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An algorithm for fractional Schrödinger equation in case of Morse potential

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ABSTRACT
Based on methods of numerical integration and Riemann–Liouville definition of the fractional derivatives, we find a numerical algorithm to find solutions of the time independent fractional Schrödinger equation for Morse potential or the quantum oscillator potential in one dimension, and the iteration formula is applied for multiple values of the fractional parameter of the space dependent fractional Schrödinger equation and multiple values of energy. We define and use the dimensionless form of the space dependent fractional Schrödinger equation of Morse potential. We employ the iteration formula of the time independent fractional Schrödinger equation of Morse potential to find the wave functions in the case of hydrogen chloride and hydrogen fluoride molecules for a certain value of the fractional parameter of the space dependent fractional Schrödinger equation and for many values of the dimensionless energy of each molecule.

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I. INTRODUCTION
The space dependent fractional Schrödinger equation is a type of linear Schrödinger equation used in fractional quantum mechanics.\(^1\)\(^\text{-}\)\(^5\) In one dimension, this equation is given by
\[
\frac{j\hbar}{\partial t} \frac{\partial \psi(r,t)}{\partial t} = -K_\alpha (\hbar \nabla)^\alpha \psi(r,t) + U(r) \psi(r,t),
\]
where \(\hbar\) is the reduced Planck constant, \(\psi(r,t)\) is the wave function of the system in space representation, \(j\) is the imaginary unit, \(K_\alpha\) is a parameter, \(U(r)\) is the interaction potential of the system, \(\alpha\) is the fractional parameter of the space dependent fractional Schrödinger equation, and \((\hbar \nabla)^\alpha\) is the space fractional operator. The space dependent fractional Schrödinger equation is written in a simpler form as follows:
\[
\frac{j\hbar}{\partial t} \frac{\partial \psi(r,t)}{\partial t} = \hat{H}_\alpha \psi(r,t).
\]
Here, \(\hat{H}_\alpha\) is the fractional Hamiltonian operator, which is given by
\[
\hat{H}_\alpha = U(r) - K_\alpha (\hbar \nabla)^\alpha.
\]
There is another type of the 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 depends on two fractional parameters; however, in this study, we focus on the space dependent type of the fractional Schrödinger equation in the stationary state. In most of the literature, the term fractional Schrödinger equation refers to the space dependent fractional Schrödinger equation; hence, in this work we use this convention.

The analytical or exact solutions of some physical applications of the fractional Schrödinger equation, in addition to some numerical solutions, were found in multiple physical and mathematical cases such as studies in Refs. 2–4, 9, 13, 14, 17, 26, 28, and 37. In this work, we apply the Riemann–Liouville definition of the fractional derivatives to find numerical solutions for the time independent fractional Schrödinger equation for Morse potential, which is used in the quantum mechanics as an oscillator potential, and this potential is given by the following formula:52–86
\[
U_M = U_0 \left[1 - e^{-a(r-r_0)}\right]^2,
\]
where $U_0$ is the well depth or Morse potential’s depth, $r_0$ is the equilibrium bond distance or the distance at which Morse potential equals zero, and $\alpha$ is a parameter that controls the width of the potential, the larger $\alpha$ is the smaller potential’s width, $a$ depends on the well depth and the force constant of the atoms or the molecules in the system at the minimum of the well. In the following, we use the dimensionless form of Morse potential in the fractional Schrödinger equation.

II. THE NUMERICAL FORMULA

We write the space dependent fractional Schrödinger equation for Morse potential as follows:

$$\frac{j\hbar}{\partial t} \frac{\partial^\alpha \Psi(r,t)}{\partial r^\alpha} = U_0[1 - e^{-a(r-r_0)}]^2\Psi(r,t) - K_0(h\nabla)^\alpha \Psi(r,t).$$  \hspace{1cm} (5)

The previous Hamiltonian does not depend explicitly on time, so we write the solution of the previous equation as follows:

$$\Psi(r,t) = e^{iEt} \Psi(r).$$ \hspace{1cm} (6)

If we substitute the previous solution in Eq. (5), we get the time independent fractional Schrödinger equation for Morse potential as follows:

$$U_0[1 - e^{-a(r-r_0)}]^2\Psi(r) - K_0(h\nabla)^\alpha \Psi(r) = E\Psi(r),$$ \hspace{1cm} (7)

where $\Psi(r)$ and $E$ are the eigenvectors and eigenvalues of the time independent fractional Schrödinger equation, respectively. We get the dimensionless version of the time independent fractional Schrödinger equation or the space formalism of the equation for Morse potential if we take the following dimensionless parameters of Morse potential

$$U_0^* = U_0/M,$$ \hspace{1cm} (8)

$$a(r - r_0) = r^*.$$ \hspace{1cm} (9)

Therefore, the dimensionless time independent fractional Schrödinger equation for Morse potential is given by the following formula:

$$(e^{-r^*} - 1)^2\tilde{\Psi}(r^*) + C^*D_{1,\alpha}\tilde{\Psi}(r^*) = E^*\tilde{\Psi}(r^*),$$ \hspace{1cm} (10)

where $\tilde{\Psi}(r^*)$ and $E^*$ are the eigenvectors and eigenvalues of the previous dimensionless fractional Schrödinger equation for Morse potential.

If we use the Riemann–Liouville definition of the fractional derivatives for increasing values of variable, which is given by

$$\frac{D_w^\alpha \Psi(r)}{\partial r^\alpha} = \frac{1}{\Gamma(w-a)} \int_0^r \frac{\partial \Psi(s)}{\partial r^\alpha} \frac{r^{1-w}}{(r-s)^{1-a}} ds; \hspace{1cm} r^* > a$$ \hspace{1cm} (11)

and the midpoint quadrature formula, we find the relation between $\Psi(r_0^*)$ and $\Psi(r_{n+1}^*)$ or the iteration formula for the wave function as follows:

$$\Psi(r_{n+1}^*) \approx \left[ E^* - (e^{-r_{n+1}^*} - 1)^2 - 2C^* \left( \frac{r_{n+1}^*}{r_{n+1}^* - a} \right)^{2-a} \right]^{-1} \times \frac{2C^*}{r_{n+1}^* - a} \left( \frac{r_{n+1}^*}{2} \right)^{2-a} \Psi(r_{n+1}^*),$$ \hspace{1cm} (12)

where $C^*$ is a dimensionless parameter and $\Delta r^*$ is the step of the dimensionless distance, i.e.,

$$\Delta r^* = r_{n}^* - r_{n-1}^*.$$ \hspace{1cm} (13)

$\Gamma(\theta)$ is the gamma function defined as

$$\Gamma(\theta) = \int_0^\infty z^{\theta-1}e^{-z} dz,$$ \hspace{1cm} (14)

where

$$Re(\theta) > 0 \land \theta \neq -q; \hspace{1cm} q \in N^+.$$ \hspace{1cm} (15)

Equation (12) is the iteration formula that we found to solve the time independent fractional Schrödinger equation in the case of Morse potential numerically.

III. RESULTS AND DISCUSSIONS

The iteration formula that we found [Eq. (12)] is used to find solutions of the fractional Schrödinger equation in the time independent form of the equation in the case of Morse potential in the dimensionless formalism; however, if we need the full solutions, we apply Eq. (6) to find them. The formula is applied in case of the system that obey Morse potential, and all we need to find the numerical solutions for the wave function of the system are the parameters and the constants in the formula that we found in addition to guessing an initial value of the wave function and a value of the space dependent Schrödinger equation’s fractional parameter, which takes its values in the range $[1, 2]$.

We applied the iteration formula that we found for the dimensionless parameter $C^* = 1$ and for multiple values of the fractional parameter of the space dependent fractional Schrödinger equation. In each case of the space dependent fractional Schrödinger equation’s fractional parameter, we took five values of the dimensionless eigenvalue of the equation. We used the MATLAB program to calculate our results and to code the formula that we found. The code of MATLAB, which is used for this purpose, was illustrated in the Appendix.

The wave function values for $\alpha = 1.1$ are shown in Table I, which includes five columns of the wave function values $\Psi_1, \Psi_2, \Psi_3, \Psi_4$, and $\Psi_5$ for five values of $E^*$, and these values of $E^*$ are $-1, 0, 0.5, 100, \text{ and } 1000$, respectively.

Results of the wave function values for $\alpha = 1.9$ are illustrated in Table II, which also includes the five columns of the wave function values $\Psi_1, \Psi_2, \Psi_3, \Psi_4$, and $\Psi_5$ for five values of $E^*$, and these values of $E^*$ are $-1, 0, 0.5, 100, \text{ and } 1000$, respectively.

As we see from Table I, the real part of the wave function for the fractional parameter of the space dependent fractional Schrödinger equation $\alpha = 1.1$ and the reduced energy $-1$ decreases when the dimensionless distance increases from about zero to $0.000 \text{,} 000 \text{,} 27$, then takes negative values and return to increase when the dimensionless distance increases from $0.002 \text{,} 286$ to $0.294 \text{,} 894$, and after that takes positive values but smaller than the previous positive values. We see the same thing for the real parts of the wave functions for the other values of the reduced energies, where these values of the real parts
The wave functions for $\alpha = 1.1$ and multiple values of $E^*$. 

| $r^*$          | $\Psi_1$       | $\Psi_2$       | $\Psi_3$       | $\Psi_4$       | $\Psi_5$       |
|---------------|----------------|----------------|----------------|----------------|----------------|
| $1.80 \times 10^{-5}$ | 2.038262       | 1.019317       | 1.019320       | 1.019931       | 1.025490       |
|               | + 0.662388 i   | + 0.331196 i   | + 0.331197 i   | + 0.331395 i   | + 0.333201 i   |
| $5.40 \times 10^{-5}$ | 1.617995       | 0.809247       | 0.809262       | 0.810968       | 0.828883       |
|               | + 1.175542 i   | + 0.587785 i   | + 0.587793 i   | + 0.589203 i   | + 0.602218 i   |
| $0.000126$     | 0.982663 i     | 0.491364 i     | 0.491380 i     | 0.494633 i     | 0.525574 i     |
|               | + 1.35232 i    | + 0.676304 i   | + 0.676327 i   | + 0.68084 i    | + 0.723390 i   |
| $0.00027$      | 0.396746 i     | 0.198405 i     | 0.198421 i     | 0.201545 i     | 0.233281 i     |
|               | + 1.221070 i   | + 0.610630 i   | + 0.610678 i   | + 0.61293 i    | + 0.717695 i   |
| $0.000558$     | $-2.512579 \times 10^{-15}$ | $-1.209404 \times 10^{-15}$ | $-1.288057 \times 10^{-15}$ | $-1.312425 \times 10^{-15}$ | $-1.930948 \times 10^{-15}$ |
|               | + 0.913568 i   | + 0.456940 i   | + 0.45909 i    | + 0.459297 i   | + 0.660529 i   |
| $0.001134$     | $-0.186775 i$  | $-0.093455 i$  | $-0.093488 i$  | $-0.100552 i$  | $-0.217602 i$  |
|               | + 0.574835 i   | + 0.287625 i   | + 0.287729 i   | + 0.309467 i   | + 0.669711 i   |
| $0.002286$     | $-0.218870 i$  | $-0.109597 i$  | $-0.109679 i$  | $-0.127680 i$  | $-0.183201 i$  |
|               | + 0.301249 i   | + 0.150848 i   | + 0.150960 i   | + 0.157735 i   | + 1.490891 i   |
| $0.00459$      | $-0.172892 i$  | $-0.086707 i$  | $-0.086838 i$  | $-0.119329 i$  | $-1.602282 i$  |
|               | + 0.125613 i   | + 0.062996 i   | + 0.063092 i   | + 0.086697 i   | + 1.164126 i   |
| $0.009198$     | $-0.108626 i$  | $-0.054644 i$  | $-0.054811 i$  | $-0.108608 i$  | $-0.486480 i$  |
|               | + 0.035294 i   | + 0.017735 i   | + 0.017809 i   | + 0.033888 i   | + 0.158067 i   |
| $0.018414$     | $-0.056769 i$  | $-0.028734 i$  | $-0.028918 i$  | $-0.148622 i$  | $0.049599 i$   |
|               | $-3.042653 \times 10^{-16}$ | $-1.567578 \times 10^{-16}$ | $-1.627916 \times 10^{-16}$ | $-8.064968 \times 10^{-16}$ | $+ 2.774853 \times 10^{-16}$ |
| $0.036846$     | $-0.024883 i$  | $-0.012749 i$  | $-0.012907 i$  | $0.284171 i$   | $-0.001944 i$  |
|               | $-0.008085 i$  | $-0.001422 i$  | $-0.001494 i$  | $+ 0.092332 i$ | $-0.000631 i$  |
| $0.07371$      | $-0.008991 i$  | $-0.004720 i$  | $-0.004838 i$  | $-0.071842 i$  | $+ 3.044152 i$ |
|               | $-0.00653246 i$ | $-0.003429 i$  | $-0.003515 i$  | $-0.052196 i$  | $+ 2.211706 i$ |
| $0.147438$     | $-0.00252618 i$ | $-0.001396 i$  | $-0.001462 i$  | $0.005395 i$   | $-1.859714 i$  |
|               | $-0.00047699 i$ | $-0.001915 i$  | $-0.002012 i$  | $+ 0.007425 i$ | $-2.559677 i$  |
| $0.294894$     | $-0.00045542 i$ | $-0.000275 i$  | $-0.000304 i$  | $-0.000121 i$  | $+ 3.795872 i$ |
|               | $-0.00140144 i$ | $-0.000847 i$  | $-0.000936 i$  | $-0.000373 i$  | $+ 1.168249 i$ |
| $0.589806$     | $3.466118 \times 10^{-18}$ | $2.518662 \times 10^{-18}$ | $3.164977 \times 10^{-18}$ | $-5.965234 \times 10^{-20}$ | $1.873473 i$   |
|               | $-0.00042144 i$ | $-0.000303 i$  | $-0.000370 i$  | $+ 7.433522 i$ | $-2.213711 i$  |
| $1.17963$      | $2.712730 \times 10^{-5}$ | $2.599738 \times 10^{-5}$ | $3.805060 \times 10^{-5}$ | $1.980743 i$   | $-5.738138 i$  |
|               | $-8.348925 \times 10^{-5}$ | $-8.001170 \times 10^{-5}$ | $-0.000117 i$  | $-6.096101 i$  | $+ 1.766017 i$ |

The wave functions decrease from the dimensionless distance about zero to take alternately positive and negative values, which means that the real parts of the wave functions of the fractional parameter of the space dependent fractional Schrödinger equation $\alpha = 1.9$ from Table II, which also have alternating and decreased values for all values of the reduced energies.

We plotted the amplitude of the wave functions, after normalizing them, vs the dimensionless distance for the fractional parameter of the space dependent fractional Schrödinger equation $\alpha = 1.1$, and...
TABLE II. The wave functions for $\alpha = 1.9$ and multiple values of $E^*$. 

| $r^*$       | $\Psi_1$          | $\Psi_2$          | $\Psi_3$          | $\Psi_4$          | $\Psi_5$          |
|-------------|-------------------|-------------------|-------------------|-------------------|-------------------|
| $1.80 \times 10^{-5}$ | $-3.549 \, 469$  | $-1.774 \, 734$  | $-1.774 \, 734$  | $-1.774 \, 735$  | $-1.774 \, 743$  |
| 5.40 $\times 10^{-5}$ | $1.618 \, 034$   | $0.809 \, 017 \, 0$  | $0.809 \, 017 \, 0$  | $0.809 \, 018 \, 6$  | $0.809 \, 032 \, 9$  |
| 0.000 126 | $-0.234 \, 375 \, 7$  | $-0.117 \, 187 \, 8$  | $-0.117 \, 187 \, 8$  | $-0.117 \, 188 \, 5$  | $-0.117 \, 194 \, 2$  |
| 0.000 27 | $0.011 \, 459 \, 38$  | $0.005 \, 729 \, 688$  | $0.005 \, 729 \, 689$  | $0.005 \, 729 \, 762$  | $0.005 \, 730 \, 422$  |
| 0.000 558 | $2.309 \, 908 \times 10^{-18}$  | $1.062 \, 558 \times 10^{-18}$  | $1.247 \, 351 \times 10^{-18}$  | $1.016 \, 375 \times 10^{-18}$  | $1.247 \, 541 \times 10^{-18}$  |
| 0.001 134 | $-1.307 \, 974 \times 10^{-5}$  | $-6.539 \, 874 \times 10^{-6}$  | $-6.539 \, 875 \times 10^{-6}$  | $-6.540 \, 260 \times 10^{-6}$  | $-6.543 \, 740 \times 10^{-6}$  |
| 0.002 286 | $3.202 \, 592 \times 10^{-7}$  | $1.601 \, 298 \times 10^{-7}$  | $1.601 \, 299 \times 10^{-7}$  | $1.601 \, 493 \times 10^{-7}$  | $1.603 \, 248 \times 10^{-7}$  |
| 0.004 59 | $-3.019 \, 185 \times 10^{-9}$  | $-1.509 \, 596 \times 10^{-9}$  | $-1.509 \, 598 \times 10^{-9}$  | $-1.509 \, 969 \times 10^{-9}$  | $-1.513 \, 335 \times 10^{-9}$  |
| 0.009 198 | $1.298 \, 148 \times 10^{-11}$  | $6.490 \, 771 \times 10^{-12}$  | $6.490 \, 788 \times 10^{-12}$  | $6.494 \, 011 \times 10^{-12}$  | $6.523 \, 265 \times 10^{-12}$  |
| 0.018 414 | $-2.670 \, 606 \times 10^{-14}$  | $-1.335 \, 316 \times 10^{-14}$  | $-1.335 \, 323 \times 10^{-14}$  | $-1.336 \, 656 \times 10^{-14}$  | $-1.348 \, 797 \times 10^{-14}$  |
| 0.036 846 | $2.660 \, 705 \times 10^{-17}$  | $1.330 \, 379 \times 10^{-17}$  | $1.330 \, 393 \times 10^{-17}$  | $1.333 \, 058 \times 10^{-17}$  | $1.357 \, 496 \times 10^{-17}$  |
| 0.073 71 | $-1.270 \, 007 \times 10^{-20}$  | $-6.350 \, 291 \times 10^{-21}$  | $-6.350 \, 419 \times 10^{-21}$  | $-6.375 \, 939 \times 10^{-21}$  | $-6.613 \, 110 \times 10^{-21}$  |
| 0.147 438 | $2.773 \, 920 \times 10^{-24}$  | $1.387 \, 072 \times 10^{-24}$  | $1.387 \, 127 \times 10^{-24}$  | $1.398 \, 315 \times 10^{-24}$  | $1.505 \, 202 \times 10^{-24}$  |
| 0.294 894 | $-2.349 \, 037 \times 10^{-28}$  | $-1.174 \, 708 \times 10^{-28}$  | $-1.174 \, 803 \times 10^{-28}$  | $-1.193 \, 864 \times 10^{-28}$  | $-1.386 \, 642 \times 10^{-28}$  |
| 0.589 806 | $-0.000 \, 000 \times 10^{-32}$  | $-0.000 \, 000 \times 10^{-32}$  | $-0.000 \, 000 \times 10^{-32}$  | $-0.000 \, 000 \times 10^{-32}$  | $-0.000 \, 000 \times 10^{-32}$  |
| 1.179 63 | $9.373 \, 408 \times 10^{-37}$  | $4.689 \, 729 \times 10^{-37}$  | $4.691 \, 243 \times 10^{-37}$  | $5.005 \, 937 \times 10^{-37}$  | $9.746 \, 642 \times 10^{-37}$  |

results of this are shown in Fig. 1 for $E^* = -1$ (the red-plus sign curve), $E^* = 0$ (the green-asterisk sign curve), $E^* = 0.5$ (the black-circle sign curve), $E^* = 100$ (the cyan-x sign curve), and $E^* = 1000$ (the magenta-rectangle sign curve).

As we note from Figs. 1 and 2, the most probable reduced energy is 100 from the dimensionless distance about zero to the dimensionless distance about 0.3, and after that the most probable energy is 0.5 for the fractional parameter of the space dependent fractional Schrödinger equation $\alpha = 1.1$, and the reduced energy 1000 is the least probable energy in this case.
Figures 3 and 4 include the amplitude of the wave functions and the probabilities for the fractional parameter of the space dependent fractional Schrödinger equation $\alpha = 1.2$ for $E^* = -1$ (the red-plus sign curve), $E^* = 0$ (the green-asterisk sign curve), $E^* = 0.5$ (the black-circle sign curve), $E^* = 100$ (the cyan-x sign curve), and $E^* = 1000$ (the magenta-rectangle sign curve).

We can see from Figs. 3 and 4 that the most probable reduced energy is 1000 from the dimensionless distance about zero to the dimensionless distance about 0.05 and after that the most probable energy is 100 from the dimensionless distance 0.05 to about 0.8, and then the most probable energy is 0.5 for the fractional parameter of the space dependent fractional Schrödinger equation $\alpha = 1.2$.

Figures 5 and 6 include the amplitude of the wave functions and the probabilities for the fractional parameter of the space dependent fractional Schrödinger equation $\alpha = 1.3$ for $E^* = -1$ (the red-plus sign curve), $E^* = 0$ (the green-asterisk sign curve), $E^* = 0.5$ (the black-circle sign curve), $E^* = 100$ (the cyan-x sign curve), and $E^* = 1000$ (the magenta-rectangle sign curve).

We can see from Figs. 5 and 6 that the most probable reduced energy is 1000 from the dimensionless distance about zero to the dimensionless distance about 0.05 and after that the most probable energy is 100 from the dimensionless distance 0.05 to about 0.8, and then the most probable energy is 0.5 for the fractional parameter of the space dependent fractional Schrödinger equation $\alpha = 1.3$. 

**FIG. 1.** Amplitude of the wave function for $\alpha = 1.1$.

**FIG. 2.** The probability vs reduced $r$ for $\alpha = 1.1$.

**FIG. 3.** Amplitude of the wave function for $\alpha = 1.2$.

**FIG. 4.** The probability vs reduced $r$ for $\alpha = 1.2$.

**FIG. 5.** Amplitude of the wave function for $\alpha = 1.3$.

**FIG. 6.** The probability vs reduced $r$ for $\alpha = 1.3$. 

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FIG. 6. The probability vs reduced $r$ for $\alpha = 1.3$.

As we can see from Figs. 5 and 6, the most probable reduced energy is 1000 from the dimensionless distance about zero to the dimensionless distance about 0.15 and after that the most probable energy is 100 from the dimensionless distance 0.15 for the fractional parameter of the space dependent fractional Schrödinger equation $\alpha = 1.3$.

Figure 7 and 8 include the amplitude of the wave functions and the probabilities for the fractional parameter of the space dependent fractional Schrödinger equation $\alpha = 1.4$ for $E^* = -1$ (the red-plus sign curve), $E^* = 0$ (the green-asterisk sign curve), $E^* = 0.5$ (the black-circle sign curve), $E^* = 100$ (the cyan-x sign curve), and $E^* = 1000$ (the magenta-rectangle sign curve).

From Figs. 7 and 8, we can see that the most probable reduced energy is 1000 from the dimensionless distance about zero to the dimensionless distance about 0.5 and after that the most probable energy is 100 from the dimensionless distance 0.5 for the fractional parameter of the space dependent fractional Schrödinger equation $\alpha = 1.4$.

Figures 9 and 10 include the amplitude of the wave functions and the probabilities for the fractional parameter of the space dependent fractional Schrödinger equation $\alpha = 1.5$ for $E^* = -1$ (the red-plus sign curve), $E^* = 0$ (the green-asterisk sign curve), $E^* = 0.5$ (the black-circle sign curve), $E^* = 100$ (the cyan-x sign curve), and $E^* = 1000$ (the magenta-rectangle sign curve).

From Figs. 9 and 10, we can see that the most probable reduced energy is 1000 from the dimensionless distance about zero to the dimensionless distance about 1 and after that the most probable energy is 100 from the dimensionless distance 1 for the fractional parameter of the space dependent fractional Schrödinger equation $\alpha = 1.5$. 

FIG. 7. Amplitude of the wave function for $\alpha = 1.4$.

FIG. 9. Amplitude of the wave function for $\alpha = 1.5$. 

FIG. 8. The probability vs reduced $r$ for $\alpha = 1.4$. 

FIG. 9. The probability vs reduced $r$ for $\alpha = 1.3$. 

(continued on the next page)
Figures 11 and 12 include the amplitude of the wave functions and the probabilities for the fractional parameter of the space dependent fractional Schrödinger equation $\alpha = 1.6$ for $E^* = -1$ (the red-plus sign curve), $E^* = 0$ (the green-asterisk sign curve), $E^* = 0.5$ (the black-circle sign curve), $E^* = 100$ (the cyan-x sign curve), and $E^* = 1000$ (the magenta-rectangle sign curve).

Figures 13 and 14 include the amplitude of the wave functions and the probabilities for the fractional parameter of the space dependent fractional Schrödinger equation $\alpha = 1.7$ for $E^* = -1$ (the red-plus sign curve), $E^* = 0$ (the green-asterisk sign curve), $E^* = 0.5$ (the black-circle sign curve), $E^* = 100$ (the cyan-x sign curve), and $E^* = 1000$ (the magenta-rectangle sign curve).

Figures 15 and 16 include the amplitude of the wave functions and the probabilities for the fractional parameter of the space dependent fractional Schrödinger equation $\alpha = 1.8$ for $E^* = -1$ (the red-plus sign curve), $E^* = 0$ (the green-asterisk sign curve), $E^* = 0.5$ (the black-circle sign curve), $E^* = 100$ (the cyan-x sign curve), and $E^* = 1000$ (the magenta-rectangle sign curve).
FIG. 15. Amplitude of the wave function for $\alpha = 1.8$.

FIG. 16. The probability vs reduced $r$ for $\alpha = 1.8$.

FIG. 17. Amplitude of the wave function for $\alpha = 1.9$.

FIG. 18. The probability vs reduced $r$ for $\alpha = 1.9$.

From Figs. 11–16, we can see that the most probable reduced energy is 1000 for the fractional parameters of the space dependent fractional Schrödinger equation $\alpha = 1.6$, $\alpha = 1.7$, and $\alpha = 1.8$ for all values of the dimensionless distance.

Figures 17 and 18 include the amplitude of the wave functions and the probabilities for the fractional parameter of the space dependent fractional Schrödinger equation $\alpha = 1.9$ for $E^* = -1$ (the red-plus sign curve), $E^* = 0$ (the green-asterisk sign curve), $E^* = 0.5$ (the black-circle sign curve), $E^* = 100$ (the cyan-x sign curve), and $E^* = 1000$ (the magenta-rectangle sign curve).

We can see from the last two figures (Figs. 17 and 18) that the probabilities of all reduced energies for the fractional parameter of the space dependent fractional Schrödinger equation $\alpha = 1.9$ are approximately equivalent. Besides, we see from all the previous figures that the most probable values are, in general, for $E^* = 0.5$ and $E^* = 100$ from $\alpha = 1.1$ to $\alpha = 1.4$ for the most reduced distance values (Figs. 1–8), but when the fractional parameter reaches 1.5, the most probable values occur for $E^* = 1000$, then from the fractional parameter $\alpha = 1.7$ and bigger than this value, the probability values for all reduced energies are semi-equal; hence we have degeneracy states.

Finally, we applied the numerical formula that we found for the space dependent fractional Schrödinger equation in the case of Morse potential in two physical systems, when the fractional parameter of the space dependent fractional Schrödinger equation equals 2 and we used an approximation to gamma function near zero in the calculations. The first case is for hydrogen fluoride (HF) molecule and the other is for hydrogen chloride (HCl) molecule. We calculated the wave function values of the hydrogen fluoride molecule, which has the following parameters of Morse potential: the well depth of the Morse potential is $U_0 = 0.6457$ eV and the equilibrium bond distance is...
where $m_i$, $m_f$, and $m_{\text{Cl}}$ are the masses of the hydrogen atom, fluorine atom, and chlorine atom, respectively. We took five values of the reduced energy in each case.

We inserted the values of wave functions for the hydrogen chloride molecule for the fractional parameter of the space dependent fractional Schrödinger equation $\alpha = 2$ in Table III, which includes five columns of the wave function values, where $\Psi 1$ corresponds to the reduced energy 0.1373, $\Psi 2$ corresponds to the reduced energy 0.3940, $\Psi 3$ corresponds to the reduced energy 0.6268, $\Psi 4$ corresponds to the reduced energy 0.8359, and $\Psi 5$ corresponds to the reduced energy 1.0211.

In addition, we inserted the values of wave functions for the hydrogen fluoride molecule for the fractional parameter of the space

| $r^*$ | $\Psi_1$  | $\Psi_2$  | $\Psi_3$  | $\Psi_4$  | $\Psi_5$  |
|-------|-----------|-----------|-----------|-----------|-----------|
| $1.80 \times 10^{-5}$ | $-224.4017071$ | $-231.4793748$ | $-233.4068203$ | $-234.201468$ | $-234.606$  |
| $5.40 \times 10^{-5}$ | $71.9114592$ | $44.38951569$ | $32.80542561$ | $26.55153208$ | $22.70627$  |
| $0.000126$ | $-1.596304311$ | $-1.55735657$ | $-0.784470049$ | $-0.494302827$ | $0.35301$  |
| $0.00027$ | $0.09768888$ | $0.012309066$ | $0.00406557$ | $0.001954844$ | $0.001155$  |
| $0.000588$ | $-0.000479595$ | $-2.33 \times 10^{-5}$ | $-4.94 \times 10^{-6}$ | $-1.80 \times 10^{-6}$ | $-8.74 \times 10^{-7}$  |
| $0.00134$ | $6.06 \times 10^{-7}$ | $1.08 \times 10^{-8}$ | $1.46 \times 10^{-9}$ | $3.99 \times 10^{-10}$ | $1.59 \times 10^{-10}$  |
| $0.00286$ | $-1.95 \times 10^{-10}$ | $-1.24 \times 10^{-12}$ | $-1.06 \times 10^{-13}$ | $-2.18 \times 10^{-14}$ | $-7.13 \times 10^{-15}$  |
| $0.00459$ | $1.58 \times 10^{-14}$ | $3.56 \times 10^{-17}$ | $1.91 \times 10^{-18}$ | $2.95 \times 10^{-19}$ | $7.90 \times 10^{-20}$  |
| $0.00996$ | $-3.21 \times 10^{-19}$ | $-2.54 \times 10^{-22}$ | $-8.57 \times 10^{-24}$ | $-9.95 \times 10^{-25}$ | $-2.18 \times 10^{-25}$  |
| $0.01841$ | $1.64 \times 10^{-24}$ | $4.53 \times 10^{-28}$ | $9.61 \times 10^{-30}$ | $8.36 \times 10^{-31}$ | $1.50 \times 10^{-31}$  |
| $0.03685$ | $-2.11 \times 10^{-30}$ | $-2.02 \times 10^{-34}$ | $-2.70 \times 10^{-36}$ | $-1.76 \times 10^{-37}$ | $-2.58 \times 10^{-38}$  |
| $0.07371$ | $7.00 \times 10^{-37}$ | $2.28 \times 10^{-41}$ | $1.90 \times 10^{-43}$ | $9.28 \times 10^{-45}$ | $1.12 \times 10^{-45}$  |
| $0.14745$ | $-6.67 \times 10^{-44}$ | $-6.66 \times 10^{-49}$ | $-3.43 \times 10^{-51}$ | $-1.25 \times 10^{-52}$ | $-1.22 \times 10^{-53}$  |
| $0.29484$ | $2.46 \times 10^{-51}$ | $5.55 \times 10^{-57}$ | $1.67 \times 10^{-59}$ | $4.43 \times 10^{-61}$ | $3.50 \times 10^{-62}$  |
| $0.58980$ | $2.75 \times 10^{-59}$ | $-1.94 \times 10^{-65}$ | $-2.67 \times 10^{-68}$ | $-4.76 \times 10^{-70}$ | $-2.91 \times 10^{-71}$  |
| $1.17963$ | $1.37 \times 10^{-68}$ | $-3.88 \times 10^{-74}$ | $3.11 \times 10^{-77}$ | $2.29 \times 10^{-79}$ | $9.20 \times 10^{-81}$  |
dependent fractional Schrödinger equation $\alpha = 2$ in Table IV, which includes five columns of the wave function values, where $\Psi_1$ corresponds to the reduced energy 0.1744, $\Psi_2$ corresponds to the reduced energy 0.4998, $\Psi_3$ corresponds to the reduced energy 0.7940, $\Psi_4$ corresponds to the reduced energy 1.0569, and $\Psi_5$ corresponds to the reduced energy 1.2885. In the calculations of Tables III and IV, we used the step 0.000 018 for the dimensionless distance in the two cases.

As we see from Table III, the values of wave functions of the hydrogen chloride molecule for the fractional parameter of the space dependent fractional Schrödinger equation $\alpha = 2$ and for all values of the dimensionless energy are alternating and decreased, and we note that the most probable dimensionless energy is 0.1373. In addition, we can see the same thing in the case of the hydrogen fluoride molecule from Table IV, where all values of the wave functions are alternating and decreased, but the most probable dimensionless energy is 0.1744 for this molecule. Besides, all values of the wave functions for all energy are real in the two cases.

IV. CONCLUSIONS

In this study, we derived a numerical algorithm [Eq. (12)] to solve the space dependent fractional Schrödinger equation in the case of Morse potential in the stationary state based on the Riemann–Liouville definition of the fractional derivatives for increasing values. The numerical algorithm that we found applied in the case of the systems that interact via Morse potential in the vibrational states and that formula depends on the dimensionless Morse potential parameters in addition to the fractional parameter of the space dependent fractional Schrödinger equation. We used the dimensionless formalism of the fractional Schrödinger equation of Morse potential because it is simple and needs less time for computational calculations.

We applied the numerical algorithm to find the wave functions and the probability functions of a system for multiple values of the fractional parameter of the space dependent fractional Schrödinger equation and for every value of the fractional parameter’s values, we found the wave functions and the probabilities for multiple values of $E^*$. We found that the probability values of a very big fractional parameter of the space dependent fractional Schrödinger equation (Figs. 16 and 18) are semi-equal. Besides, we applied the iteration formula that we derived for the fractional Schrödinger equation of the Morse potential to find the values of wave functions for the hydrogen chloride (HCl) molecule and for the hydrogen fluoride (HF) molecule, and we found that all values of the wave functions in these two cases are purely real.

We found that the wave function values are alternating and decreased for all cases we calculated and are acceptable for all cases of the fractional parameter of the space dependent fractional Schrödinger equation and all energy values that we used because they move to zero when the distance increases. We believe that the formula that we derived for the fractional Schrödinger equation in the case of Morse potential can be applied in the systems described by Morse potential in the vibrational states.

APPENDIX: THE CODE OF THE ALGORITHM

In the Appendix, we illustrate the MATLAB code used to calculate our results for the following reduced $r$ range $r^* = [\Delta r^*:\Delta r^*:2.5]$ and for multiple values of reduced energy and fractional parameter.

```matlab
%Marwan file for fractional Morse. run consfileoffathing tic %Start the time. % E MorseRedMrseFRACTALMorse = 2500:0.1:2500; CCFULLMorsefractalformn = -3:0.1:3; % nEE = length(E MorseRedMrseFRACTALMorse); % %The fractal. sfullMORSEfullam = 1.001:0.001:1.999; % for w1 = 1:nEE nCC = length(CCFULLMorsefractalformn); for w2 = 1:nCC nsf = length(sfullMORSEfullam); for frctalnumber = 1:length(sfullMORSEfullam) TaMrseFRACTAL0 = ; TaMrseFRACTALMorse = Ta0; na = round((max(rr)-min(rr))/ddr) for wa = 1:(na-1)./2 TaMrseFRACTALMorse(2*wa+1) = [E MorseRedMrseFRACTALMorse(w1)- (1-exp(-rr(wa))).^2... (2*CCFULLMorsefractalformn(w2)^2*(ddr./2)... ./(2-sfullMORSEfullam(frctalnumber)))].
```
end
end
end
end

\% 
TasparMrseFRACTALMorse = sparse(TasparMrseFRACTALMorse);
\% 
 siaTaMrseFRACTALMorse = find(TasparMrseFRACTALMorse);
\% 
wwwa = size(siaTaMrseFRACTALMorse);
for wwa = 1:wwwa(2)
  rrfull(wwa) = rr(siaTaMrseFRACTALMorse(wwa));
end
Ta=(nonzeros(TasparMrseFRACTALMorse))';
\% 
save thefractionalMarwanMALFA1Morse19.mat
\%
Thetime = toc./60;
\%End time.
\%
fprintf(’The time of all file = %6.3f min\n’, Thetime);
\%
\% 
Thecpuetime = cputime./60;
\%
fprintf(’The cpuetime of all file = %6.3f min\n’, Thecpuetime);
\%

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