



Research article

Numerical simulation of the space dependent fractional Schrödinger equation for London dispersion potential type

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ABSTRACT

In this study, we apply the definition of one of the fractional derivatives definitions of increasing values of the variable, which is the fractional derivative of Riemann-Liouville, and the numerical-integral methods to find numerical solutions of the fractional Schrödinger equation with the time-independent form for Van Der Waals potential type. We use the dimensionless formalism of the fractional Schrödinger equation in the space-dependent form in case of London dispersion potential in the stationary state. The solutions are found for multiple values of the space-dependent fractional Schrödinger equation parameter with a certain value of the energy. We find that the numerical solutions are physically acceptable for some values of the space dependent fractional parameter of the fractional Schrödinger equation but are not physically acceptable for others for a specific case. The numerical solutions can be applied for the systems that obey London dispersion potential type, which is resulted from the polarization of the instantaneous multi-poles of two moieties, such as soft materials systems and fluids of the inert gases.

1. Introduction

The linear fractional Schrödinger equation or the fractional Schrödinger equation is a type of the linear Schrödinger equations used in the fractional quantum mechanics and this equation use one of the physical potentials to give the probability. The fractional Schrödinger equation in the general space representation form with a space fractional parameter α is given in the linear formalism as follows [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19]:

$$j \frac{\hbar}{2\pi} \frac{\partial \Psi(\mathbf{r}, t)}{\partial t} = \hat{H}_\alpha \Psi(\mathbf{r}, t) \quad (1)$$

Where \hbar is Planck constant, $\Psi(\mathbf{r}, t)$ is the wave function of the system in space-representation, j is the imaginary unit and \hat{H}_α is Hamiltonian operator in the fractional type which is defined by the following formula:

$$\hat{H}_\alpha = U(\mathbf{r}) + K_\alpha (-\hbar^2 \Delta)^{\alpha/2} \quad (2)$$

K_α is a coefficient, $U(\mathbf{r})$ is the interaction potential of the system and $(-\hbar^2 \Delta)^{\alpha/2}$ is the space fractional operator which is given by:

$$(-\hbar^2 \Delta)^{\alpha/2} \Psi(\mathbf{r}, t) = \frac{1}{h^3} \int d^3 \Pi e^{i\mathbf{r} \cdot \mathbf{\Pi}} |\Pi|^\alpha \Phi(\mathbf{\Pi}, t) \quad (3)$$

The $\Phi(\mathbf{\Pi}, t)$ is the wave function of the system in the momentum-representation which relates to the wave function in space-representation by Fourier transforms. In one dimension, the fractional Schrödinger equation in the space-dependent form is written as:

$$j\hbar \frac{\partial \Psi(r, t)}{\partial t} = -K_\alpha (\hbar \nabla)^\alpha \Psi(r, t) + U(r) \Psi(r, t) \quad (4)$$

There is another type of linear fractional Schrödinger equation called the time-dependent fractional Schrödinger equation and the two types can be derived from the general fractional Schrödinger equation which depending on two fractional parameters but in this work we focus on the space-dependent type in the stationary state. In most of literatures, the term fractional Schrödinger equation refers to the space-dependent fractional Schrödinger equation type so in this work we use this convention. The analytical or exact solutions of some applications of the fractional Schrödinger equation in the space form are found in multiple physical cases, the first case is free particle in one and three dimensions [7], the second case is infinite potential well and barrier penetration [14], the third case is δ function [7, 8], the fourth case is linear potential

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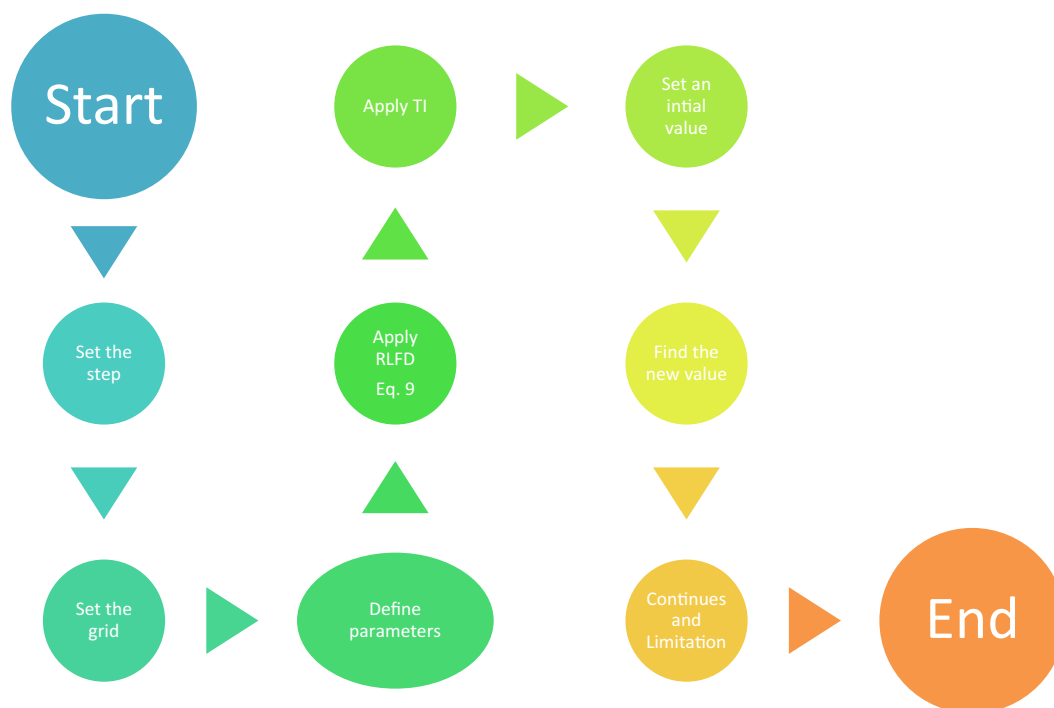


Figure 1. A schematic plot of the algorithm.

Table 1. The wave function values for $\alpha = 1.10$ and $\alpha = 1.20$.

$r/ \alpha \times 10^{-2}$	ψ_1	ψ_2
7.275445	3.456413e-20 - 2.182293e-19j	121301.6-373328.1j
7.279520	-2.865280e-14 - 2.865280e-14j	843181.8 + 1.491311e-09j
7.279811	-7.805082e-14 + 5.670724e-14j	275677.9-848449.3j
7.280102	1.043058e-13 + 2.047117e-13j	-763800.1-554933.3j
7.280393	5.204921e-13 - 1.691181e-13j	-808511.8 + 587418.2j
7.294362	528751.4 + 727763.9j	6281216-1.933159e+07j
7.294653	1931785 - 984293.4j	-1.761264e+07-1.279633e+07j
7.294944	-1615136 - 4970877j	-1.886835e+07 + 1.370866e+07j
7.295235	-1.244800e+07 + 1971569j	7722752 + 2.376819e+07j
7.295526	-3.567037e-07 + 3.039739e+07j	2.678595e+07 + 2.288803e-07j
7.295817	7.242974e+07 + 1.147175e+07j	8873822-2.731082e+07j

Table 2. The wave function values for $\alpha = 1.30$ and $\alpha = 1.40$.

$r/ \alpha \times 10^{-2}$	ψ_3	ψ_4
7.275445	3.442973e+07-6.757215e+07j	4.716548e+07-6.491772e+07j
7.275737	-1.506902e+07-2.074072e+07j	-2274032 - 6998752j
7.277192	17768.81-112187.9j	45.56454-14.80482j
7.279811	2.067761 + 6.363915j	-1.817333e-08 - 1.320369e-08j
7.280102	2.242230 + 0.3551344j	-1.966322e-09 + 6.388968e-10j
7.284176	-5.552231e-07 - 2.829003e-07j	-3.901252e-24 + 5.369612e-24j
7.284467	-1.716519e-07 + 1.247124e-07j	1.894529e-25 + 5.830760e-25j
7.284758	1.130399e-08 + 7.137056e-08j	5.387197e-26 + 1.750406e-26j
7.287960	-1.621969e-13 + 4.991906e-13j	-1.949834e-37 + 1.416638e-37j
7.292615	-1.852927e-20 + 1.700233e-35j	0.000000 + 0.000000j
7.292907	-2.884208e-21 + 5.660576e-21j	0.000000 + 0.000000j

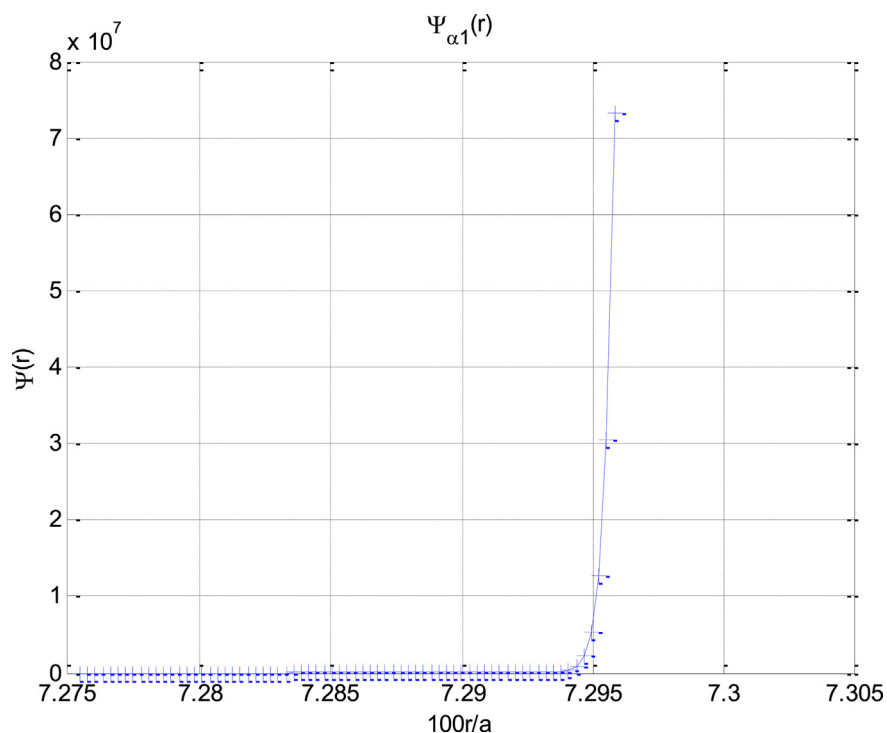


Figure 2. Amplitude of the wave function for $\alpha = 1.10$.

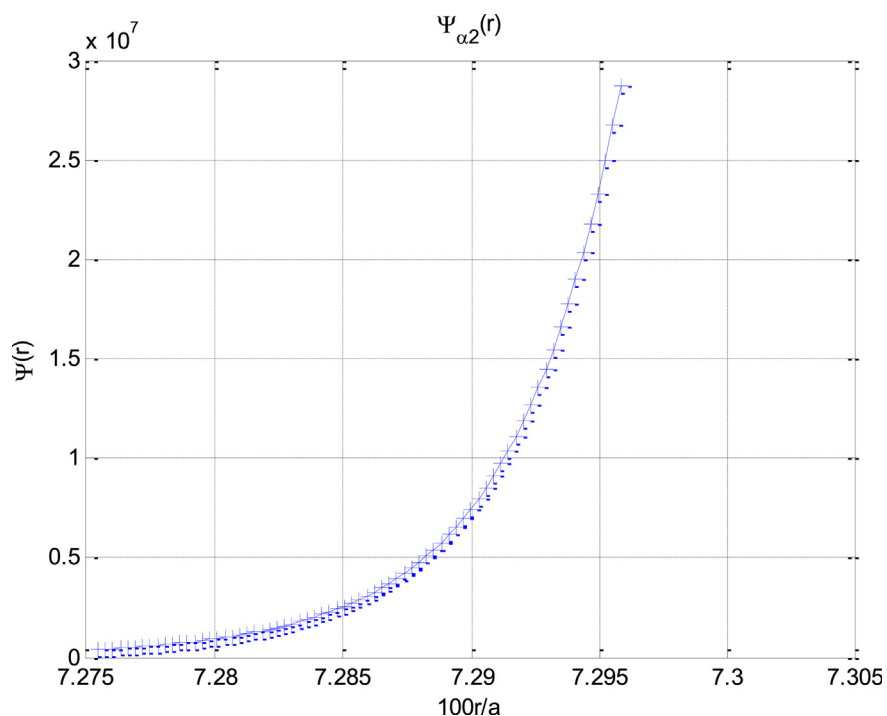


Figure 3. Amplitude of the wave function for $\alpha = 1.20$.

field and Coulomb's potential in one dimension [7, 8, 14] and the fifth case is the energy level of stationary states for one dimension fractional oscillator by semi classical approximation [7], in addition to a number of other mathematical solutions.

In the following, we find an algorithm to solve the space-dependent fractional Schrödinger equation in one dimension in case of potential of London dispersion forces which is important in case of some macro-molecular such as polymers and proteins, the simple relation that gives

potential of London dispersion forces between two atoms or molecules is given as follows [20, 21, 22, 23, 24, 25, 26]:

$$U_{ij}^{disp}(r) = -\frac{C_{ij}}{r^6} \approx -\frac{3I_i I_j}{2(I_i + I_j)} \frac{\lambda_i \lambda_j}{r^6} \tag{5}$$

Where I is the first ionization energy, λ is the dipole polarizability and C_{ij} is a constant can be calculated from the first ionization energy and dipole

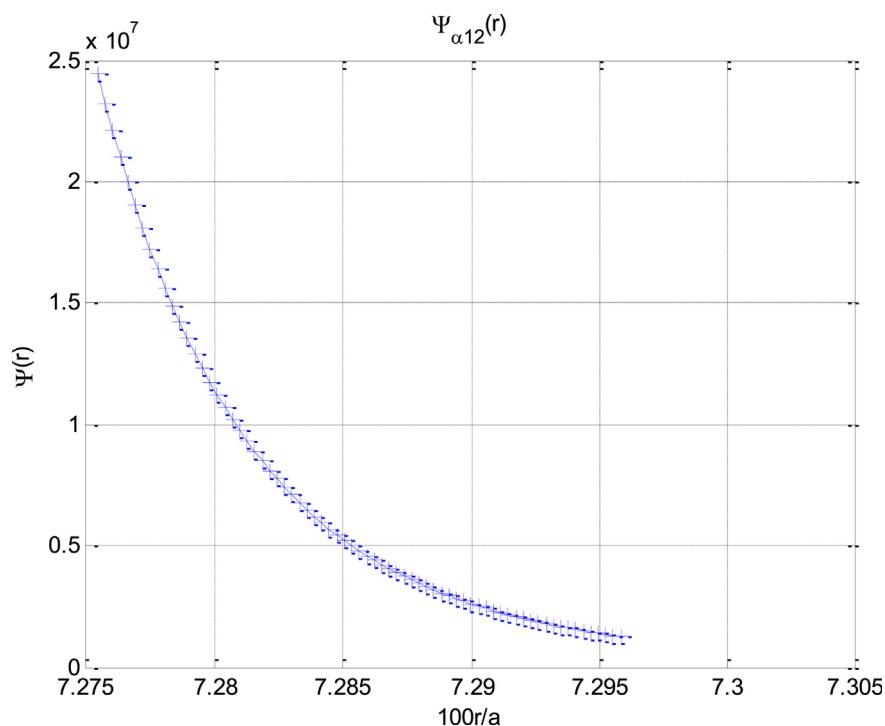


Figure 4. Amplitude of the wave function for $\alpha = 1.21$.

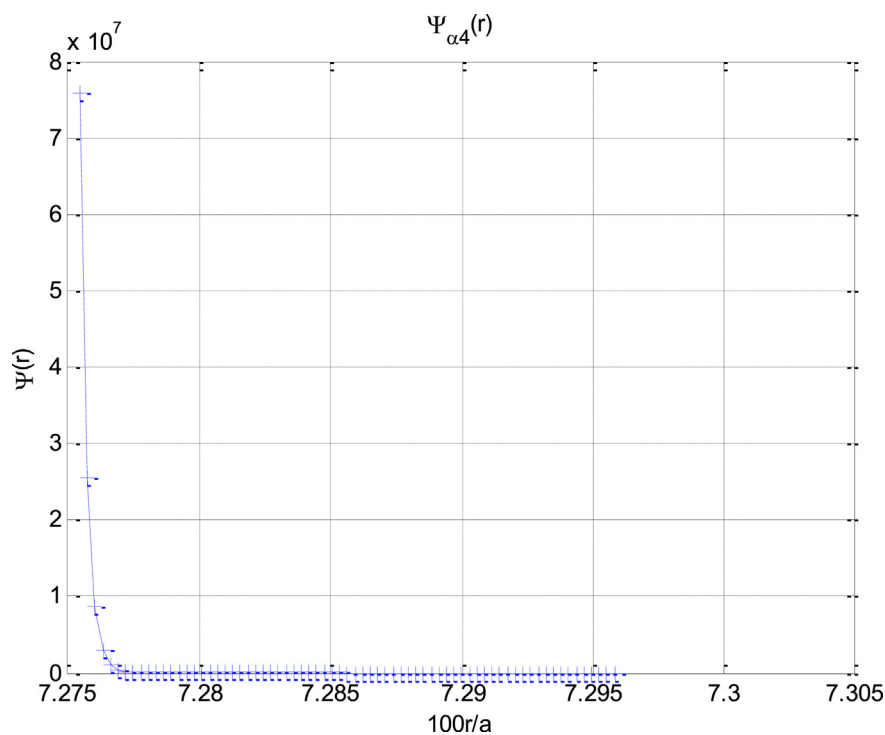


Figure 5. Amplitude of the wave function for $\alpha = 1.40$.

polarizability or from Hamaker constant of each component in the system.

The fractional Schrödinger equation in the fractional quantum mechanics is very similar to the traditional Schrödinger equation in the traditional quantum mechanics. It is well known that the traditional Schrödinger equation is considered the most important equation in quantum mechanics where we can find a lot of properties for a certain system described by a specific potential by solving the traditional

Schrödinger equation either by an exact solution or by a numerical solution. The same thing can be seen from the fractional Schrödinger equation in the fractional quantum mechanics because if we find a solution of the fractional Schrödinger equation, we can determine a lot of properties of the system. In this study, we find a numerical solutions of the fractional Schrödinger equation in the stationary state in case of London dispersion potential type which is considered an important potential for describing the weak forces between particles which is resulted

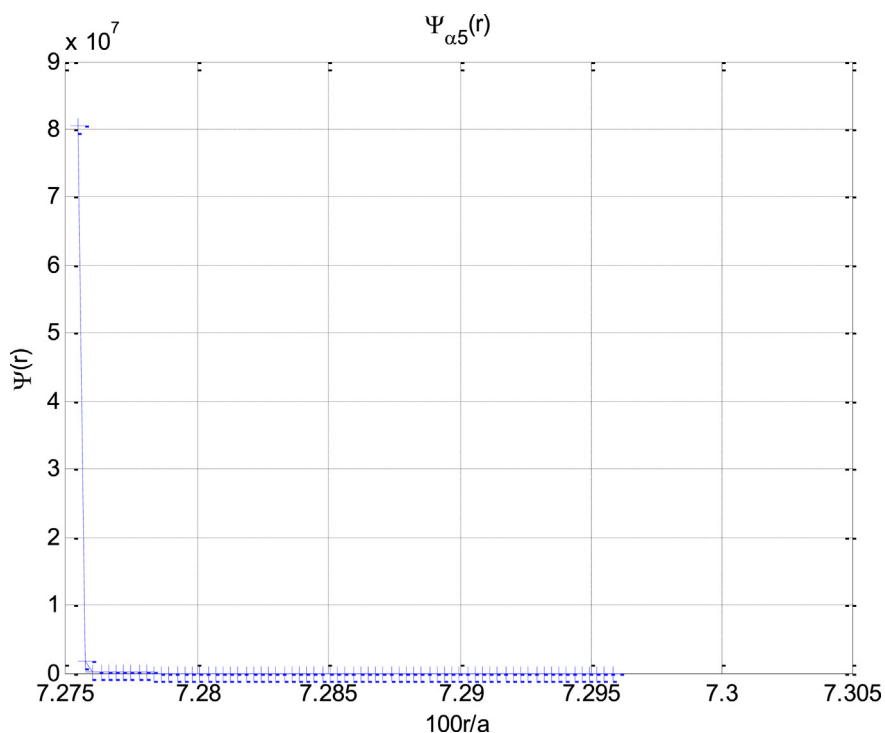


Figure 6. Amplitude of the wave function for $\alpha = 1.50$.

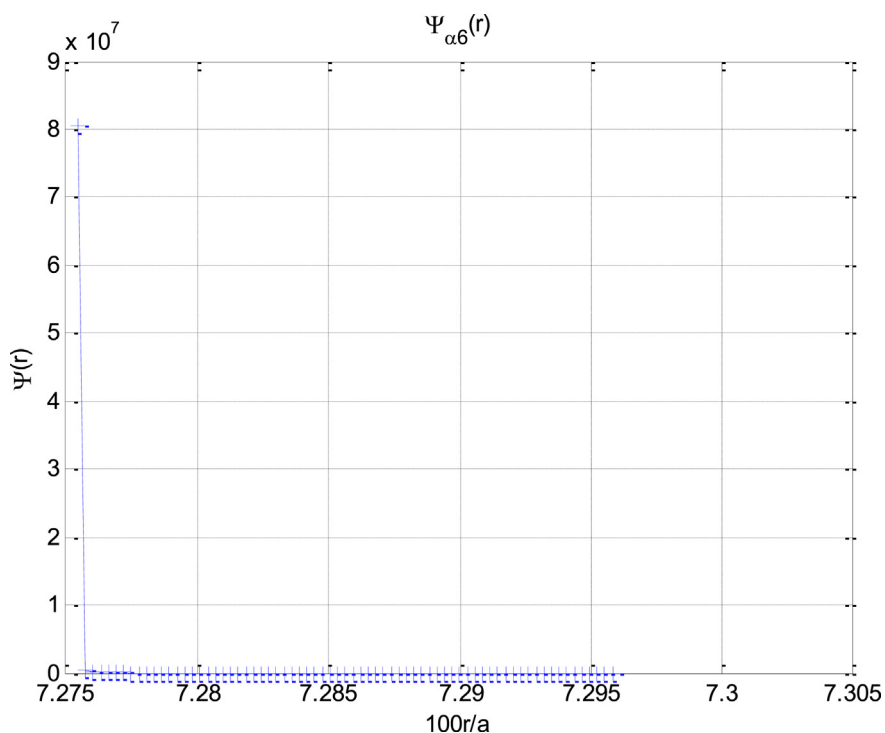


Figure 7. Amplitude of the wave function for $\alpha = 1.60$.

from the fluctuating polarization of neighbour particles in a specific system which has an interaction between the instantaneous multi-poles particles such as polymers, proteins and inert gases. This study is arranged as follows: in the second section, we illustrate the algorithm which we use for finding the numerical solutions of the fractional Schrödinger for London dispersion potential type. In the third section, we

insert computational results of the study and the discussion of these results and in the last section, we illustrate a conclusion of the study.

2. The iteration method

The fractional Schrödinger equation in the space-dependent form for London dispersion potential can be written as follows:

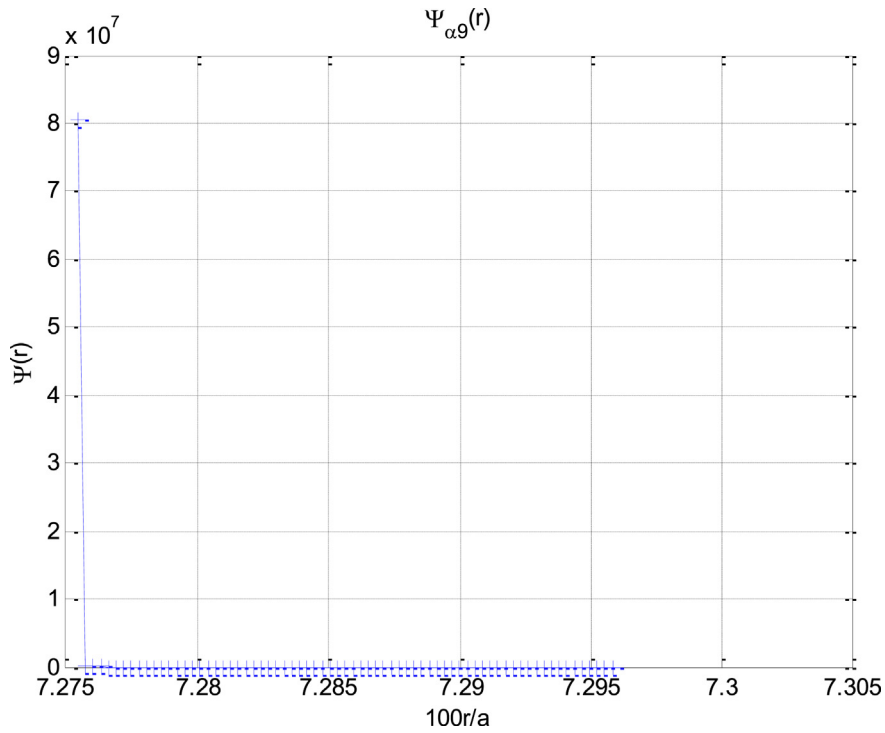


Figure 8. Amplitude of the wave function for $\alpha = 1.90$.

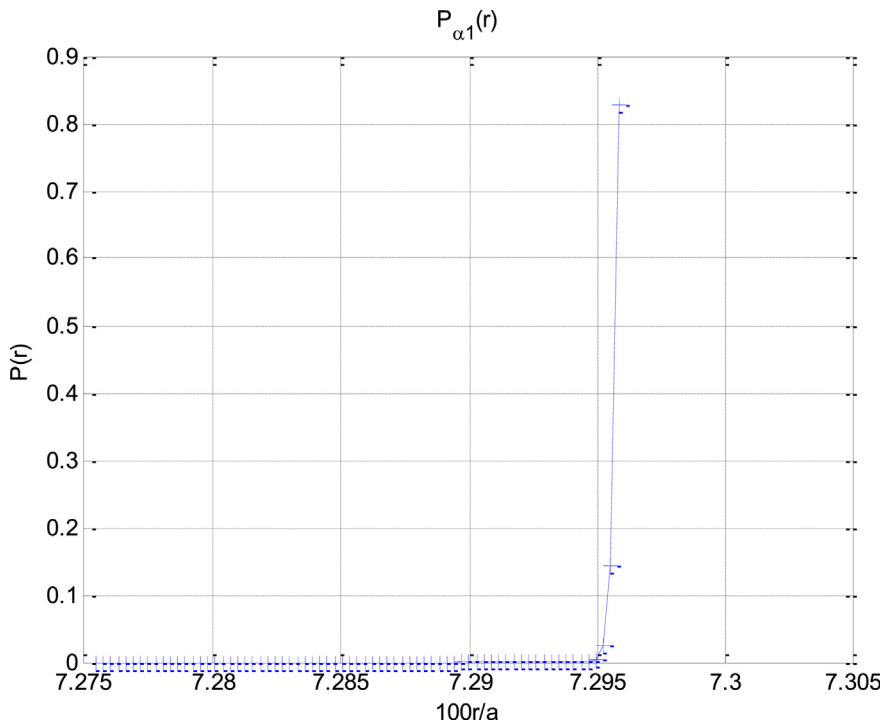


Figure 9. The probability versus distance for $\alpha = 1.10$.

$$j\hbar \frac{\partial \Psi(r, t)}{\partial t} = -K_\alpha (\hbar \nabla)^\alpha \Psi(r, t) - \frac{3I_i I_j}{2(I_i + I_j)} \frac{\lambda_i \lambda_j}{r^6} \Psi(r, t) \quad (6)$$

$$\hat{H}_\alpha \psi(r) = E_\alpha \psi(r) \quad (8)$$

As we see, the Hamiltonian of this case does not explicitly depend on the time and then we write the special solution of the last equation as follows:

$$\Psi(r, t) = e^{-j\frac{E_\alpha}{\hbar}t} \psi(r) \quad (7)$$

Where E_α and $\psi(r)$ are the eigenvalues and eigenvectors of the Hamiltonian operator. The previous equation in the dimensionless formalism is written as follows:

$$D_r^\alpha \psi(r^*) + \lambda^* r^{*-6} \psi(r^*) + E^* \psi(r^*) = 0 \quad (9)$$

This leads to:

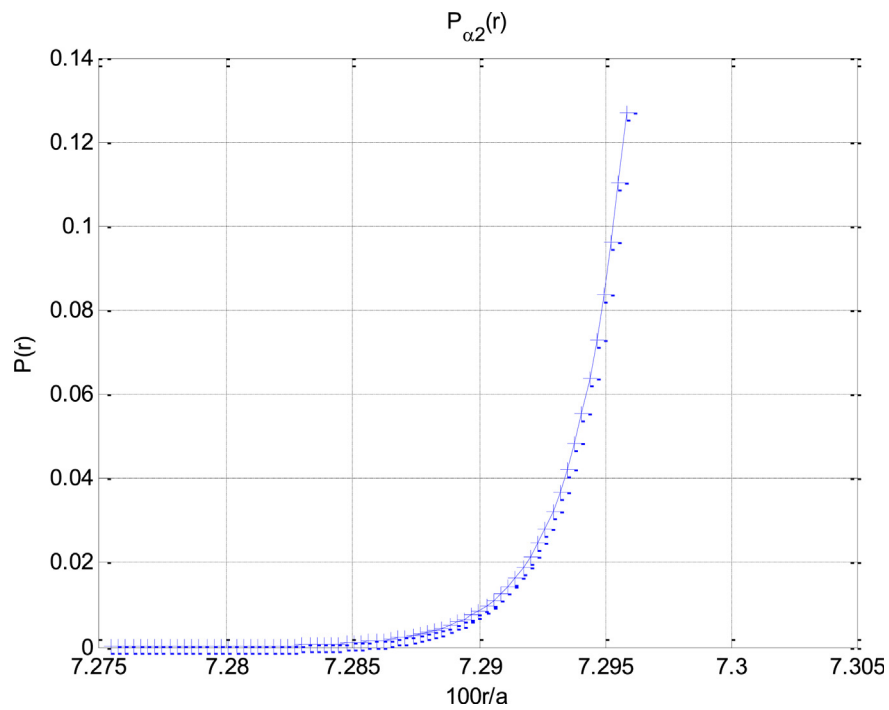


Figure 10. The probability versus distance for $\alpha = 1.20$.

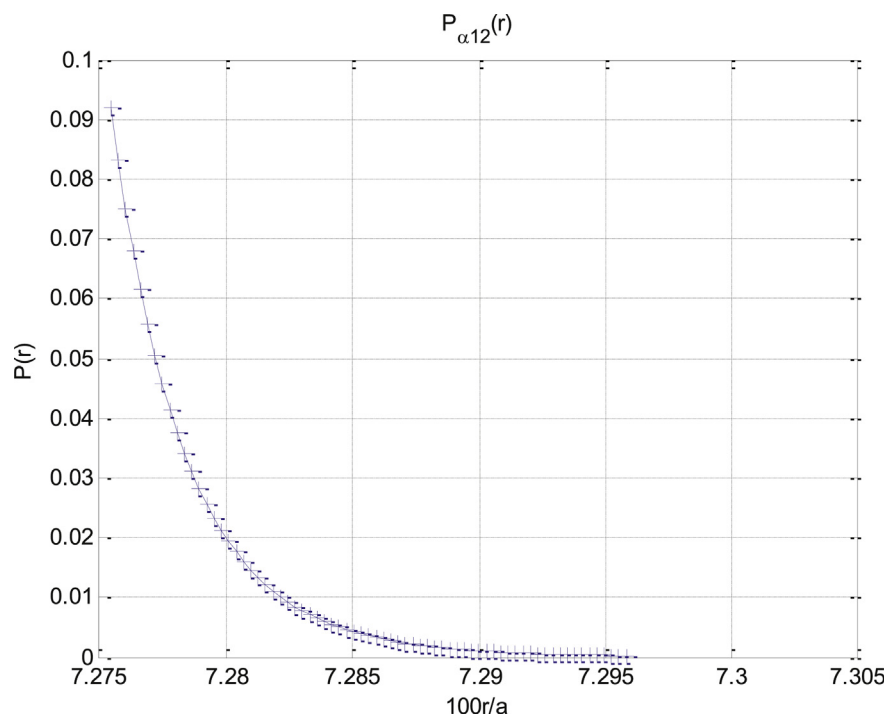


Figure 11. The probability versus distance for $\alpha = 1.21$.

Where r^* is the dimensionless distance, D_r^α is the fractional derivative operator of the α order with respect to the dimensionless distance, $\psi(r^*)$ is the wave function in the stationary formalism as a function of the dimensionless distance, λ^* is the reduced dipole polarizability and E^* is the eigenvalues of the energy in the dimensionless formalism.

For purpose of finding the numerical solutions of the previous equation, we apply the fractional derivative of Riemann-Liouville [27, 28, 29] and the Runge-Kutta methods. We use Wolfram Mathematica programming language to code the method and we apply it for multiple values of the space-dependent fractional parameter. We apply the method for the range $]0, 10000a_0]$ of the distance. We insert and plot some values of the

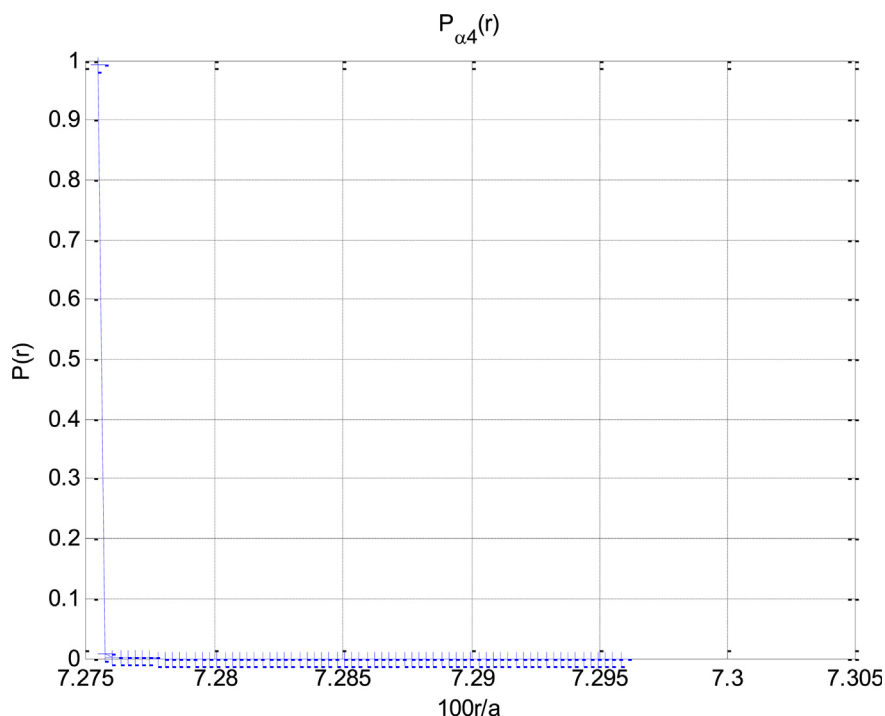


Figure 12. The probability versus distance for $\alpha = 1.40$.

calculated results in the following section. The full results are ready when requested. Figure 1 shows the algorithm used for this method.

3. Results and discussion

We apply the previous method to compute the wave functions of the stationary state, however, if we need to find the total wave function, we apply equation. 7 to find the full wave function. The method must be used only with $1 < \alpha < 2$ because we only use Riemann-Liouville definition of

the fractional derivatives for the last range of the space dependent fractional parameter. So, the method can be applied for all values of the fractional parameter of the space-dependent fractional Schrodinger equation except α equals to the limited value. The wave functions must be physical so it must be continuous, single-valued and limited, i. e. when the distance increases to infinity, the wave function should be decreased. The method can be applied in case of systems that obeys London dispersion forces which have induced multi-poles between moieties such as soft materials system like proteins and some other polymers and

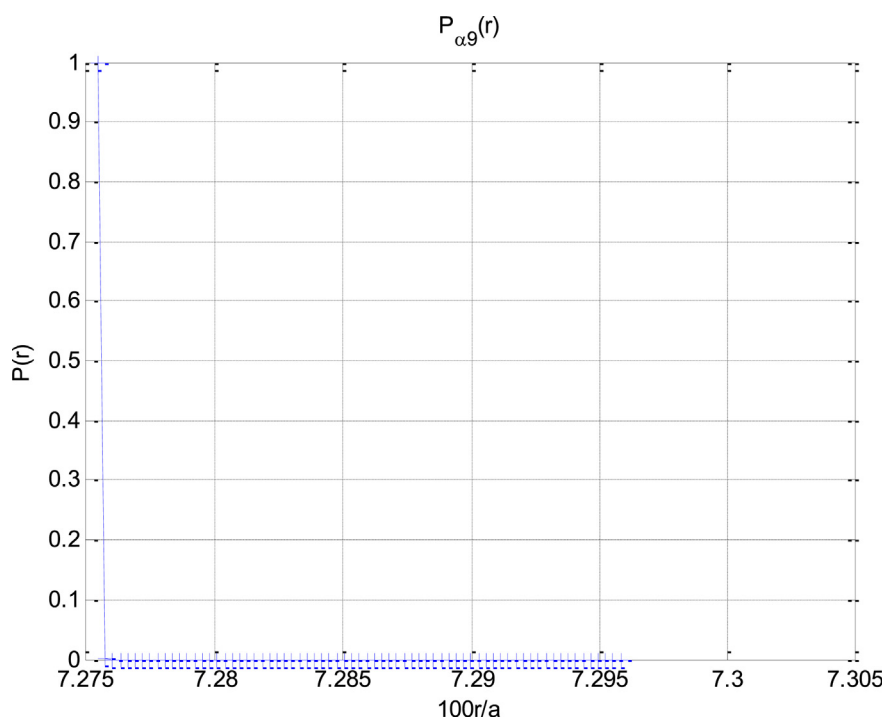


Figure 13. The probability versus distance for $\alpha = 1.90$.

macromolecules. In this work, we applied the numerical method in case of Polyethylene [24, 30] for multiple values of the space dependent fractional parameter in case of the ground state. The values of the wave function were calculated for values of the space dependent fractional parameter of the fractional Schrödinger equation from $\alpha = 1.10$ to $\alpha = 1.90$. Some of the results for $\alpha = 1.10$ and $\alpha = 1.20$ were inserted in Table 1 and for $\alpha = 1.30$ and $\alpha = 1.40$ in Table 2 where a is Bohr radius. However, for the full values of the wave functions for the previous space dependent fractional parameters of the fractional Schrödinger equation, see supplementary materials file of this article.

As we notice from Table 1, the wave functions values increase with distance for the two values of the space dependent fractional parameter of the fractional Schrödinger equation $\alpha = 1.10$ and $\alpha = 1.20$, and the same thing we can see from all values less than $\alpha = 1.20$ which mean they are not acceptable for physical reasons. While, for the other values of the space dependent parameters of the fractional Schrödinger equation, i. e. for the values more than $\alpha = 1.20$ as it can be seen from Table 2 for two values, the values of the wave functions decrease when the distance increase. Also, we can see from the two tables and from the tables illustrated in the supplementary materials file that the most values of the wave functions for the previous values of the space dependent fractional parameters are complex. Besides, we see from Table 2 that the values of the wave function for $\alpha = 1.40$ go to zero for the greatest values of the distance.

We plotted the amplitude of wave function versus the distance for the following four values of the space dependent fractional parameter of the fractional Schrödinger equation $\alpha = 1.10$, $\alpha = 1.20$, $\alpha = 1.21$, $\alpha = 1.40$, $\alpha = 1.50$, $\alpha = 1.60$ and $\alpha = 1.90$, the results were depicted in Figure 2, Figure 3, Figure 4, Figure 5, Figure 6, Figure 7 and Figure 8 for these values of the space dependent fractional parameter of the fractional Schrödinger equation. Also, we plotted the probability versus distance for the space dependent fractional parameters $\alpha = 1.10$, $\alpha = 1.20$, $\alpha = 1.21$, $\alpha = 1.40$ and $\alpha = 1.90$ and the results were depicted in Figure 9 for $\alpha = 1.10$, Figure 10 for $\alpha = 1.20$, Figure 11 for $\alpha = 1.21$, Figure 12 for $\alpha = 1.40$ and Figure 13 for $\alpha = 1.90$.

We have not illustrated the other values of the wave function and the probability for the space-dependent fractional parameter of the fractional Schrödinger equation which is greater than 1.9 because these values are similar to the values for resulted for the space dependent fractional Schrödinger equation more than $\alpha = 1.3$. However, all values in the full range of the fractional parameter of the fractional Schrödinger equation are ready when requested.

We see from the previous figures and tables, all results of the wave functions for the space-dependent fractional parameter of the fractional Schrödinger equation greater than 1.2 are limited so they do not give unlimited probability while the results for the space-dependent fractional parameter smaller than or equals to 1.2 increase with the distance.

4. Conclusion

We used a numerical algorithm to solve the space-dependent fractional Schrödinger equation in the stationary state for Van Der Waals potential type based on Riemann-Liouville definition of the fractional derivatives in addition to the Runge-Kutta quadrature method. We used the dimensionless form of the space-dependent fractional Schrödinger equation in case of London dispersion potential because it is more useful for reducing the consumed time in the computational calculations. We did the computational calculations in Wolfram Mathematica software.

We found the wave functions values (Table 1, Table 2 and the tables in supplementary materials file and Figure 2, Figure 3, Figure 4, Figure 5, Figure 6, Figure 7 and Figure 8) and the probability values (Figure 9, Figure 10, Figure 11, Figure 12 and Figure 13) in case of system obeys London dispersion potential in the ground state, for multiple values of the space dependent fractional parameter except for the limited value of the space dependent fractional parameter. We found that the values of the space-dependent fractional parameter which give limited wave functions

are greater than 1.2 while the values those are smaller than or equals 1.2 give increasing wave functions so these values are not accepted for physical reasons.

We believe that the numerical method we used in this study can be applied for multiple systems interact via London dispersion potential type such as soft materials system and fluid of the inert gases, all we need to apply the method: the parameters of the systems. So, if we find the numerical solutions of the fractional Schrödinger equation of London dispersion potential type, i. e. finding the probability, we can find a lot of physical properties of the considered system by applying the integration over the required properties using the probability functions which were found by the numerical solutions.

Declarations

Author contribution statement

Marwan Al-Raei: Conceived and designed the experiments; Performed the experiments; Analyzed and interpreted the data; Contributed reagents, materials, analysis tools or data; Wrote the paper.

Moustafa Sayem El-Daher: Contributed reagents, materials, analysis tools or data; Wrote the paper.

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Competing interest statement

The authors declare no conflict of interest.

Additional information

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