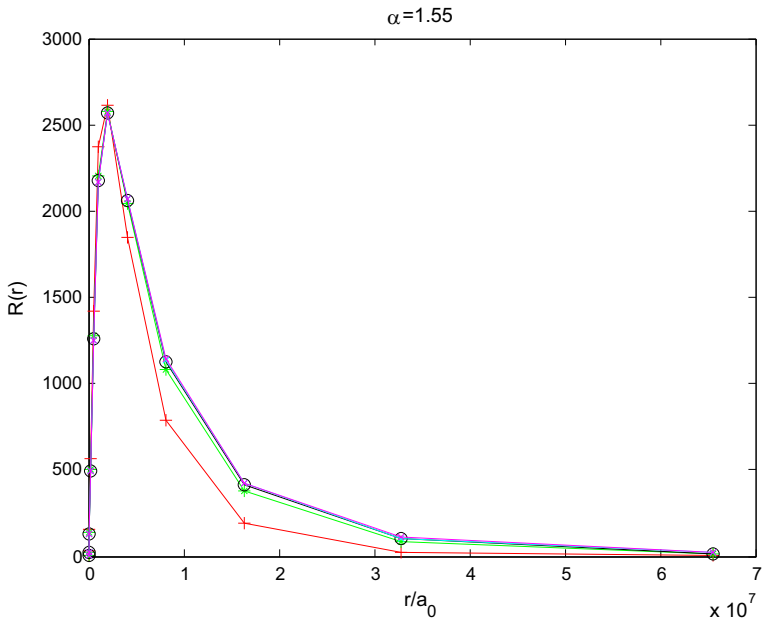

Figure 1. Amplitude of wave function vs. distance (in Bohr's radius unit) for $\alpha = 1.55$.

$$R(r_{n+1}) \approx \frac{2\pi C_\alpha \varepsilon_0}{\Delta r}\Gamma^{-1}(2-\alpha)\left[\left(\frac{\Delta r}{2}\right)^{2-\alpha} R(r_n) + r_n^{-1}\Delta r\left(-\frac{r_n}{2}\right)^{2-\alpha} R\left(\frac{r_n}{2}\right)\right] \times [\pi\varepsilon_0(r_n+\Delta r)E_\alpha - 2^{-2}q_1q_2]^{-1}. \quad (11)$$

The previous numerical formula that we derived is applied to find solutions of the time-independent fractional Schrödinger equation in the systems that interact through the simple Coulomb's potential in one dimension, i.e. finding the time-independent wave function values. We can apply eq. (8) to find and calculate the full wave function. The iteration formula is applied for the fractional parameter of the space-dependent form of the fractional Schrödinger equation values in the interval $1 < \alpha < 2$.

3. Results and discussion

3.1 *The computational information*

We used MATLAB software to code the derived iteration formula for multiple values of space-dependent

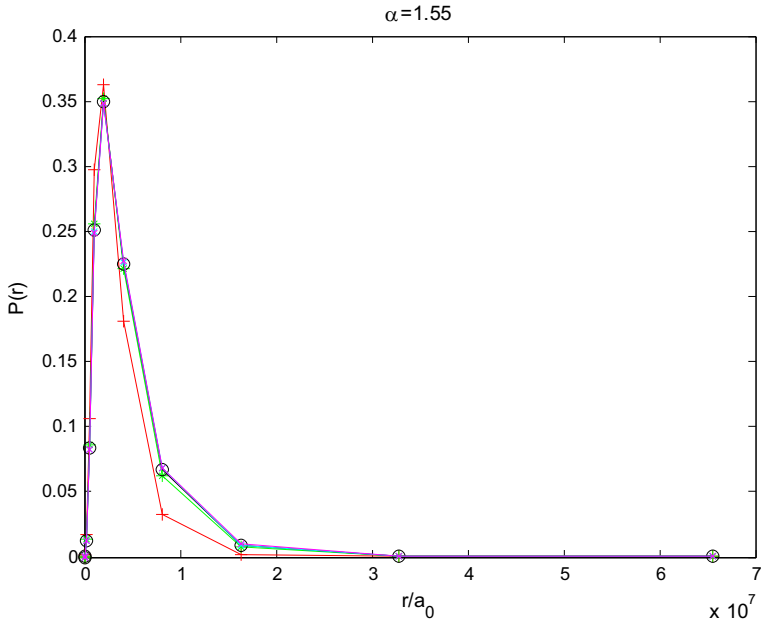

Figure 2. Probability vs. distance (in Bohr's radius unit) for $\alpha = 1.55$.

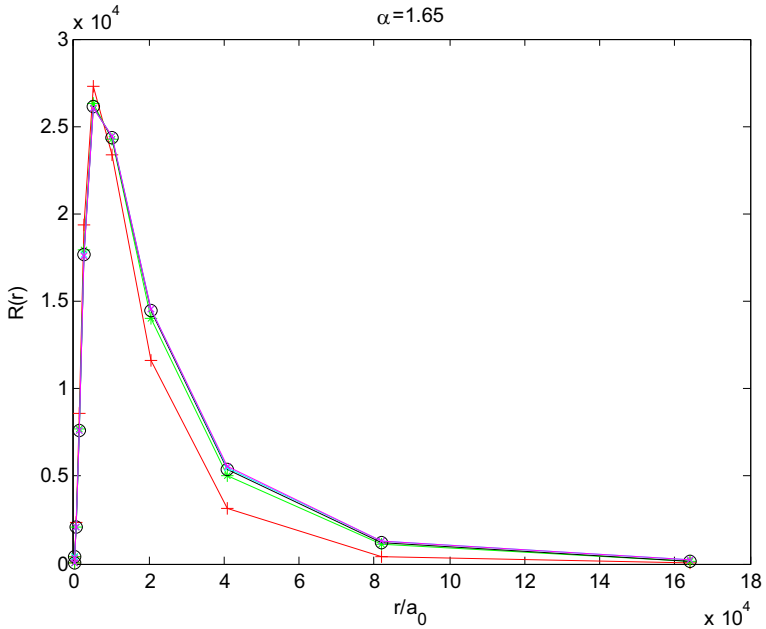

Figure 3. Amplitude of wave function vs. distance (in Bohr's radius unit) for $\alpha = 1.65$.

fractional parameter of the fractional Schrödinger equation. We applied the formula for multiple interval of the distance in each case of the space-dependent fractional parameter of the fractional Schrödinger equation.

3.2 *The convergence of the formula*

In this subsection, we discuss the convergence of the iteration formula which we found for the space-dependent fractional Schrödinger equation in the

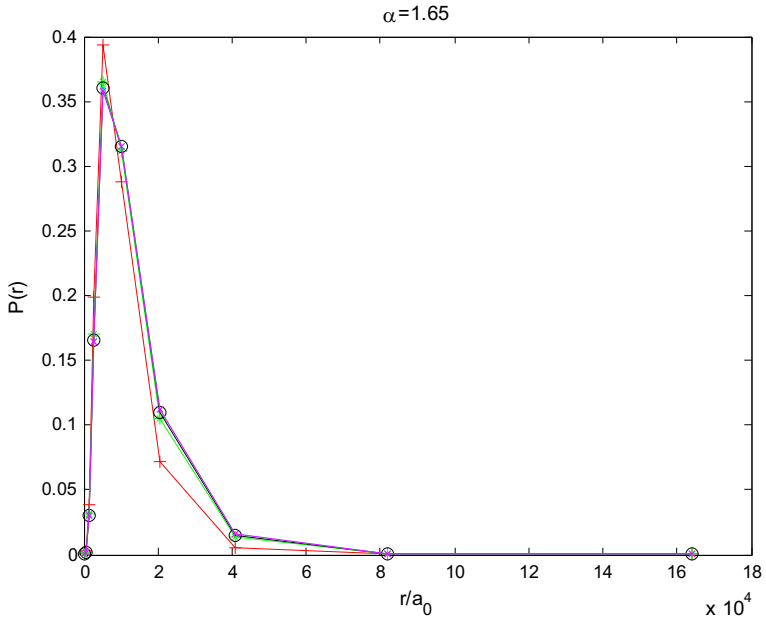

Figure 4. Probability vs. distance (in Bohr's radius unit) for $\alpha = 1.65$.

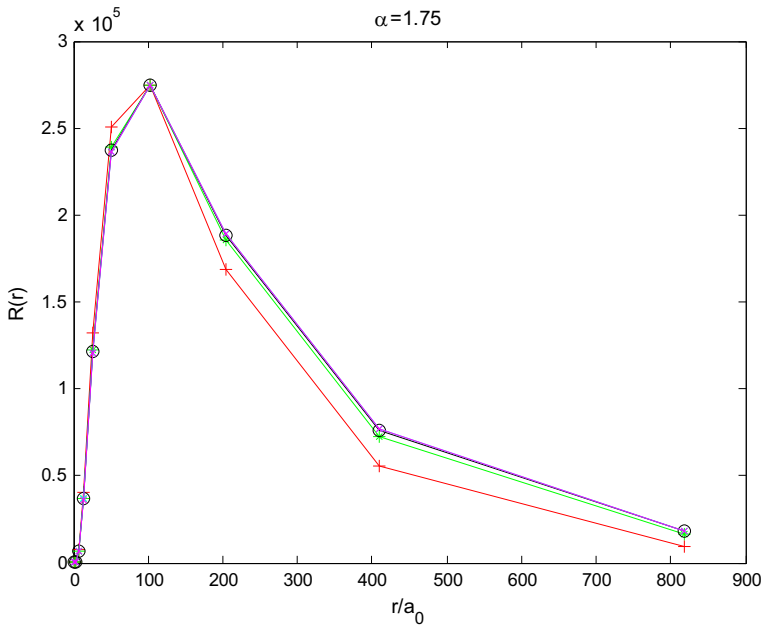

Figure 5. Amplitude of wave function vs. distance (in Bohr's radius unit) for $\alpha = 1.75$.

case of Coulomb's potential with respect to the space-dependent fractional parameter. For this purpose, we return to the iteration formula, i.e. eq. (11), where we can see that the iteration formula is diverged for the limited case of the fractional parameter of the space-dependent fractional Schrödinger equation. Therefore, we can apply the iteration formula for all values of the space-dependent fractional Schrödinger equation parameter except for the limited case of the parameter.

3.3 *The numerical calculations*

We applied numerical formula for an electron in the nucleus field to find the wave function values $R(r)$ and

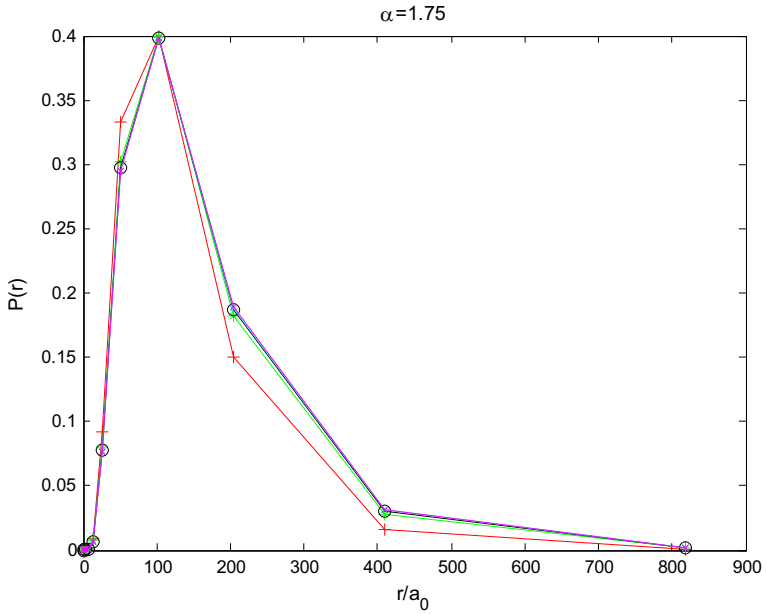

Figure 6. Probability vs. distance (in Bohr's radius unit) for $\alpha = 1.75$.

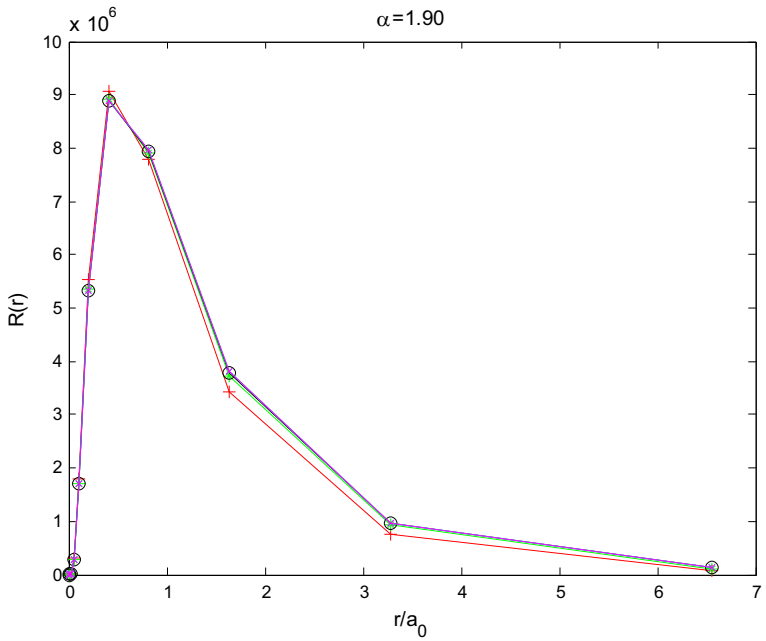

Figure 7. Amplitude of wave function vs. distance (in Bohr's radius unit) for $\alpha = 1.90$.

the probability values for some values of the fractional parameter of the space-dependent form of the fractional Schrödinger equation. For every value of the space-dependent fractional parameter, we tested multiple values of energy and we took sign of this energies as negative to represent a bound state. We took $q_1 = -e$ and $q_2 = Ze$ where e is the elementary charge. We used $Z = 1$ to study the fractional hydrogen atom.

Values of wave function for the space-dependent fractional parameter of the fractional Schrödinger equation $\alpha = 1.95$ and energies E_1, E_2, E_3, E_4 and E_5 are listed in table 1 where R_1 is the value of wave function at $E_1 = -4.9026\,\text{eV}$, R_2 is the value at

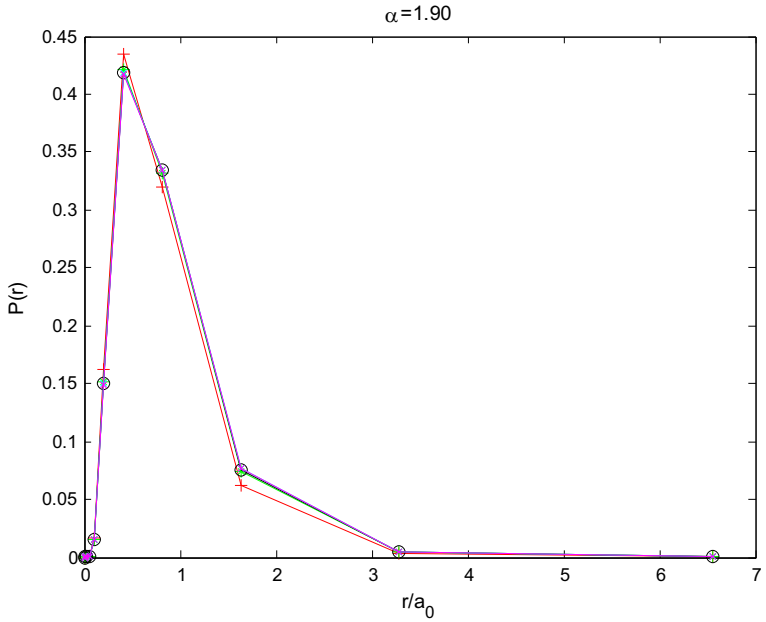

Figure 8. Probability vs. distance (in Bohr's radius unit) for α = 1.90.

$E_2 = -1.1817$ eV, R_3 is the value at $E_3 = -0.5141$eV, R_4 is the value at $E_4 = -0.2849$ eV and R_5 is the value at $E_5 = -0.1802$ eV, and a_0 is Bohr's radius. The wave function values for the space-dependent fractional parameter of the fractional Schrödinger equation $\alpha = 1.50$ are shown in table 2 for multiple values of energy.

We set wave function vs. distance and probability vs. distance for $\alpha = 1.55$, 1.65, 1.75 and 1.90 for multiple values of energy and we listed the results in figures 1–8 respectively.

As we notice from figures 2, 4, 6 and 8, the probability vs. distance curves, for a certain value of the space-dependent fractional parameter and for each value of energy, reach the peaks in the figures, at a certain value of distance. Also, those values of distances at the probability peaks go towards smaller values when the space-dependent fractional parameter value increases. The same trend can be seen in tables 1, 2, figures 1, 3, 5 and 7 but with the wave function values.

We listed the distance at which the probability takes its maximum value r_{Max} in Bohr's radius unit for multiple values of space-dependent fractional parameters in table 3.

We see from table 3 that the most probable values for $\alpha = 1.50$ and 1.55 are at distances of order of millimetres, for $\alpha = 1.60$ are at distances of order of micrometres, for $\alpha = 1.65$ and 1.70 are at distances of order of parts of micrometres, for $\alpha = 1.75$ are at distances of order of nanometres, for $\alpha = 1.80$ are at distances of order of Angstroms, for the space-dependent fractional parameter values bigger than 1.80 and smaller than 1.95 are at distances of order of parts of nanometres and for $\alpha = 1.95$ and more, are at distances of order of picometres.

Table 3. The distance at which the probability takes their maximum value.

α	r_{Max}/a_0
1.50	8.191×10^{7}
1.55	2.047×10^{6}
1.60	1.023×10^{5}
1.65	5.111×10^{3}
1.70	5.110×10^{2}
1.75	1.020×10^{2}
1.80	1.023×10^{1}
1.85	2.047×10^{0}
1.90	4.095×10^{-1}
1.95	8.191×10^{-2}

3.4 *The energy eigenvalues*

Finally, in order to compare our results with other results, we used the energy formula of the fractional Bohr atom derived by Laskin [1] and this formula is given by

$$E_K = (1-\alpha)E_0 k^{\frac{\alpha}{1-\alpha}}, \tag{12}$$

Table 4. The energies corresponding to the maximum peak from this work and the ground-state energies from the fractional Bohr atom formula.

α	E_0 (eV)	E_0^* (eV)	$\lvert\Delta E_0\rvert$ (eV)	$\Delta E_0/E_0$
1.50	-2.4998×10^{-8}	-2.3808×10^{-8}	1.1904×10^{-9}	0.0476
1.55	-9.5952×10^{-7}	-9.1383×10^{-7}	4.5691×10^{-8}	0.0476
1.60	-2.0151×10^{-5}	-1.9192×10^{-5}	9.5958×10^{-7}	0.0475
1.65	-2.6599×10^{-4}	-2.5332×10^{-4}	1.2666×10^{-5}	0.0476
1.70	-0.0024	-0.0023	1.1603×10^{-4}	0.0476
1.75	-0.0033	-0.0159	0.0126	3.8065
1.80	-0.0898	-0.0855	0.0043	0.0476
1.85	-0.3978	-0.3788	0.0189	0.0476
1.90	-1.4962	-1.4249	0.0712	0.0476
1.95	-4.9026	-4.6691	0.2335	0.0476

where Laskin derived the formula in the CGS system units and the formula has the same form in SI units, the only difference being in the ground-state energy that is given in the IS system as

$$E_0 = \left[\frac{1}{K_\alpha}\left(\frac{Ze^2}{4\pi\varepsilon_0\alpha\hbar}\right)^\alpha\right]^{\frac{1}{\alpha-1}}. \tag{13}$$

We compared the energy corresponding to the maximum peak of the probability E_0 which is calculated from the numerical formula derived in this work (eq. (11)) with the ground-state energy from the fractional Bohr atom energy formula E_0^* (eqs. (12) and (13)). The results for these comparisons are listed in table 4 for multiple values of the space-dependent fractional parameter.

As we see from table 4, the energy corresponding to the maximum peak of the probability from our results based on the numerical formula that we found and the ground-state energy from the energy formula of the fractional Bohr energy (except for $\alpha = 1.75$) are close to each other.

4. Conclusions

In this study, we derived a numerical formula to get solutions of the time-independent fractional Schrödinger equation in the case of Coulomb's potential in one dimension (eq. (11)) by applying the right definition of Riemann–Liouville fractional derivative. The iteration formula we found is applied in systems interacting through the static electric interaction.

We applied the numerical formula in the case of electron in the nucleus electric field of the atom assuming that the gravitational interaction is negligible. We found wave functions and probabilities for multiple values of fractional parameters of the space-dependent form of the fractional Schrödinger equation in the stationary state and we obtained distances corresponding to the maximum value of probability in each case of the space-dependent fractional parameter (table 3) and from these distances we showed that each range of the space-dependent fractional parameter must be applied in a range of distances and we concluded that the distance's ranges in the order of nanometres and picometres occur for the greatest values of the space-dependent fractional parameter of the fractional Schrödinger equation.

We found energies corresponding to the maximum values of probability and we compared these values of energy with the ground-state energy values from the fractional Bohr's atom formula for multiple values of space-dependent fractional parameter. We concluded that the results calculated from Laskin formula of the fractional Bohr's atom, which is considered semi-classical, agreed well with the results we obtained from this work.

References

[1] N Laskin, *Fractional quantum mechanics* (World Scientific Publishing, Singapore, 2018)
[2] J Dong and M Xu, *J. Math. Phys.* **48**, 072105 (2007), https://doi.org/10.1063/1.2749172
[3] M Al-Raeei and M S El-Daher, *AIP Adv.* **10**, 035305 (2020), https://doi.org/10.1063/1.5113593
[4] J Banerjee, U Ghosh, S Sarkar and S Das, *Pramana – J. Phys.* **88**: 70 (2017), https://doi.org/10.1007/s12043-017-1368-1
[5] M Al-Raeei and M S El-Daher, *Pramana – J. Phys.* **94**: 9 (2020), https://doi.org/10.1007/s12043-019-1877-1
[6] Mostafa M A Khater, Aly R Seadawy and D Lu, *Pramana – J. Phys.* **90**: 59 (2018), https://doi.org/10.1007/s12043-018-1547-8

[7] M Al-Raeei and M S El-Daher, *Phys. Lett. A* **383**, 125831 (2019), https://doi.org/10.1016/j.physleta.2019.07.019
[8] N Laskin, *Phys. Lett. A* **268**, 298 (2000)
[9] M Al-Raeei, *Using methods of statistical mechanics in the study of soft condensed matter materials and complex structures* (Syrian Arab Republic, Damascus, 2018)
[10] F Pinsker, W Bao, Y Zhang, H Ohadi, A Dreismann and J J Baumberg, *Phys. Rev. B* **92**, 195310 (2015), https://doi.org/10.1103/PhysRevB.92.195310
[11] M Al-Raeei and M S El-Daher, *Pramana – J. Phys.* **90**: 60 (2018). https://doi.org/10.1007/s12043-018-1550-0
[12] N Laskin, *Chaos* **10**, 780 (2000), https://doi.org/10.1063/1.1050284
[13] M Al-Raeei, *AIP Adv.* **10**, 065325 (2020), https://doi.org/10.1063/5.0014275
[14] M Al-Raeei and M S El-Daher, *Polym. Bull.* (2020), https://doi.org/10.1007/s00289-020-03166-8
[15] C Li and F Zeng, *Numerical methods for fractional calculus* (CRC Press, Boca Raton, 2015)
[16] C J Song, *Phys. Lett. A* **383**, 125914 (2019), https://doi.org/10.1016/j.physleta.2019.125914
[17] M Al-Raeei and M El-Daher, *Chem. Phys. Lett. A* **734**, 136729 (2019), https://doi.org/10.1016/j.cplett.2019.136729
[18] T Das, U Ghosh, S Sarkar and S Das, *Pramana – J. Phys.* **93**, 76 (2019), https://doi.org/10.1007/s12043-019-1836-x
[19] H A Fallahgoul, S M Focardi and F J Fabozzi, *Fractional calculus and fractional processes with applications to financial economics* (Elsevier, Amsterdam, 2017)
[20] A M Mathai and H J Houbold, *Matrix methods and fractional calculus* (World Scientific Publishing, Singapore, 2017)
[21] Y Zhou, J R Wang and L Zhang, *Basic theory of fractional differential equations* (World Scientific Publishing, Singapore, 2017)
[22] D Feng, J Jiao and G Jiang, *Phys. Lett. A* **382**, 2081 (2018), https://doi.org/10.1016/j.physleta.2018.05.028
[23] Y Xie, Z Yang and L Li, *Phys. Lett. A* **382**, 2506 (2018), https://doi.org/10.1016/j.physleta.2018.06.023
[24] I K Mylonas, C B Ward, P G Kevrekidis, V M Rothos and D J Frantzeskakis, *Phys. Lett. A* **381**, 3965 (2017), https://doi.org/10.1016/j.physleta.2017.10.043
[25] H Y Wu and L H Jiang, *Pramana – J. Phys.* **89**: 40 (2017), https://doi.org/10.1007/s12043-017-1438-04
[26] W X Ma, T Huang and Y Zhang, *Phys. Scr.* **82**, 065003 (2010), https://doi.org/10.1088/0031-8949/82/06/065003
[27] W X Ma, *Appl. Math. Lett.* **102**, 106161 (2020), https://doi.org/10.1016/j.aml.2019.106161
[28] W X Ma and L Zhang, *Pramana – J. Phys.* **94**: 43 (2020), https://doi.org/10.1007/s12043-020-1918-9
[29] W X Ma, *Mod. Phys. Lett. B* **33**, 1950457 (2019), https://doi.org/10.1142/S0217984919504578