




The generalized fractional NU method for the diatomic molecules in the Deng–Fan model

M. Abu-Shady^{1,a}, E. M. Khokha^{2,b} , and T. A. Abdel-Karim^{1,c}

¹ Department of Mathematics and Computer Science, Faculty of Science, Menoufia University, Shibin El Kom, Egypt

² Department of Basic Science, Modern Academy for Engineering and Technology, Maadi, Egypt

Received 22 June 2022 / Accepted 10 August 2022

© The Author(s) 2022

Abstract. A solution of the fractional N -dimensional radial Schrödinger equation (SE) with the Deng–Fan potential (DFP) is investigated by the generalized fractional Nikiforov–Uvarov (NU) method. The analytical formulas of energy eigenvalues and corresponding eigenfunctions for the DFP are generated. Furthermore, the current results are applied to several diatomic molecules (DMs) for the DFP as well as the shifted Deng–Fan potential (SDFP). For both the DFP and its shifted potential, the effect of the fractional parameter (δ) on the energy levels of various DMs is examined numerically and graphically. We found that the energy eigenvalues are gradually improved when the fractional parameter increases. The energy spectra of various DMs are also evaluated in three-dimensional space and higher dimensions. It is worthy to note that the energy spectrum raises as the number of dimensions increases. In addition, the dependence of the energy spectra of the DFP and its shifted potential on the reduced mass, screening parameter, equilibrium bond length and rotational and vibrational quantum numbers is illustrated. To validate our findings, the energy levels of the DFP and SDFP are estimated at the classical case ($\delta = 1$) for various DMs and found that they are entirely compatible with earlier studies.

1 Introduction

Fractional calculus (FC) has attracted a huge number of researchers throughout the last decades in the last and present century. The prominence of FC in diverse disciplines of science and engineering has grown considerably [1–3]. The foundations of FC are non-integer order differentiation and integration. In the literature, numerous definitions have been suggested for the fractional differential equations. The definitions of Jumarie [4], Riemann–Liouville [5] and Caputo [6] are the most appropriate for physical circumstances and have received a lot of attention.

By using Jumarie-type derivative rules, Das et al. [7, 8] investigated the approximate solutions of the N -dimensional fractional SE for generalized Mie-type potentials [7] and pseudoharmonic potential [8] for a typical DM, and they obtained the mass spectra of quarkonia with the Cornell potential corresponds to the fractional parameter $\alpha = 0.5$. In addition, they employed the power series approach to investigate the solution of the fractional Klein–Gordon (KG) equation with fractional scalar and vector and potentials [9].

Al-Raei and El-Daher relied on the definition of Riemann–Liouville fractional derivative with a numerical technique to solve the space-dependent fractional SE for the Coulomb potential [10], Van Der Walls potential [11], Lennard–Jones potential [12] and Morse potential [13].

Recently, Khalil [14] has proposed a new definition of fractional derivative termed conformable fractional derivative (CFD) which upholds essential classical characteristics. Abdeljawad [15] extended the definition and established the fundamental notions of the CFD. Depending on the CFD, Karayer et al. [16] presented conformable fractional (CF) NU method to investigate the solutions of the SE with different potentials.

Chung et al. [17] used the Heun function to investigate the CF SE for the Killingbeck and hyperbolic potentials. Within the context of CF quantum mechanics, the three-dimensional fractional harmonic oscillator was explored and some expectation values were obtained in Ref. [18]. The CF NU approach was used to obtain the one-dimensional KG equation for the generalized Hulthén potential [19]. In Ref. [20], the fractional SE for a particle with position-dependent mass in an infinite potential well was studied using the CFD. In the context of the CFD, the N -dimensional radial SE was used to investigate the properties of heavy quarkonia for the dependent temperature potential [21], Trigonometric Rosen–Morse potential [22], hot-magnetized inter-

^a e-mail: dr.abushady@gmail.com

^b e-mail: emad.mohammed@eng.modern-academy.edu.eg (corresponding author)

^c e-mail: tabdelkarim63@yahoo.com

action potential [23], and generalized Cornell potential [24]. The impact of fraction-order and dimensional number on heavy-quarkonium masses was also examined. Hammad et al. [25] used the CF NU method to develop the solutions of the CF Bohr Hamiltonian with the Kratzer potential for triaxial nuclei. Abu-Shady [26] explored the mathematical model for the Coronavirus Disease 2019 using the concept of the CFD. The fractional SE with the screened Kratzer potential [27] and Morse potential [28] was solved using the CF NU technique and the energies of several DMs were estimated for various fractional values.

The investigation of DMs is a prominent branch of chemistry and molecular physics. Several authors have recently examined the solution of relativistic and non-relativistic wave equations in order to understand the characteristics of some DMs using different molecular potentials. There is a considerable number of empirical potentials in the literature that provide a proper description of the interactions between atoms in the DM as the Kratzer [29], Morse [30], Pöschl–Teller [31], Manning–Rosen [32], Hulthén [33], Schlöberg [34], and Tietz–Hua potentials [35].

The DFP is generally renowned as one of the most empirical potentials for accurately describing the DM energy spectrum and electromagnetic transitions. In 1957, Deng and Fan [36] postulated the DFP to explain the ro-vibrational spectrum of the DM, also called the generalized Morse potential. The DFP is regarded an empirical potential because it has the proper physical boundary conditions at the origin and infinity. The DFP takes the form [37, 38]

$$V(r) = D_e \left(1 - \frac{be^{-\alpha r}}{1 - e^{-\alpha r}} \right)^2, \\ b = e^{\alpha r_e} - 1, \quad r \in (0, \infty). \quad (1)$$

The SDFP is also defined as [39]

$$V(r) = D_e \left(1 - \frac{be^{-\alpha r}}{1 - e^{-\alpha r}} \right)^2 - D_e, \quad (2)$$

where D_e , r_e and α are the dissociation energy, the equilibrium bond length and the screening parameter which indicates the radius of the potential, respectively.

Copious theoretical studies were reported to derive the solutions of the DFP and SDFP in both relativistic and non-relativistic regimes. For example, the approximate solutions of the DFP were investigated using the hypergeometric functions with the SE [37] and with KG equation [38]. Zhang et al. [39] solved the SE with the DFP using the supersymmetric shape invariance formalism and also computed the rotational transition frequencies for HF molecule. By using the exact quantization rule method, Falaye et al. [40] obtained the solutions of the SE with the DFP and calculated the ro-vibrational energy of some DMs. Ikhdair [41] studied the solutions of the Dirac equation for the DFP with spin and pseudospin symmetries by the NU method. Oluwadare et al. [42] solved the KG and Dirac equa-

tions using the NU method with the DFP. Mustafa [43] calculated the vibrational energies of Li_2 DM with the SE for the DFP. The NU technique was used to solve the SE with the DFP [44] and SDFP [45], as well as the energy levels for a set of DMs were also reported.

The solutions of the SE with the SDFP were found and the ro-vibrational energies for various DMs were also computed using the asymptotic iteration method [46], and the generalized pseudospectral method [47]. Oluwadare and Oyewumi [48] used the proper quantization rule to explore the approximate solutions of the SE with the SDFP, as well as the energy levels and the expectation values of DMs were investigated. The Feynman path integral method [49] was employed to explore the approximate solutions of the SDFP. Furthermore, the energy eigenvalues and the eigenfunctions were investigated for some DMs. Omugbe [50] used the WKB method to estimate the energy spectrum of the SE with the DFP for HCl, LiH and ScH molecules. Nath and Roy [51] utilized the NU method to evaluate the ro-vibrational energy and thermodynamic characteristics of the DFP for H_2 , LiH, HCl and CO molecules. The numerical values of energy and thermodynamic quantities of K_2 molecule with the DFP were reported by Onyenegecha et al. [52] using the formula technique. The KG equation with the DFP was examined by the SWKB and WKB methods [53]. Furthermore, the vibrational energies and scattering phase shift of HCl and LiH molecules were discussed in the higher dimensions using the NU functional analysis [54].

The study of diverse problems of quantum mechanics in the higher dimensional space has recently attracted the attention of theoretical physicists. Since the higher dimension studies aid in a broad approach to the problem, allowing the desired outcomes in the lower dimensions to be obtained directly by selecting appropriate with N . Therefore, a wide number of works [55–66] have been reported to derive the energy spectra of SE solutions in N -dimensional space.

Abu-Shady and Kaabar [67] recently proposed a new definition for the fractional derivative known as the generalized fractional derivative (GFD). The GFD definition is regarded as a comprehensive type for the fractional derivative because it provides more features than the other definitions [4–6, 14] where the CFD can be simply obtained as a special case from the GFD.

As a novel investigation, we employ the perception of the GFD to derive the bound state solutions of the N -dimensional SE with the DFP via the GF NU method motivated by the recent work [67]. Moreover, we explore the impact of the fractional order and the dimensional number on the ro-vibrational energy spectra of multiple DMs.

This investigation is organized as follows: In Sect. 2, the theoretical tools required for this investigation are displayed. In Sect. 3, we get the bound state solutions of the N -dimensional SE for the DFP via the GF NU method. In Sect. 4, the numerical estimates of the ro-vibrational energy levels of several DMs are reported. Finally, in Sec. 5, we provide the conclusion of our investigation.

2 Mathematical tools

2.1 Overview of the fractional derivative definitions

Here, we introduce some of the basic definitions of the fractional derivative. For $\delta \in (n - 1, n)$, the Riemann–Liouville definition is defined as [68,69]

$$\mathcal{D}^{RL} f(r) = \frac{1}{\Gamma(n - \delta)} \frac{d^n}{dr^n} \int_{r_0}^r \frac{f(s)}{(x - s)^{\delta - n + 1}} ds \quad (3)$$

and the Caputo definition is also defined as [68,69]

$$\mathcal{D}^C f(r) = \frac{1}{\Gamma(n - \delta)} \int_{r_0}^r \frac{f^n(s)}{(r - s)^{\delta - n + 1}} ds. \quad (4)$$

Due to the fact that the Riemann–Liouville and Caputo fractional derivative formulas do not satisfy some classical features such as the chain rule and the product or quotient of two functions, Khalil et al. suggested a new formula for the fractional derivative defined as the conformable fractional derivative (CFD) to overcome this problem. The CFD has the following form [14]

$$\begin{aligned} \mathcal{D}^{CF} f(r) &= \lim_{\varphi \rightarrow 0} \frac{f(r + \varphi r^{1-\delta}) - f(r)}{\varphi}; \\ 0 < \varphi \leq 1, \quad \mathcal{D}^{CF} f(0) &= \lim_{r \rightarrow 0^+} f^{CF}(r). \end{aligned} \quad (5)$$

where \mathcal{D}^{CF} is the local fractional derivative operator which satisfies the interesting properties that traditional fractional derivatives do not, such as the formula of the derivative of the product or quotient of two functions and the chain rule.

More recently, Abu-Shady and Kaabar [67] proposed a new definition for the fractional derivative known as the GFD that has the form:

$$\begin{aligned} \mathcal{D}^{GF} f(r) &= \lim_{\varphi \rightarrow 0} \frac{f\left(r + \frac{\Gamma(\gamma)}{\Gamma(\gamma - \delta + 1)} \varphi r^{1-\delta}\right) - f(r)}{\varphi}; \\ \gamma > -1, \gamma \in R^+, \quad \mathcal{D}^{GF} f(0) &= \lim_{r \rightarrow 0^+} f^{GF}(r). \end{aligned} \quad (6)$$

The main advantage of the GFD is that it fulfills the property: $\mathcal{D}^\delta \mathcal{D}^\gamma f(r) = \mathcal{D}^{\delta + \gamma} f(r)$, for a differentiable function $f(r)$, which is not satisfied by the CFD.

2.2 Generalized fractional NU method

In this subsection, our aim is to generalize the NU method into the framework of GFD. The NU method is an effective technique for solving second-order differential equations. Furthermore, it has been used successfully to solve both relativistic and nonrelativistic quantum mechanical problems. The NU method [70] is utilized to solve the second-order differential equation

which has the following form:

$$\mathcal{H}''(\rho) + \frac{\tilde{\tau}(\rho)}{\sigma(\rho)} \mathcal{H}'(\rho) + \frac{\tilde{\sigma}(\rho)}{\sigma^2(\rho)} \mathcal{H}(\rho), \quad (7)$$

where $\sigma(\rho)$ and $\tilde{\sigma}(\rho)$ are functions of maximum second degree and $\tilde{\tau}(\rho)$ is a function of maximum first degree.

The generalized fractional differential equation is defined as follows:

$$\mathcal{D}^\delta [\mathcal{D}^\delta \mathcal{H}(\rho)] + \frac{\tilde{\tau}(\rho)}{\sigma(\rho)} \mathcal{D}^\delta \mathcal{H}(\rho) + \frac{\tilde{\sigma}(\rho)}{\sigma^2(\rho)} \mathcal{H}(\rho), \quad (8)$$

Using the key property of the GFD,

$$\begin{aligned} \mathcal{D}^\delta \mathcal{H}(\rho) &= Q \rho^{1-\delta} \mathcal{H}'(\rho), \\ \mathcal{D}^\delta [\mathcal{D}^\delta \mathcal{H}(\rho)] &= Q^2 \left[\rho^{2(1-\delta)} \mathcal{H}''(\rho) \right. \\ &\quad \left. + (1 - \delta) \rho^{1-2\delta} \mathcal{H}'(\rho) \right], \end{aligned} \quad (9) \quad (10)$$

where

$$Q = \frac{\Gamma(\gamma)}{\Gamma(\gamma - \delta + 1)} \quad (11)$$

and substituting Eqs. (9) and (10) into Eq. (8) leads to

$$\begin{aligned} \mathcal{H}''(\rho) + \frac{Q(1 - \delta) \rho^{-\delta} \sigma(\rho) + \tilde{\tau}(\rho)}{Q \rho^{1-\delta} \sigma(\rho)} \mathcal{H}'(\rho) \\ + \frac{\tilde{\sigma}(\rho)}{Q^2 \rho^{2-2\delta} \sigma^2(\rho)} \mathcal{H}(\rho). \end{aligned} \quad (12)$$

Equation (12) can be reduced to a hypergeometric type equation as follows:

$$\mathcal{H}''(\rho) + \frac{\tilde{\tau}_{GF}(\rho)}{\sigma_{GF}(\rho)} \mathcal{H}'(\rho) + \frac{\tilde{\sigma}(\rho)}{\sigma_{GF}^2(\rho)} \mathcal{H}(\rho), \quad (13)$$

where

$$\begin{aligned} \tilde{\tau}_{GF}(\rho) &= Q(1 - \delta) \rho^{-\delta} \sigma(\rho) + \tilde{\tau}(\rho), \\ \sigma_{GF}(\rho) &= Q \rho^{1-\delta} \sigma(\rho). \end{aligned} \quad (14)$$

where the subscript GF stands for the generalized fractional, and $\sigma(\rho)$ and $\tilde{\sigma}(\rho)$ are polynomials of maximum 2δ th degree and $\tilde{\tau}(\rho)$ is a function at most δ th degree.

Setting

$$\mathcal{H}(\rho) = \chi(\rho) \mathcal{V}(\rho). \quad (15)$$

Substituting Eq. (15) into Eq. (13) gives

$$\sigma_{GF}(\rho) \mathcal{V}''(\rho) + \tau_{GF}(\rho) \mathcal{V}'(\rho) + \lambda(\rho) \mathcal{V}(\rho) = 0, \quad (16)$$

where $\chi(\rho)$ satisfies the following relation

$$\frac{\chi'(\rho)}{\chi(\rho)} = \frac{\pi_{GF}(\rho)}{\sigma_{GF}(\rho)} \quad (17)$$

and

$$\lambda(\rho) = k(\rho) + \pi'_{GF}(\rho). \tag{18}$$

Here, $\mathcal{V}(\rho) = \mathcal{V}_n(\rho)$ is a hypergeometric-type function, whose polynomial solutions are given by the Rodrigues formula

$$\mathcal{V}_n(\rho) = \frac{G_n}{\omega(\rho)} \frac{d^n}{d\rho^n} [\sigma^n_{GF}(\rho)\omega(\rho)], \tag{19}$$

where G_n is the normalization constant, and $\omega(\rho)$ is a weight function that defined as follows [51]:

$$\omega(\rho) = [\sigma_{GF}(\rho)]^{-1} \exp\left(\int \frac{\tau_{GF}(\rho)}{\sigma_{GF}(\rho)} d\rho\right). \tag{20}$$

The function $\pi_{GF}(\rho)$ has the following form:

$$\begin{aligned} \pi_{GF}(\rho) = & \frac{\sigma'_{GF}(\rho) - \tilde{\tau}_{GF}(\rho)}{2} \\ & \pm \sqrt{\left[\frac{\sigma'_{GF}(\rho) - \tilde{\tau}_{GF}(\rho)}{2}\right]^2 - \tilde{\sigma}(\rho) + k(\rho)\sigma_{GF}(\rho)}. \end{aligned} \tag{21}$$

The value of $k(\rho)$ can be determined if the function under the square root is the square of a polynomial. Thus, the equation of the eigenvalues can be obtained from the following relation:

$$\lambda(\rho) = \lambda_n(\rho) = -n\left[\tau'_{GF}(\rho) + \frac{(n-1)}{2}\sigma''_{GF}(\rho)\right], \tag{22}$$

where

$$\tau_{GF}(\rho) = \tilde{\tau}_{GF}(\rho) + 2\pi_{GF}(\rho). \tag{23}$$

Finally, the eigenfunctions $\mathcal{H}(\rho)$ can be determined from Eq. (15) using Eq. (17) and Eq. (19).

3 Solution of the generalized fractional SE for the DFP

The N -dimensional radial SE for a DM can be written as [55–66]

$$\left\{ \frac{d^2}{dr^2} + \frac{N-1}{r} \frac{d}{dr} - \frac{l(l+N-2)}{r^2} + \frac{2\mu}{\hbar^2} (E - V(r)) \right\} \phi(r) = 0, \tag{24}$$

where μ, \hbar, E and N are the reduced mass, the reduced Planck's constant, the energy spectrum and the dimen-

sional number, respectively. By setting,

$$\phi(r) = \frac{1}{r^{\frac{N-1}{2}}} F(r), \tag{25}$$

Equation (24) becomes

$$\frac{d^2 F(r)}{dr^2} + \left[\frac{2\mu}{\hbar^2} (E - V(r)) - \frac{(\eta^2 - \frac{1}{4})}{r^2} \right] F(r) = 0, \tag{26}$$

with

$$\eta = l + \frac{N-2}{2}. \tag{27}$$

Here we consider a general form of the DFP as follows:

$$\begin{aligned} V(r) = & D_e \left(1 - \frac{be^{-\alpha r}}{1 - e^{-\alpha r}}\right)^2 + V_0, \quad b = e^{\alpha r_e} - 1, \\ & r \in (0, \infty). \end{aligned} \tag{28}$$

The DFP can be found by setting $V_0 = 0$. In the case if $V_0 = -D_e$, Eq. (28) turns to the SDFP. Inserting Eq. (28) into Eq. (26) gives

$$\frac{d^2 F(r)}{dr^2} + \left\{ \frac{2\mu}{\hbar^2} \left[E - D_e \left(1 - \frac{be^{-\alpha r}}{1 - e^{-\alpha r}}\right)^2 - V_0 \right] - \frac{(\eta^2 - \frac{1}{4})}{r^2} \right\} F(r) = 0, \tag{29}$$

now we utilize a proper approximation for the term $1/r^2$ as [51]

$$\begin{aligned} \frac{1}{r^2} \approx & \alpha^2 \left[c_0 + \frac{e^{-\alpha r}}{(1 - e^{-\alpha r})} + \frac{e^{-2\alpha r}}{(1 - e^{-\alpha r})^2} \right]; \\ c_0 = & \frac{1}{12}. \end{aligned} \tag{30}$$

Inserting Eq. (30) into Eq. (29) yields

$$\begin{aligned} \frac{d^2 F(r)}{dr^2} + & \left\{ \frac{2\mu}{\hbar^2} \left[E - D_e \left(1 - \frac{be^{-\alpha r}}{1 - e^{-\alpha r}}\right)^2 - V_0 \right] \right. \\ & \left. - \alpha^2 \left(\eta^2 - \frac{1}{4} \right) \left[c_0 + \frac{e^{-\alpha r}}{(1 - e^{-\alpha r})} + \frac{e^{-2\alpha r}}{(1 - e^{-\alpha r})^2} \right] \right\} \\ & F(r) = 0. \end{aligned} \tag{31}$$

By defining the variable $\rho = e^{-\alpha r}$, Eq. (31) turns to

$$F''(\rho) + \frac{(1-\rho)}{\rho(1-\rho)} F'(\rho) + \frac{1}{\rho^2(1-\rho)^2} [-\mathcal{A}\rho^2 + \mathcal{B}\rho - \mathcal{C}] F(\rho) = 0, \tag{32}$$

where

$$\pi_{GF}(\rho) = \frac{(Q\delta - 1) + (1 - 2Q\delta)\rho^\delta}{2} \pm \sqrt{\left[\frac{(1 - 2Q\delta)^2}{4} + \mathcal{A} - Qk\rho^{1-\delta}\right]\rho^{2\delta} + \left[\frac{(Q\delta - 1)(1 - 2Q\delta)}{2} - \mathcal{B} + Qk\rho^{1-\delta}\right]\rho^\delta + \left[\frac{(Q\delta - 1)^2}{4} + \mathcal{C}\right]}. \tag{40}$$

$$\mathcal{A} = c_0\left(\eta^2 - \frac{1}{4}\right) + \frac{2\mu}{\alpha^2\hbar^2} [V_0 + D_e(b + 1)^2] - \epsilon, \tag{33}$$

$$\mathcal{B} = (2c_0 - 1)\left(\eta^2 - \frac{1}{4}\right) + \frac{4\mu}{\alpha^2\hbar^2} [V_0 + D_e(b + 1)] - 2\epsilon, \tag{34}$$

$$\mathcal{C} = c_0\left(\eta^2 - \frac{1}{4}\right) + \frac{2\mu}{\alpha^2\hbar^2} (V_0 + D_e) - \epsilon, \tag{35}$$

with

$$\epsilon = \frac{2\mu E}{\alpha^2\hbar^2}. \tag{36}$$

The generalized fractional form of the SE for the DFP can be stated by changing integer orders with fractional orders in Eq. (32) as follows:

$$\mathcal{D}^\delta \mathcal{D}^\delta F(\rho) + \frac{(1-\rho^\delta)}{\rho^\delta(1-\rho^\delta)} \mathcal{D}^\delta F(\rho) + \frac{1}{\rho^{2\delta}(1-\rho^\delta)^2} [-\mathcal{A}\rho^{2\delta} + \mathcal{B}\rho^\delta - \mathcal{C}] F(\rho) = 0. \tag{37}$$

Substituting Eqs. (9) and (10) into Eq. (37) gives

$$F''(\rho) + \frac{[1 + Q(1 - \delta)](1 - \rho^\delta)}{Q\rho(1 - \rho^\delta)} F'(\rho) + \frac{1}{Q^2\rho^2(1 - \rho^\delta)^2} [-\mathcal{A}\rho^{2\delta} + \mathcal{B}\rho^\delta - \mathcal{C}] F(\rho) = 0, \tag{38}$$

By comparing Eq. (38) with Eq. (13), the following functions are obtained:

$$\begin{aligned} \tilde{\tau}_{GF}(\rho) &= (1 + Q(1 - \delta))(1 - \rho^\delta), \\ \sigma_{GF}(\rho) &= Q\rho(1 - \rho^\delta), \\ \tilde{\sigma}_{GF}(\rho) &= -\mathcal{A}\rho^{2\delta} + \mathcal{B}\rho^\delta - \mathcal{C}. \end{aligned} \tag{39}$$

The function $\pi_{GF}(\rho)$ can be defined after substituting Eq. (39) into Eq. (21) as follows:

Equation (40) can be written in the following form:

$$\pi_{GF}(\rho) = \frac{(Q\delta - 1) + (1 - 2Q\delta)\rho^\delta}{2} \pm \sqrt{P\rho^{2\delta} + W\rho^\delta + R}, \tag{41}$$

where

$$\begin{aligned} P &= T_1 - Qk\rho^{1-\delta}, & W &= T_2 + Qk\rho^{1-\delta}, \\ R &= T_3, \end{aligned} \tag{42}$$

with

$$\begin{aligned} T_1 &= \frac{(1 - 2Q\delta)^2}{4} + \mathcal{A}, & T_2 &= \frac{(Q\delta - 1)(1 - 2Q\delta)}{2} - \mathcal{B}, \\ T_3 &= \frac{(Q\delta - 1)^2}{4} + \mathcal{C}. \end{aligned} \tag{43}$$

The two possible roots of k can be found by employing the condition that the discriminant of the expression under the square root of Eq. (41) must be zero, this leads to the following:

$$\begin{aligned} k_{\pm} &= \Lambda \left[-(T_2 + 2T_3) \pm 2\sqrt{T_3(T_1 + T_2 + T_3)} \right] \rho^{\delta-1}; \\ \Lambda &= \frac{1}{Q}. \end{aligned} \tag{44}$$

Inserting Eq. (44) into Eq. (41) gives

$$\begin{aligned} \pi_{GF}(\rho) &= \frac{(Q\delta - 1) + (1 - 2Q\delta)\rho^\delta}{2} \\ &\pm \begin{cases} (\sqrt{T_3} - \sqrt{T_1 + T_2 + T_3})\rho^\delta - \sqrt{T_3}, & k = k_+ \\ (\sqrt{T_3} + \sqrt{T_1 + T_2 + T_3})\rho^\delta - \sqrt{T_3}, & k = k_- \end{cases}. \end{aligned} \tag{45}$$

In order to obtain a physically acceptable solution, the negative sign in Eq. (45) is chosen. The function $\pi_{GF}(\rho)$ becomes

$$\pi_{GF}^-(\rho) = \frac{(Q\delta - 1) + (1 - 2Q\delta)\rho^\delta}{2} - \left[(\sqrt{T_3} + \sqrt{T_1 + T_2 + T_3})\rho^\delta - \sqrt{T_3} \right] \quad (46)$$

and

$$k_- = -\Lambda \left[T_2 + 2T_3 + 2\sqrt{T_3(T_1 + T_2 + T_3)} \right] \rho^{\delta-1}. \quad (47)$$

Therefore, the functions $\lambda(\rho)$, $\tau_{GF}(\rho)$ and $\lambda_n(\rho)$ can be found as follows:

$$\lambda(\rho) = \left[-\Lambda(T_2 + 2T_3) + \delta \left(\frac{1}{2}(1 - 2Q\delta) - \sqrt{T_3} \right) - \sqrt{T_1 + T_2 + T_3} (\delta + 2\Lambda\sqrt{T_3}) \right] \rho^{\delta-1}, \quad (48)$$

$$\tau_{GF}(\rho) = \left(2\sqrt{T_3} + Q \right) - \left[Q(\delta + 1) + 2 \left(\sqrt{T_3} + \sqrt{T_1 + T_2 + T_3} \right) \right] \rho^\delta, \quad (49)$$

$$\lambda_n(\rho) = n\delta \left[\frac{Q(n+1)(\delta+1)}{2} + 2 \left(\sqrt{T_3} + \sqrt{T_1 + T_2 + T_3} \right) \right] \rho^{\delta-1}. \quad (50)$$

By equating Eqs. (48) and (50), the energy spectrum formula for a DM in the N -dimensional space can be written as follows:

$$E_{nl}^N = \frac{\alpha^2 \hbar^2}{2\mu} \left\{ \xi_3 - \left(\frac{\delta \left[\frac{1}{2}(1 - 2Q\delta - Qn(n+1)(\delta+1)) - (2n+1)\sqrt{\xi_1 + \xi_2 + \xi_3} \right] - \Lambda(\xi_2 + 2\xi_3)}{\delta(2n+1) + 2\Lambda\sqrt{\xi_1 + \xi_2 + \xi_3}} \right)^2 \right\}, \quad (51)$$

where

$$\xi_1 = \frac{(1 - 2Q\delta)^2}{4} + c_0 \left(\eta^2 - \frac{1}{4} \right) + \frac{2\mu}{\alpha^2 \hbar^2} \left[V_0 + D_e(b+1)^2 \right], \quad (52)$$

$$\xi_2 = \frac{(Q\delta - 1)(1 - 2Q\delta)}{2} - (2c_0 - 1) \left(\eta^2 - \frac{1}{4} \right) - \frac{4\mu}{\alpha^2 \hbar^2} \left[D_e(b+1) + V_0 \right], \quad (53)$$

$$\xi_3 = \frac{(Q\delta - 1)^2}{4} + c_0 \left(\eta^2 - \frac{1}{4} \right) + \frac{2\mu}{\alpha^2 \hbar^2} \left(D_e + V_0 \right). \quad (54)$$

Now we determine the corresponding eigenfunctions. Using Eq. (17) the function $\chi(\rho)$ is

$$\chi(\rho) = \rho^\Lambda \left(\frac{(Q\delta-1) + \sqrt{\xi_3 - \epsilon}}{2} \right) (1 - \rho^\delta)^{\left(\frac{1}{2} + \frac{\Lambda}{\delta} \sqrt{\xi_1 + \xi_2 + \xi_3} \right)}. \quad (55)$$

The weight function $\omega(\rho)$ is found using Eq. (20) as

$$\omega(\rho) = \Lambda \rho^{\left(2\Lambda\sqrt{\xi_3 - \epsilon} \right)} (1 - \rho^\delta)^{\left(\frac{2\Lambda}{\delta} \sqrt{\xi_1 + \xi_2 + \xi_3} \right)}. \quad (56)$$

Using Eq. (19), the expression for the function $\mathcal{V}_n(\rho)$ takes the form

$$\mathcal{V}_n(\rho) = G_n \rho^{\left(-2\Lambda\sqrt{\xi_3 - \epsilon} \right)} (1 - \rho^\delta)^{\left(\frac{-2\Lambda}{\delta} \sqrt{\xi_1 + \xi_2 + \xi_3} \right)} \times \frac{d^n}{d\rho^n} \left[Q^n \rho^{\left(n+2\Lambda\sqrt{\xi_3 - \epsilon} \right)} (1 - \rho^\delta)^{\left(n + \frac{2\Lambda}{\delta} \sqrt{\xi_1 + \xi_2 + \xi_3} \right)} \right]. \quad (57)$$

Using Eq. (15), the complete solution of Eq. (32) can be expressed as

$$F(\rho) = G_n \rho^{\Lambda \left(\frac{(Q\delta-1) - \sqrt{\xi_3 - \epsilon}}{2} \right)} (1 - \rho^\delta)^{\left(\frac{1}{2} - \frac{\Lambda}{\delta} \sqrt{\xi_1 + \xi_2 + \xi_3} \right)} \times \frac{d^n}{d\rho^n} \left[Q^n \rho^{\left(n+2\Lambda\sqrt{\xi_3 - \epsilon} \right)} (1 - \rho^\delta)^{\left(n + \frac{2\Lambda}{\delta} \sqrt{\xi_1 + \xi_2 + \xi_3} \right)} \right]. \quad (58)$$

4 Results and discussion

In this part, we employ the previously obtained solutions to analyze the energy spectra of numerous DMs for both the DFP and the SDFP under the influence of the fractional parameter (δ) in N -dimensional space. The spectroscopic values for the selected DMs: HCl, CO, O₂ and NO used in this study are reported in Table 1. The criteria for the choice of these molecules are mainly based on the purposes that they play in many aspects of chemical, physical and related disciplines. In our computations, we use the following replacements [71]: $\hbar c = 1973.29 \text{ eV\AA}$, $1 \text{ cm}^{-1} = 1.239841875 \times 10^{-4} \text{ eV}$, and $1 \text{ amu} = 931.494028 \text{ MeV}/c^2$.

In Fig. 1, the variation of the DFP and its shifted is indicated at $r = r_e$ for some DMs. In Tables 2, 3, 4 and 5, the numerical results of the energy spectra for various DMs: CO, I₂, NO and N₂ with the DFP are displayed at diverse values of the fractional parameter (δ) and the dimensional number (N). It is found that increasing the fractional parameter (δ) causes a

Table 1 Spectroscopic parameters for various DMs [48]

Molecule	r_e (Å)	α (Å ⁻¹)	μ (a.m.u.)	D_e (cm ⁻¹)
NO	1.1508	2.7534	7.468441	64877.06229
CO	1.1282	2.2994	6.860586	87471.42567
I ₂	2.6620	1.8643	63.452235	12758.0129
N ₂	1.0940	2.6989	7.00335	96288.03528
O ₂	1.2070	2.6636	7.997457504	41591.26201
H ₂	0.7416	1.9426	0.50391	38267.78314
HF	0.9170	2.2266	0.96367	49382
LiH	1.5956	1.1280	0.8801221	20287.13295
ScH	1.7080	1.5068	10.682771	36778.8836
HCl	1.2746	1.8677	0.9801045	37255.24414

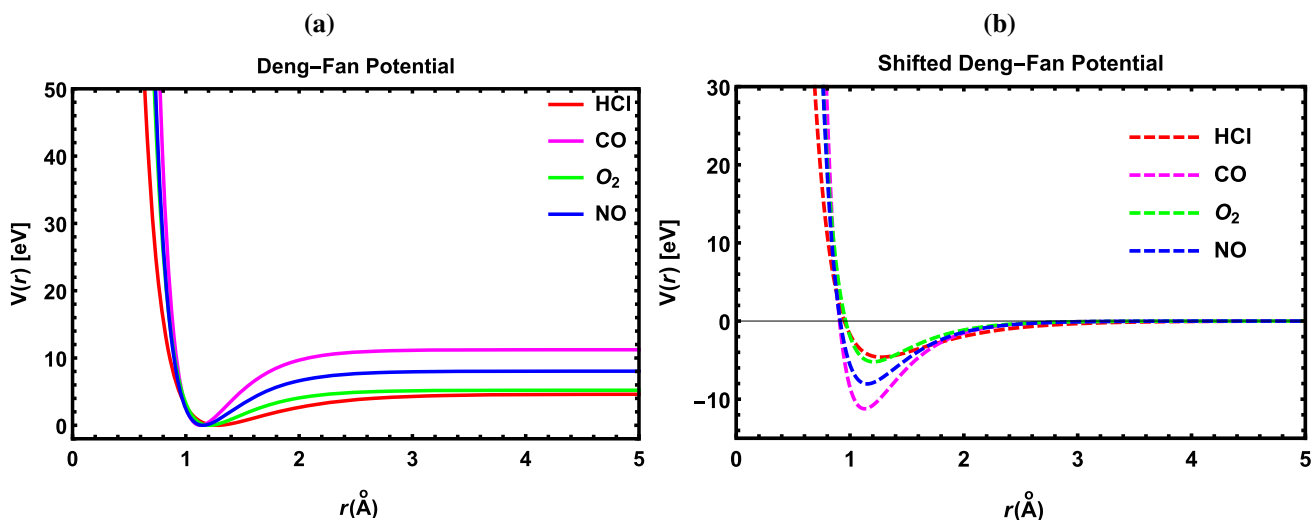


Fig. 1 Shape of DFP and SDFP for some DMs

Table 2 E_{nl} (eV) of DFP for CO molecule

n	l	$N = 3$			$N = 3$ $\delta = 1$	$\delta = 1$ $N = 4$	$N = 5$	$N = 6$
		$\delta = 0.2$	$\delta = 0.5$	$\delta = 0.8$				
0	0	0.03089963	0.08051605	0.12410601	0.14236930	0.14257464	0.14291688	0.14339599
1	0	0.09208239	0.24044444	0.36996537	0.42399536	0.42419921	0.42453895	0.42501458
	1	0.09263068	0.24099063	0.37050972	0.42453895	0.42501458	0.42562610	0.42637351
2	0	0.15310157	0.39912230	0.61277480	0.70157568	0.70177804	0.70211529	0.70258745
	1	0.15364899	0.39966624	0.61331569	0.70211529	0.70258745	0.70319450	0.70393644
	2	0.15474383	0.40075410	0.61439745	0.70319450	0.70393644	0.70481328	0.70582499
3	0	0.21395707	0.55655092	0.85254182	0.97512297	0.97532384	0.97565862	0.97612730
	1	0.21450363	0.55709261	0.85307925	0.97565862	0.97612730	0.97672990	0.97746640
	2	0.21559675	0.55817599	0.85415410	0.97672990	0.97746640	0.97833679	0.97934108
	3	0.21723640	0.55980101	0.85576633	0.97833679	0.97934108	0.98047926	0.98175131

significant increase in the energy eigenvalues. Concurrently, as the dimensional number (N) rises, so do the energy eigenvalues. Furthermore, the impact of fractional parameter (δ) and the dimensional number (N) on the energy eigenvalues for the SDFP is explored in Tables 6, 7, 8 and 9. We also observe here that the energy eigenvalues move to higher values as δ and N rise.

According to the results reported in Tables 2, 3, 4, 5, 6, 7, 8 and 9, the energy of the diatomic molecule is more constrained in the fractional case than in the classical one. Therefore, it can be deduced that the fractional parameter has a major effect on the rovibrational energy of the diatomic molecule. The influence of the fractional parameter on the behavior of the energy spectra for both the DFP and SDFP with var-

Table 3 E_{nl} (eV) of DFP for I₂ molecule

n	l	$N = 3$			$N = 3$ $\delta = 1$	$\delta = 1$		
		$\delta = 0.2$	$\delta = 0.5$	$\delta = 0.8$		$N = 4$	$N = 5$	$N = 6$
0	0	0.00290217	0.00757848	0.01168805	0.01341022	0.01341798	0.01343092	0.01344903
1	0	0.00866328	0.02266887	0.03492991	0.04005490	0.04006266	0.04007558	0.04009368
	1	0.00868398	0.02268957	0.03495060	0.04007558	0.04009368	0.04011695	0.04014539
2	0	0.01441374	0.03768510	0.05799444	0.06646580	0.06647355	0.06648647	0.06650456
	1	0.01443444	0.03770578	0.05801512	0.06648647	0.06650456	0.06652781	0.06655623
	2	0.01447584	0.03774715	0.05805647	0.06652781	0.06655623	0.06658982	0.06662857
3	0	0.02015357	0.05262715	0.08088166	0.09264296	0.09265070	0.09266361	0.09268169
	1	0.02017427	0.05264783	0.08090232	0.09266361	0.09268169	0.09270493	0.09273333
	2	0.02021566	0.05268918	0.08094365	0.09270493	0.09273333	0.09276689	0.09280562
	3	0.02027774	0.05275121	0.08100563	0.09276689	0.09280562	0.09284952	0.09289857

Table 4 E_{nl} (eV) of DFP for NO molecule

n	l	$N = 3$			$N = 3$ $\delta = 1$	$\delta = 1$		
		$\delta = 0.2$	$\delta = 0.5$	$\delta = 0.8$		$N = 4$	$N = 5$	$N = 6$
0	0	0.02958454	0.07685720	0.11839178	0.13579494	0.13599984	0.13634133	0.13681943
1	0	0.08794744	0.22923250	0.35239340	0.40372140	0.40392501	0.40426436	0.40473945
	1	0.08849444	0.22977770	0.35293702	0.40426436	0.40473945	0.40535028	0.40609683
2	0	0.14610481	0.38010256	0.58275773	0.66683706	0.66703939	0.66737660	0.66784869
	1	0.14665108	0.38064583	0.58329836	0.66737660	0.66784869	0.66845566	0.66919750
	2	0.14774361	0.38173235	0.58437963	0.66845566	0.66919750	0.67007422	0.67108582
3	0	0.20405658	0.52946844	0.80949102	0.92515259	0.92535363	0.92568870	0.92615780
	1	0.20460211	0.53000977	0.81002867	0.92568870	0.92615780	0.92676092	0.92749807
	2	0.20569316	0.53109243	0.81110397	0.92676092	0.92749807	0.92836923	0.92937441
	3	0.20732971	0.53271639	0.81271689	0.92836923	0.92937441	0.93051361	0.93178682

Table 5 E_{nl} (eV) of DFP for N₂ molecule

n	l	$N = 3$			$N = 3$ $\delta = 1$	$\delta = 1$		
		$\delta = 0.2$	$\delta = 0.5$	$\delta = 0.8$		$N = 4$	$N = 5$	$N = 6$
0	0	0.03680223	0.09579693	0.14763020	0.16934841	0.16957830	0.16996144	0.17049785
1	0	0.10957917	0.28598430	0.43994427	0.50415932	0.50438779	0.50476857	0.50530166
	1	0.11019288	0.28659602	0.44055425	0.50476857	0.50530166	0.50598707	0.50682477
2	0	0.18214266	0.47458659	0.72841609	0.83388317	0.83411023	0.83448865	0.83501843
	1	0.18275555	0.47519618	0.72902278	0.83448865	0.83501843	0.83569959	0.83653210
	2	0.18398134	0.47641535	0.73023614	0.83569959	0.83653210	0.83751597	0.83865120
3	0	0.25449260	0.66160500	1.01305263	1.15853183	1.15875747	1.15913354	1.15966002
	1	0.25510469	0.66221245	1.01365603	1.15913354	1.15966002	1.16033694	1.16116427
	2	0.25632884	0.66342735	1.01486282	1.16033694	1.16116427	1.16214202	1.16327018
	3	0.25816506	0.66524968	1.01667299	1.16214202	1.16327018	1.16454875	1.16597773

ied potential parameters is depicted in Figs. 2, 3, 4, 5 and 6 for a more illustration. For various values of the fractional parameter $\delta = 0.1, \delta = 0.3, \delta = 0.5, \delta = 0.7, \delta = 0.9$ and $\delta = 1$, the variations of the energy spectra with the vibrational (n) and rotational (l) quantum numbers are shown in Figs. 2 and 3, respectively. Figure 2 reveals that the energy spectra gradually grow as the vibrational quantum number (n) increases.

In line with this inspection, Fig. 3 illustrates a progressive rise also in the energy spectra as the rotational quantum number (l) rises. In Fig. 4, the behavior of the energy spectra with the screening param-

eter (α) for different values of the fractional parameter is displayed. As seen in Fig. 4, the energy spectra elevate in a consistent manner as the screening parameter is increased. In Fig. 5, the energy spectra are plotted with the equilibrium bond length (r_e) at $\delta = 0.1, \delta = 0.3, \delta = 0.5, \delta = 0.7, \delta = 0.9$ and $\delta = 1$. As shown in Fig. 5, the energy spectra decrease by increasing the equilibrium bond length. The behavior of the energy spectra with the reduced mass (μ) is depicted in Fig. 6. Obviously, increasing the reduced mass leads to a drop in the energy spectra. Due to our investigation being innovative, we are unable to compare the

Table 6 $-E_{nl}$ (eV) of SDFP for CO molecule

n	l	$N = 3$			$N = 3$	$\delta = 1$		
		$\delta = 0.2$	$\delta = 0.5$	$\delta = 0.8$	$\delta = 1$	$N = 4$	$N = 5$	$N = 6$
0	0	10.8141740	10.7645575	10.7209676	10.7027043	10.7024990	10.7021568	10.7016776
1	0	10.7529912	10.6046292	10.4751082	10.4210782	10.4208744	10.4205347	10.4200591
	1	10.7524429	10.6040830	10.4745639	10.4205347	10.4200591	10.4194475	10.4187001
2	0	10.6919720	10.4459513	10.2322988	10.1434979	10.1432956	10.1429583	10.1424862
	1	10.6914246	10.4454074	10.2317579	10.1429583	10.1424862	10.1418791	10.1411372
	2	10.6903298	10.4443195	10.2306761	10.1418791	10.1411372	10.1402604	10.1392486
3	0	10.6311165	10.2885227	9.99253181	9.86995067	9.86974980	9.86941502	9.86894634
	1	10.6305700	10.2879810	9.99199438	9.86941502	9.86894634	9.86834374	9.86760724
	2	10.6294768	10.2868976	9.99091954	9.86834374	9.86760724	9.86673685	9.86573256
	3	10.6278372	10.2852726	9.98930730	9.86673685	9.86573256	9.86459438	9.86332233

Table 7 $-E_{nl}$ (eV) of SDFP for I₂ molecule

n	l	$N = 3$			$N = 3$	$\delta = 1$		
		$\delta = 0.2$	$\delta = 0.5$	$\delta = 0.8$	$\delta = 1$	$N = 4$	$N = 5$	$N = 6$
0	0	1.55269782	1.54802152	1.54391195	1.54218978	1.54218201	1.54216908	1.54215097
1	0	1.54693672	1.53293112	1.52067008	1.51554509	1.51553734	1.51552441	1.51550631
	1	1.54691602	1.53291043	1.52064939	1.51552441	1.51550631	1.51548304	1.51545460
2	0	1.54118625	1.51791490	1.49760555	1.48913420	1.48912645	1.48911353	1.48909544
	1	1.54116556	1.51789421	1.49758488	1.48911353	1.48909544	1.48907219	1.48904377
	2	1.54112416	1.51785284	1.49754353	1.48907219	1.48904377	1.48901018	1.48897142
3	0	1.53544642	1.50297285	1.47471833	1.46295704	1.46294929	1.46293638	1.46291831
	1	1.53542573	1.50295217	1.47469767	1.46293638	1.46291831	1.46289507	1.46286667
	2	1.53538434	1.50291081	1.47465635	1.46289507	1.46286667	1.46283310	1.46279437
	3	1.53532225	1.50284878	1.47459436	1.46283310	1.46279437	1.46275048	1.46270142

Table 8 $-E_{nl}$ (eV) of SDFP for NO molecule

n	l	$N = 3$			$N = 3$	$\delta = 1$		
		$\delta = 0.2$	$\delta = 0.5$	$\delta = 0.8$	$\delta = 1$	$N = 4$	$N = 5$	$N = 6$
0	0	8.01414531	7.96687265	7.92533807	7.90793492	7.90773002	7.90738852	7.90691043
1	0	7.95578242	7.81449736	7.69133645	7.64000845	7.63980484	7.63946549	7.63899040
	1	7.95523541	7.81395215	7.69079283	7.63946549	7.63899040	7.63837958	7.63763302
2	0	7.89762504	7.66362729	7.46097213	7.37689279	7.37669047	7.37635326	7.37588117
	1	7.89707877	7.66308403	7.46043149	7.37635326	7.37588117	7.37527420	7.37453235
	2	7.89598625	7.66199750	7.45935023	7.37527420	7.37453235	7.37365563	7.37264404
3	0	7.83967328	7.51426141	7.23423884	7.11857727	7.11837622	7.11804115	7.11757206
	1	7.83912775	7.51372008	7.23370118	7.11804115	7.11757206	7.11696893	7.11623179
	2	7.83803670	7.51263743	7.23262589	7.11696893	7.11623179	7.11536062	7.11435544
	3	7.83640014	7.51101347	7.23101296	7.11536062	7.11435544	7.11321624	7.11194304

obtained results for different values of the fractional parameter. As a consequence, the classical solutions of the DFP and its shifted are recovered by setting $\delta = 1$, and our results are compared to those found in the literature. In Tables 10, 11 and 12, the numerical results for the ro-vibrational energy spectra of the DFP for several DMs: LiH, ScH, HCl, CO, O₂ and H₂ are reported in comparison with the found in Refs. [40, 44, 50]. Furthermore, the ro-vibrational energy spectra of the SDFP for numerous DMs: LiH, ScH, HCl, CO, H₂ and I₂ are displayed in Tables 13, 14 and 15 compared to the findings in Refs. [46, 48, 49].

As can be shown in Tables 10, 11, 12, 13, 14 and 15, the ro-vibrational energy spectra of all selected DMs rise as the vibrational and rotational quantum numbers increase. To the best of our knowledge, no one has previously investigated the solutions of the N -dimensional SE with the DFP in the framework of the GFD. Furthermore, in the case of $\delta = 1$, one can see that our estimates are perfectly consistent with previous works that used other techniques. Therefore, we hope that the current findings will be helpful in future studies.

Table 9 $-E_{nl}$ (eV) of SDFP for N_2 molecule

n	l	$N = 3$			$N = 3$ $\delta = 1$	$\delta = 1$		
		$\delta = 0.2$	$\delta = 0.5$	$\delta = 0.8$		$N = 4$	$N = 5$	$N = 6$
0	0	11.9013916	11.8423969	11.7905636	11.7688454	11.7686155	11.7682324	11.7676960
1	0	11.8286147	11.6522095	11.4982495	11.4340345	11.4338060	11.4334252	11.4328922
	1	11.8280009	11.6515978	11.4976396	11.4334252	11.4328922	11.4322067	11.4313690
2	0	11.7560512	11.4636072	11.2097777	11.1043106	11.1040836	11.1037052	11.1031754
	1	11.7543833	11.4629976	11.2091710	11.1037052	11.1031754	11.1024942	11.1016617
	2	11.7542125	11.4617785	11.2079577	11.1024942	11.1016617	11.1006778	11.0995426
3	0	11.6837012	11.2765888	10.9251412	10.7796620	10.7794364	10.7790603	10.7785338
	1	11.6830891	11.2759814	10.9245378	10.7790603	10.7785338	10.7778569	10.7770296
	2	11.6818650	11.2747665	10.9233310	10.7778569	10.7770296	10.7760518	10.7749236
	3	11.6800288	11.2729441	10.9215208	10.7760518	10.7749236	10.7736451	10.7722161

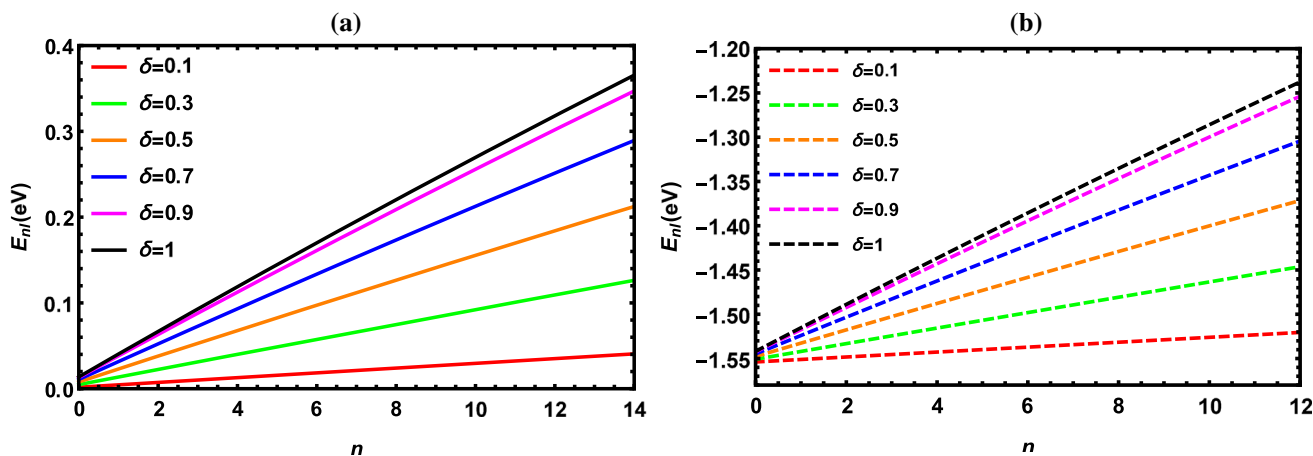


Fig. 2 Energy levels of I_2 molecule with n at numerous values of δ for **a** DFP and **b** SDFP

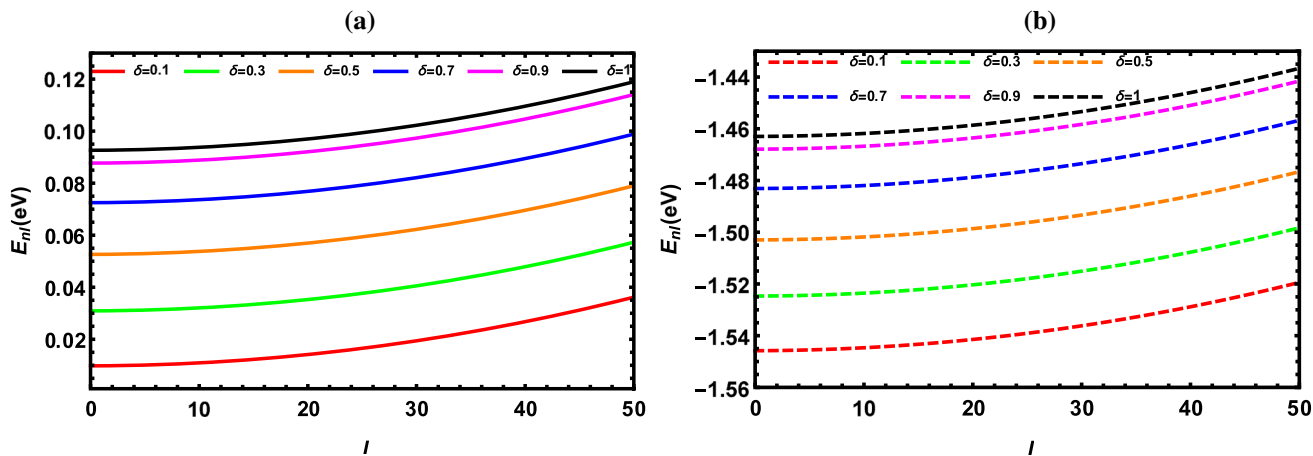


Fig. 3 Energy levels of I_2 molecule with l at numerous values of δ for **a** DFP and **b** SDFP

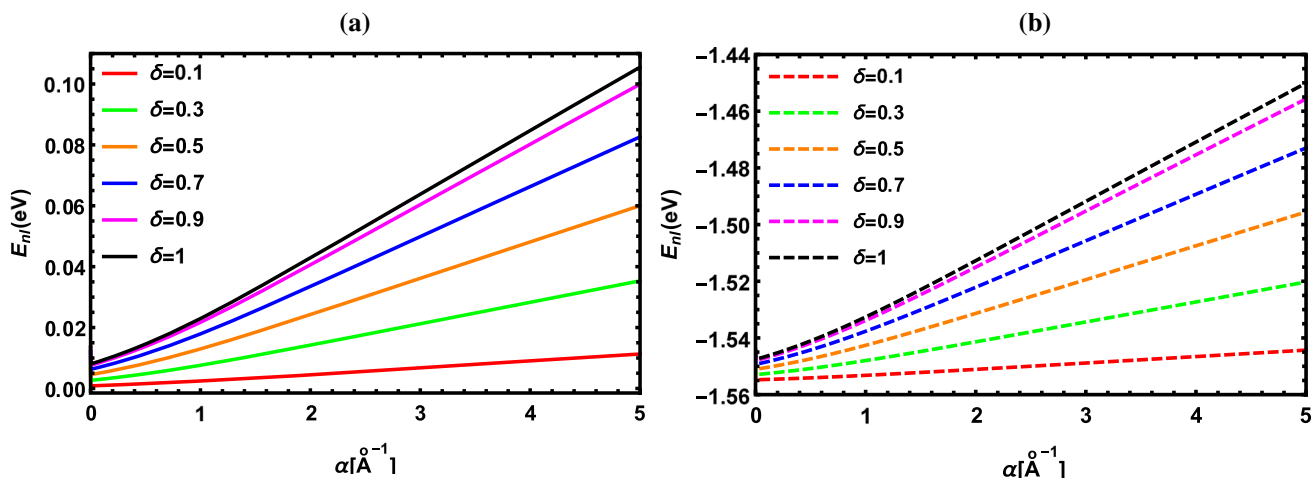


Fig. 4 Energy levels of I_2 molecule with α at numerous values of δ for a DFP and b SDFP

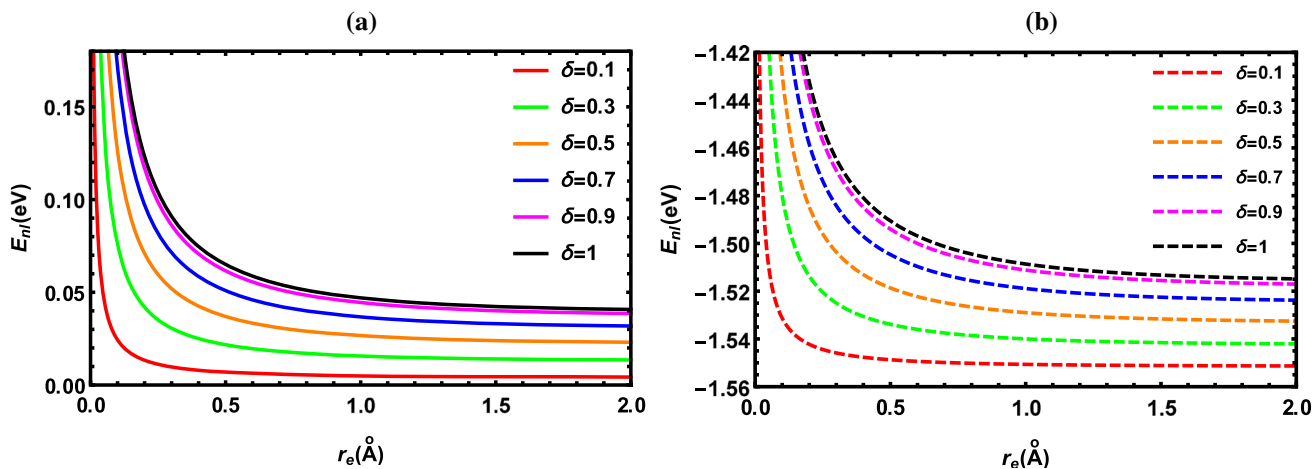


Fig. 5 Energy levels of I_2 molecule with r_e at numerous values of δ for a DFP and b SDFP

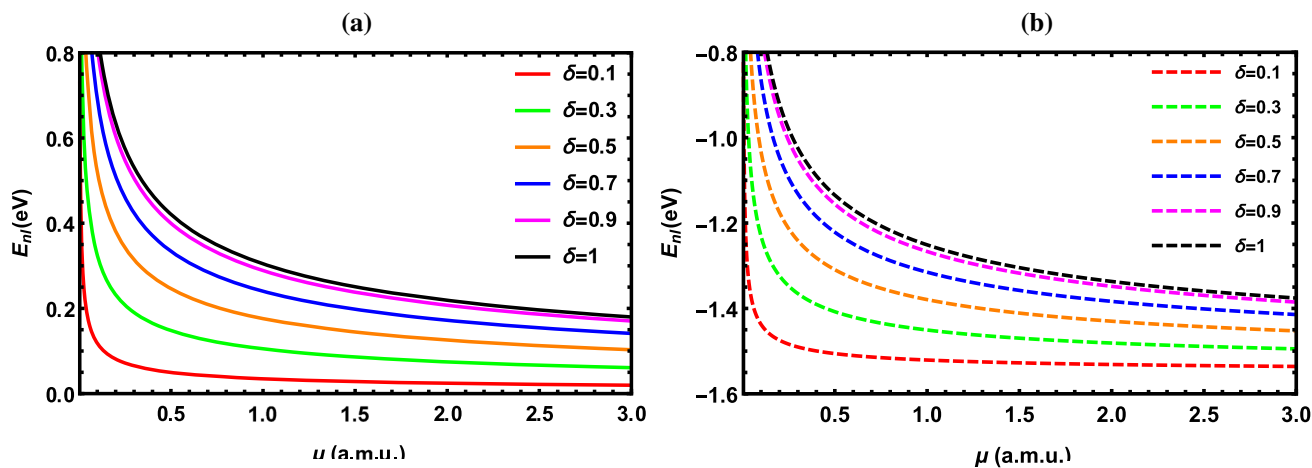


Fig. 6 Energy levels of I_2 molecule with μ at numerous values of δ for a DFP and b SDFP

Table 10 E_{nl} (eV) of DFP for LiH and ScH molecules

n	l	LiH			ScH		
		Present	[44]	[50]	Present	[44]	[50]
0	0	0.103334307	0.103334650	0.103397595	0.104850693	0.104850694	0.104938646
1	0	0.302004929	0.302005955	0.302068901	0.306246537	0.306246538	0.306334489
	1	0.303837626	0.303838653	0.303901531	0.307704128	0.307704129	0.307791993
2	0	0.490684151	0.490685861	0.490748806	0.496950687	0.496950687	0.497038637
	1	0.492449049	0.492450759	0.492513638	0.498367396	0.498367397	0.498455260
	2	0.495977286	0.495978997	0.496041760	0.501200315	0.501200316	0.501288002
3	0	0.669598629	0.669601019	0.669663964	0.677093198	0.677093198	0.677181146
	1	0.671297257	0.671299648	0.671362527	0.678469522	0.678469522	0.678557384
	2	0.674692995	0.674695388	0.674758151	0.681221677	0.681221677	0.681309362
	3	0.679782810	0.679785205	0.679847770	0.685348676	0.685348677	0.685436100
4	0	0.838967494	0.838970564	0.839033509	0.846801672	0.846801673	0.846889620
	1	0.840601332	0.840604402	0.840667281	0.848138097	0.848138097	0.848225957
	2	0.843867529	0.843870601	0.843933363	0.850810460	0.850810460	0.850898144
	3	0.848763128	0.848766203	0.848828768	0.854817790	0.854817791	0.854905213
	4	0.855283702	0.855286782	0.855349091	0.860158632	0.860158632	0.860245696
5	0	0.999002656	0.999006401	0.999069346	1.006201313	1.006201313	1.006289259
	1	1.000573134	1.000576880	1.000639759	1.007498315	1.007498315	1.007586174
	2	1.003712649	1.003716397	1.003779159	1.010091841	1.010091841	1.010179523
	3	1.008418320	1.008422072	1.008484637	1.013980933	1.013980933	1.014068354
	4	1.014685833	1.014689589	1.014751899	1.019164157	1.019164157	1.019251220
	5	1.022509444	1.022513206	1.022575209	1.025639600	1.025639693	1.025726220

Table 11 E_{nl} (eV) of DFP for HCl and CO molecules

n	l	HCl			CO	
		Present	[44]	[40]	Present	[50]
0	0	0.201983505	0.201984174	0.202139134	0.144850105	0.144969072
1	0	0.590745819	0.590747827	0.590902787	0.431437877	0.430178995
	1	0.593535604	0.593537612	0.593692401	0.431981483	0.430719631
2	0	0.960007699	0.960011044	0.960166004	0.713979856	0.711910800
	1	0.962718245	0.962721591	0.962876380	0.714519556	0.712447561
	2	0.968138299	0.968141645	0.968296136	0.715598945	0.713521071
3	0	1.310023186	1.310027865	1.310182826	0.992488526	0.989632352
	1	1.312655523	1.312660203	1.312814994	0.993024333	0.990165249
	2	1.317919173	1.317923855	1.318078347	0.994095934	0.991231033
	3	1.325812091	1.325816775	1.325970803	0.995703306	0.992829678
4	0	1.641041232	1.641047243	1.641202203	1.266976312	1.263355977
	1	1.643596366	1.643602379	1.643757170	1.267508237	1.263885023
	2	1.648705629	1.648711644	1.648866136	1.268572075	1.264943104
	3	1.656367005	1.656373023	1.656527052	1.270167801	1.266530195
	4	1.666577476	1.666583499	1.666736911	1.272295381	1.268646261
5	0	1.953305816	1.953313156	1.953468116	1.537455578	1.533093944
	1	1.955784737	1.955792078	1.955946871	1.537983633	1.533619151
	2	1.960741588	1.960748932	1.960903424	1.539039731	1.534669552
	3	1.968174386	1.968181734	1.968335762	1.540623848	1.536245125
	4	1.978080159	1.978087513	1.978240925	1.542735948	1.538345834
	5	1.990454948	1.990462308	1.990614950	1.545375984	1.540971631

Table 12 E_{nl} (eV) of DFP for HF, O₂ and H₂ molecules

n	l	HF		O ₂		H ₂	
		Present	[40]	Present	[40]	Present	[40]
0	0	0.291247434	0.296644754	0.349980220	0.365141571	0.101919228	0.102043850
1	0	0.848733535	0.848791378	0.996777053	0.998213655	0.302577426	0.3015750557
	1	0.853910381	0.853968904	1.010323238	1.011736491	0.303043144	0.3020376575
2	0	1.374650333	1.374741414	1.580248366	1.582601950	0.499057714	0.4974222630
	1	1.379631880	1.379723603	1.592700793	1.595035333	0.499520138	0.4978816054
	2	1.389590976	1.389683982	1.617539648	1.619836697	0.500444979	0.4988002821
3	0	1.869636743	1.869756985	2.104086156	2.107302268	0.691370318	0.6891297288
	1	1.874426923	1.874547769	2.115507769	2.118708590	0.691829458	0.6895858196
	2	1.884003381	1.884125435	2.138289195	2.141459973	0.692747730	0.6904979933
	3	1.898358314	1.898482178	2.172307398	2.175434452	0.694125117	0.6918662339
4	0	2.334312319	2.334457762	2.571680443	2.575691305	0.879525427	0.8767075389
	1	2.338914946	2.339060957	2.582129083	2.586127919	0.879981291	0.8771603861
	2	2.348116388	2.348263535	2.602968445	2.606943719	0.880893009	0.8780660724
	3	2.361909031	2.362057878	2.634083222	2.638024369	0.882260567	0.8794245822
	4	2.380281458	2.380432567	2.675301759	2.679199648	0.884083941	0.8812358915
5	0	2.769277951	2.769444752	2.986148433	2.990875171	1.063533190	1.0601657396
	1	2.773696723	2.773864056	2.995677323	3.000394872	1.063985785	1.0606153510
	2	2.782530546	2.782698944	3.014680784	3.019380399	1.064890966	1.0615145658
	3	2.795771983	2.795941975	3.043050669	3.047724487	1.066248719	1.0628633684
	4	2.813409888	2.813582001	3.080625975	3.085267435	1.068059018	1.0646617349
	5	2.835429422	2.835604179	3.127194276	3.131798515	1.070321833	1.0669096339

Table 13 $-E_{nl}$ (eV) of SDFP for CO and HCl molecules

n	l	CO			HCl		
		Present	[46]	[49]	Present	[46]	[49]
0	0	11.08074990	11.08075178	11.08074989	4.417047400	4.417077001	4.417047400
	5	11.07253746	11.07253985	11.07360695	4.374033861	4.374065784	4.378422991
	10	11.05064208	11.05064581	11.05456479	4.259723835	4.259761948	4.275898727
5	0	9.688144422	9.688146187	9.688144422	2.665725089	2.665748019	2.665725089
	5	9.680224016	9.680226284	9.681355403	2.628575957	2.628601192	2.633922445
	10	9.659107308	9.659110919	9.663257003	2.529874313	2.529905688	2.549565348
7	0	9.159162287	9.159164003	9.159162288	2.096504515	2.096524802	2.096504516
	5	9.151357442	9.151359661	9.152513419	2.061597436	2.061620020	2.067315382
	10	9.130548864	9.130552425	9.134788734	1.968863331	1.968892038	1.989918464

Table 14 $-E_{nl}$ (eV) of SDFP for LiH and ScH molecules

n	l	LiH			ScH		
		Present	[46]	[49]	Present	[46]	[48]
0	0	2.411932904	2.411949045	2.411932904	2.145149306	2.1451493060	2.145149306
	5	2.383459166	2.383476249	2.384580437	2.122682696	2.1226840150	2.122682696
	10	2.308127882	2.308147473	2.312283846	2.062960535	2.0629653710	–
5	0	1.516264555	1.516277294	1.516264555	1.243798687	1.2437986870	–
	5	1.492757768	1.492771433	1.494210023	1.224360400	1.2243617190	–
	10	1.430598166	1.430614300	1.435969432	1.172700118	1.1727049540	–
7	0	1.223382139	1.223393538	1.223382139	0.955436772	0.9554367725	–
	5	1.201712023	1.201724343	1.203290365	0.937159725	0.9371610441	–
	10	1.144423818	1.144438594	1.150257886	0.888590944	0.8885957808	–

Table 15 $-E_{nl}$ (eV) of SDFP for H₂ and I₂ molecules

n	l	H ₂			I ₂		
		Present	[46]	[49]	Present	[46]	[48]
0	0	4.394619779	4.394619779	4.394619776	1.542189775	1.542189775	1.542189775
	5	4.176613157	4.176618048	4.180734836	1.541879304	1.541879340	1.541879304
	10	3.621820491	3.621838424	3.637874575	1.541051381	1.541051513	–
5	0	1.758451567	1.758451567	1.758451566	1.411303767	1.411303767	–
	5	1.617405724	1.617410615	1.624065481	1.410994355	1.410994391	–
	10	1.260433707	1.260451640	1.285780199	1.410169257	1.410169388	–
7	0	1.077636993	1.077636993	1.077636991	1.360584943	1.360584943	–
	5	0.961809891	0.961814782	0.969361194	1.360275954	1.360275990	–
	10	0.669826131	0.669844065	0.698426418	1.359451985	1.359452116	–

5 Conclusion

Based on the generalized fractional derivative (GFD), the generalized fractional NU method has been derived and utilized to obtain the bound state solutions of the N -dimensional SE with the DFP. The formulas of energy eigenvalues and corresponding eigenfunctions for the DFP as a function of the fractional parameter have been produced for arbitrary values of the vibrational and rotational quantum numbers in the N -dimensional space. As an application, the ro-vibrational energy levels of varied diatomic molecules (DMs) have been evaluated for both the DFP and its shifted potential at different values of the fractional parameter. The effect of the fractional parameter on the energy levels has also been graphically illustrated. It is observed that decreasing fractional parameter (δ) significantly lowers the energy eigenvalues. As a consequence, we conclude that the diatomic molecule's energy is more bounded at lower fractional parameter values than in the classical case ($\delta = 1$). Furthermore, the energy levels of numerous DMs have been estimated in three-dimensional space as well as higher dimensions. It is notable that as the number of dimensions grows, the energy spectrum grows as well. The variation of the energy levels of the DFP and its shifted potential for the I₂ DM has been graphically depicted with the reduced mass, screening parameter, equilibrium bond length, rotational and vibrational quantum numbers. To prove the validity of our findings, the energy levels of numerous DMs have been calculated at $\delta = 1$, and compared the results with previous studies. As it can be observed, our findings are in perfect accord with those of others. We infer that the fractional parameter has a significant impact on the ro-vibrational energy levels of DMs. Consequently, exploring the solutions of the N -dimensional SE within the framework of the GFD, and the study of the impact of the fractional number on various features of diverse systems in molecular and atomic physics should be investigated. Finally, we indicate that this work would be extended in the future to derive the solutions of the N -dimensional SE within the scope of the GFD for further molecular potentials such

as the Kratzer potential, Morse potential, Pöschl-Teller potential, Hulthén potential, and so on.

Author contributions

All authors contributed to the study conception and design. Material preparation, data collection and analysis were performed by MAS, EMK and TAA-K. The first draft of the manuscript was written by EMK and all authors commented on previous versions of the manuscript. All authors read and approved the final manuscript.

Funding Information Open access funding provided by The Science, Technology & Innovation Funding Authority (STDF) in cooperation with The Egyptian Knowledge Bank (EKB).

Data Availability Statement This manuscript has no associated data or the data will not be deposited. [Authors' comment: All data included in this study are available on request by contacting the corresponding author.]

Declarations

Conflict of interest The author declares no conflict of interest.

Open Access This article is licensed under a Creative Commons Attribution 4.0 International License, which permits use, sharing, adaptation, distribution and reproduction in any medium or format, as long as you give appropriate credit to the original author(s) and the source, provide a link to the Creative Commons licence, and indicate if changes were made. The images or other third party material in this article are included in the article's Creative Commons licence, unless indicated otherwise in a credit line to the material. If material is not included in the article's Creative Commons licence and your intended use is not permitted by statutory regulation or exceeds the permitted use, you will need to obtain permission directly from the copyright holder. To view a copy of this licence, visit <http://creativecommons.org/licenses/by/4.0/>.

References

1. R. Hilfer, *Applications of Fractional Calculus in Physics* (World Scientific, Singapore, 2000)
2. M. Dalir, M. Bashour, *Appl. Math. Sci.* **4**(21), 1021–1032 (2010)
3. Y.A. Rossikhin, M.V. Shitikova, *App. Mech. Rev.* **50**(1), 15–67 (1997)
4. G. Jumarie, *Comput. Math. Appl.* **51**, 1367–1376 (2006)
5. K.S. Miller, B. Ross, *An Introduction to the Fractional Calculus and Fractional Differential Equations* (Wiley, New York, 1993)
6. M. Caputo, *Geophysical. J. Int.* **13**(5), 529–539 (1967)
7. T. Das, U. Ghosh, S. Sarkar, S. Das, *J. Math. Phys.* **59**(2), 022111 (2018)
8. T. Das, U. Ghosh, S. Sarkar, S. Das, *Pramana J. Phys.* **93**, 76 (2019)
9. T. Das, U. Ghosh, S. Sarkar, S. Das, *Pramana J. Phys.* **94**, 33 (2020)
10. M. Al-Raei, M.S. El-Daher, *Pramana J. Phys.* **94**, 157 (2020)
11. M. Al-Raei, M.S. El-Daher, *Heliyon* **6**(7), e04495 (2020)
12. M. Al-Raei, M.S. El-Daher, *Phys. Lett. A* **383**(26), 125831 (2019)
13. M. Al-Raei, M.S. El-Daher, *AIP Adv.* **10**(3), 035305 (2020)
14. R. Khalil, M. Al Horani, A. Yousef, M. Sababheh, *J. Comput. Appl. Math.* **264**, 65–70 (2014)
15. T. Abdeljawad, *J. Comput. Appl. Math.* **279**, 57–66 (2015)
16. H. Karayer, D. Demirhan, F. Büyükkılıç, *Commun. Theor. Phys.* **66**, 12–18 (2016)
17. W.S. Chung, S. Zare, H. Hassanabadi, *Commun. Theor. Phys.* **67**, 250–254 (2017)
18. F.S. Mozaffari, H. Hassanabadi, H. Sobhani, *J. Kor. Phys. Soc.* **72**(9), 980–986 (2017)
19. H.H. Karayer, A.D. Demirhan, F. Büyükkılıç, *Turk. J. Phys.* **41**, 551–559 (2017)
20. N. Jamshir, B. Lari, H. Hassanabadi, *Physica A: Stat. Mech. Appl.* **565**, 125616 (2021)
21. M. Abu-Shady, *Int. J. Mod. Phys. A* **34**(31), 1950201 (2019)
22. M. Abu-Shady, Sh.Y. Ezz-Alarab, *Few-Body Syst.* **62**(2), 1–8 (2021)
23. M. Abu-Shady, A. I. Ahmadov, H. M. Fath-Allah, V. H. Badalov, (2021) [arXiv:2105.01607](https://arxiv.org/abs/2105.01607)
24. A. Al-Jamel, *Int. J. Mod. Phys. A* **34**(10), 1950054 (2019)
25. M.M. Hammad, A.S. Yaqut, M.A. Abdel-Khalek, S.B. Doma, *Nuc. Phys. A* **1015**, 122307 (2021)
26. M. Abu-Shady, *Fur. App. Math.* **1**(2), 34–42 (2021)
27. U. S. Okorie, A. N. Ikot, P. O. Amadi, G. J. Rampho, (2020) [arXiv:2103.14064](https://arxiv.org/abs/2103.14064)
28. U.S. Okorie et al., *Mod. Phys. Lett. A* **36**(7), 2150041 (2021)
29. O. Bayrak, I. Boztosun, H. Ciftci, *Int. J. Quant. Chem.* **107**(3), 540–544 (2007)
30. D.A. Morales, *Chem. Phys. Lett.* **394**(1–3), 68–75 (2004)
31. S.H. Dong, R. Lemus, *Int. J. Quant. Chem.* **86**(3), 265–272 (2002)
32. A.K. Roy, *Mod. Phys. Lett. (29)* **9**, 1450042 (2014)
33. X.Y. Gu, J.Q. Sun, *J. Math. Phys.* **51**(2), 022106 (2010)
34. D. Schiöberg, *Mol. Phys.* **59**(5), 1123–1137 (1986)
35. A.K. Roy, *J. Math. Chem.* **52**(5), 1405–1413 (2014)
36. Z.H. Deng, Y.P. Fan, *Shandong Univ. J.* **7**, 162 (1957)
37. S.H. Dong, X.Y. Gu, *J. Phys. Conf. Ser.* **96**(1), 012109 (2008)
38. S.H. Dong, *Commun. Theor. Phys.* **55**, 969–971 (2011)
39. L.H. Zhang, X.P. Li, C.S. Jia, *Int. J. Quant. Chem.* **111**(9), 1870–1878 (2011)
40. B.J. Falaye, S.M. Ikhdair, M. Hamzavi, *Z. Naturforsch.* **70**(2), 85–90 (2015)
41. S.M. Ikhdair, *J. Math. Phys.* **52**(5), 052303 (2011)
42. O.J. Oluwadare, K.J. Oyewumi, C.O. Akoshile, O.A. Babalola, *Phys. Scr.* **86**(3), 035002 (2012)
43. O. Mustafa, *J. Phys. B At. Mol. Opt. Phys.* **48**(6), 065101 (2015)
44. K.J. Oyewumi et al., *J. Math. Chem.* **51**(3), 976–991 (2013)
45. M. Hamzavi, S.M. Ikhdair, K.E. Thylwe, *J. Math. Chem.* **51**(1), 227–238 (2013)
46. K.J. Oyewumi et al., *Mol. Phys.* **112**(1), 127–141 (2014)
47. A.K. Roy, *Int. J. Quant. Chem.* **114**(6), 383–391 (2014)
48. O.J. Oluwadare, K.J. Oyewumi, *Eur. Phys. J. Plus* **133**(10), 422 (2018)
49. H. Boukabcha, M. Hachamab, A. Diaf, *App. Math. Comp.* **321**, 121–129 (2018)
50. E. Omugbe, *Asian J. Phys. Chem. Sci.* **8**(1), 26–36 (2020)
51. D. Nath, A.K. Roy, *Int. J. Quant. Chem.* **121**(10), e26616 (2021)
52. C. P. Onyenegecha et al., (2021) <https://doi.org/10.21203/rs.3.rs-763444/v1>
53. E. Omugbe, O.E. Osafire, E.P. Inyang, A. Jahanshir, *Phys. Scr.* **96**(12), 125408 (2021)
54. A.N. Ikot et al., *Few-Body Syst.* **62**, 101 (2021)
55. E.M. Khokha, M. Abu-Shady, T.A. Abdel-Karim, *Int. J. Theor. Appl. Math.* **2**(2), 86–92 (2016)
56. M. Abu-Shady, T.A. Abdel-Karim, E.M. Khokha, *Adv. High Energy Phys.* **2018**, 7356843 (2018)
57. M. Abu-Shady, T.A. Abdel-Karim, E.M. Khokha, *SciFed J. Quant. Phys.* **2**, 1000017 (2018)
58. M. Abu-Shady, E.M. Khokha, *Adv. High Energy Phys.* **2018**, 7032041 (2018)
59. M. Abu-Shady, T.A. Abdel-Karim, Sh.Y. Ezz-Alarab, *J. Egypt. Math. Soc.* **27**, 14 (2019)
60. M. Abu-Shady, Sh.Y. Ezz-Alarab, *Few-Body Syst.* **60**(4), 1–11 (2019)
61. M. Abu-Shady, H.M. Fath-Allah, *Int. J. Mod. Phys. A* **35**(21), 2050110 (2020)
62. M. Abu-Shady, H.M. Fath-Allah, *J. Found. Appl. Phys.* **6**, 163 (2019)
63. M. Abu-Shady, A.N. Ikot, *Eur. Phys. J. Plus* **134**(7), 321 (2019)
64. M. Abu-Shady, *J. Egypt. Math. Soc.* **25**(1), 86–89 (2019)
65. M. Abu-Shady, *Adv. Math. Phys.* **2016**, 4935940 (2016)

66. M. Abu-Shady, Int. J. Appl. Math. Theor. Phys. **2**(2), 16 (2016)
67. M. Abu-Shady, M.K.A. Kaabar, Math. Prob. Eng. **2021**, 9444803 (2021)
68. I. Podlubny, *Fractional Differential Equations* (Academic Press, USA, 1999)
69. A. Kilbas, H. Srivastava, J. Trujillo, Theory and Applications of Fractional Differential Equations, in: Math. Studies., North-Holland, New York, 2006
70. A.F. Nikivorof, V.B. Uvarov, *Special Functions of Mathematical, Physics-A Unified Introduction with Applications* (Basel, Birkhäuser, 1988)
71. U.S. Okorie et al., Int. J. Thermophys. **41**(7), 1–15 (2020)