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Gohar Fractional Effect on the Diatomic Structure and Ro-vibrational Spectroscopy in the Molecular Kratzer Model

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Abstract

Solving the Schrödinger equation (SE) for the wavefunction and binding energy levels of the diatomic molecular system is essential for modeling its structure and analyzing its spectral properties, as the complete wave function inherently involves all the necessary information to analyze its physical properties. In contrast, the obtained energy levels reveal its spectroscopic characteristics. In this work, the Nikiforov-Uvarov (NU) analytical method is brought into the domain of Gohar fractional calculus (GFC). We use the Gohar fractional NU (GFNU) method to solve the fractional hyper-radial SE for the binding rovibrational energy spectra of some homo-nuclear and hetero-nuclear diatomic molecules (DMs) in the molecular Kratzer model for arbitrary values of the vibrational and rotational quantum numbers. Graphical analysis is used to explore the effect of the fractional parameter on the obtained diatomic energy levels and their corresponding normalized hyper-radial wave functions. Interestingly, the fractional parameter was found to have a significant effect on the diatomic structure and spectral properties. The graphical behavior of the Kratzer potential (KP) model and its modified version was analyzed for various DMs. It was observed that the characteristic features of both potential models were affected by the variation of the fractional parameter. We also investigated the dependence of the diatomic energies in both potentials on dimensionality, equilibrium inter-nuclear distance, reduced mass, and quantum numbers. This study provided entirely new results for the energy levels of HCL, LiH, ScH, H₂, O₂, and I₂ DMs in the modified Kratzer potential (MKP) that had not been previously reported in the literature.

Keywords: Gohar Fractional Effect. Nikiforov-Uvarov Method. Schrödinger Equation. Analytical Solutions. Kratzer Potential

1. Introduction

The analytical techniques for solving SE are critical in analyzing the spectroscopic characteristics, the electronic structure, and the energetic properties of the DMs. The literature presents several analytical techniques for solving SE, including the asymptotic iteration method (AIM) [1], the super-symmetric Quantum Mechanics (SUSYQM) [2], the

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NU method [3], the Exact Quantization Rule (EQR) [4], and the Laplace Transform Approach (LTA) [5].

Diatomic molecular vibrational and rotational spectroscopy is a critical field of research in chemistry and molecular physics. Several authors in contemporary literature have examined the bound-state solutions of SE for the DMs [6-9] to gain a deeper understanding of their physical features and chemical characteristics. Several theoretical potential models have been proposed for the diatomic structures, but only a limited number of these models allow for exact analytical solutions of SE for all values of the vibrational and rotational quantum numbers. These models include Morse [10], Yukawa [11], Woods-Saxon [12], Hua [13], Mie-type [14] and Pseudo-harmonic [15] potentials.

In 1920, A. Kratzer [16] introduced an "exactly solvable" potential model for the diatomic structure to investigate the ro-vibrational energy spectra of the DMs. The KP takes the form

$$V(r) = -\mathcal{D}_e \left(\frac{2r_e}{r} - \frac{r_e^2}{r^2} \right), \quad (1.1)$$

where \mathcal{D}_e is the dissociation energy between two atoms in the DM separated by an equilibrium inter-nuclear distance r_e . A recent modification has been made to KP model [17] by adding the dissociation energy to it, resulting in a shift by amount \mathcal{D}_e . The MKP takes the form:

$$V(r) = \mathcal{D}_e \left(\frac{r - r_e}{r} \right)^2. \quad (1.2)$$

The KP is a combination of the Coulomb potential, which exhibits a long-range attractive effect, and a centrifugal potential barrier that is associated with the electronic kinetic energy and possesses a short-range repulsive effect. Their superposition creates an effective molecular potential to explore various aspects of the DMs, including their molecular structure, inter-nuclear vibration, chemical interactions, and ro-vibrational energy spectra. Z. Yalçın et al. [18] demonstrated that the KP well exhibits greater sharpness and depth in comparison to the purely Coulombic potential well. With the KP, Shi-hai Dong and Gus-hua Sun [19] were able to solve the hyper-radial SE and study the impact of dimensionality on the obtained energy spectra. As a result of the remarkable precision with which the KP and its modified version model the diatomic molecular structures, S. M. Ikhdair and R. Sever [20] used the EQR to solve the hyper-radial SE with KP and MKP for various DMs. The KP and its modified form have been investigated through the AIM [21], the ansatz method [22], and the polynomial solutions [23].

In recent years, fractional calculus has come to be recognized for its vast potential to offer more accurate models for natural phenomena than what was achievable with ordinary integer-order calculus. In the literature, many fractional derivatives have been proposed, expanding the scope of applicability of fractional calculus. Among the fractional derivatives introduced thus far, the Riemann-Liouville derivative [24], the Caputo derivative [24], and the conformable derivative (CD) [25] are the most often used fractional derivatives in applications. Al-Raei and El-Daher used the Riemann-Liouville fractional

derivative to numerically solve the space-dependent fractional SE for various potentials, including Lennard-Jones potential [26], Coulomb potential [27], and Morse potential [28]. With the CD, Hadi Rezazadeh et al. solved the conformable Schrödinger-kdv equation and obtained the traveling wave solutions using the G'/G -expansion technique. M. Bilal and J. Ahmad [29] obtained exact optical soliton solutions of the generalized (2+1)-dimensional conformable fractional SE by means of three novel integration norms [30], Hale Y. Karayer et al. [31] used the CD to generalize the NU method and introduced the conformable fractional NU method to solve SE with three different "exactly solvable" potentials. M. M. Hammad et al. [32] used the Conformable fractional NU method to solve the conformable fractional Bohr Hamiltonian with the KP for the tri-axial nuclei.

A. A. Gohar et al. [33] have recently introduced a novel, local, and well-behaved fractional calculus. Its locality imposes simplicity and accuracy in modeling fractional order systems, and its fractional derivative possesses more properties compared to all the previously defined fractional derivatives. In this work, we aim to study the effect of Gohar fractional parameter on the structure and ro-vibrational energy spectra of some homo-nuclear and hetero-nuclear DMs. To this end, we formulate the NU method in the context of GFC and apply the GFNU method to solve the hyper-radial fractional SE with the molecular KP and its modified version. This work is structured as follows: Section 2 presents the basic definition and essential properties of the GFD, which will be subsequently used in our investigation, along with the formulation of the GFNU technique. In Sect. 3, the bound-state energy spectra are obtained, and their corresponding normalized hyper-radial wave functions are analytically formulated in a closed form by solving the hyper-radial Gohar fractional SE by means of the GFNU method for the KP and MKP. Sect. 4 presents numerical computations and graphical representations of the ro-vibrational energy spectra for certain DMs. Finally, our work is concluded in Sect. 5 with a summary and conclusions.

2. Mathematical tools

2.1. Overview of Gohar Fractional Calculus

Definition 2.1.1. Given a function $f : [0, \infty) \rightarrow \mathbb{R}$, the GFD of f of order α , denoted by G_α , is defined by

$$G_\alpha f(x) = \lim_{\Delta x \rightarrow 0} \frac{1}{\Delta x} [f(x + \ln(1 + \Delta x g(\alpha, \eta)x^{-\alpha})) - f(x)],$$

for $x > 0, \alpha \in (0, 1), \eta \in \mathbb{R}^+, g(\alpha, \eta) = \frac{\Gamma(\eta)}{\Gamma(\eta - \alpha + 1)}$.

Theorem 2.1.1. For $\alpha \in (0, 1), \eta \in \mathbb{R}^+$. Suppose that $f, \varphi : [0, \infty) \rightarrow \mathbb{R}$ are G_α -differentiable functions at $x > 0$. Then they satisfy the following properties

(I) *Linearity:* $G_\alpha(\lambda f + \mu \varphi)(x) = \lambda G_\alpha f(x) + \mu G_\alpha \varphi(x); \lambda, \mu \in \mathbb{R}.$

(II) *Product rule:* $G_\alpha(f\varphi)(x) = f(x)G_\alpha \varphi(x) + \varphi(x)G_\alpha f(x).$

(III) *Quotient rule:* $G_\alpha(f/\varphi)(x) = [\varphi(x)G_\alpha f(x) - f(x)G_\alpha \varphi(x)]/\varphi^2(x), \varphi(x) \neq 0.$

(IV) Chain rule: $G_\alpha(f \circ \varphi)(x) = G_\alpha(\varphi(x)) f'(\varphi(x)).$

(V) Derivative of a constant: $G_\alpha(c) = 0, c \in \mathbb{R}.$

Theorem 2.1.2. If $f : [0, \infty) \rightarrow \mathbb{R}$ is a G_α -differentiable function at $x > 0$, then

$$G_\alpha f(x) = g(\alpha, \eta) x^{1-\alpha} f'(x),$$

for $\alpha \in (0, 1), \eta \in \mathbb{R}^+.$

Definition 2.1.2. For $x > 0$, if f is a function defined on $(0, x]$, then the Gohar fractional integral of f of order α , denoted by \mathfrak{T}^α , is defined by

$$\mathfrak{T}^\alpha f(x) = \frac{\Gamma(\eta - \alpha + 1)}{\Gamma(\eta)} \int_0^x \frac{f(t)}{t^{1-\alpha}} dt,$$

where $\alpha \in (0, 1), \eta \in \mathbb{R}^+.$

Theorem 2.1.3. For $x > 0$, If f is a continuous \mathfrak{T}^α -integrable function, then

$$G_\alpha(\mathfrak{T}^\alpha f(x)) = f(x),$$

$$\mathfrak{T}^\alpha(G_\alpha(f(x))) = f(x) - f(0),$$

where $\alpha \in (0, 1), \eta \in \mathbb{R}^+.$

2.2. The GFNU method

The GFNU method can be applied to solve the second-order differential equations of hypergeometric type, which commonly arise in time-independent problems, by means of orthogonal polynomials. It provides us with an exact solution of the SE for the exactly solvable potentials. In spherical coordinates, the SE reduces to a typical hypergeometric-type equation with the following form:

$$G_\alpha^{(2)}\psi(x) + \frac{\tilde{\tau}(x)}{\sigma(x)} G_\alpha\psi(x) + \frac{\tilde{\sigma}(x)}{\sigma^2(x)}\psi(x) = 0, \quad (2.1)$$

where $\psi(x)$ is a hypergeometric-type function, $\sigma(x)$ and $\tilde{\sigma}(x)$ are polynomials of degree at most 2α , $\tilde{\tau}(x)$ is a polynomial of degree at most α .

With the assumption

$$\psi(x) = \varphi(x)\chi(x), \quad (2.2)$$

we write (2.1) as

$$G_\alpha^{(2)}\chi(x) + \left[2\frac{G_\alpha\varphi(x)}{\varphi(x)} + \frac{\tilde{\tau}(x)}{\sigma(x)} \right] G_\alpha\chi(x) + \left[\frac{G_\alpha^{(2)}\varphi(x)}{\varphi(x)} + \frac{\tilde{\tau}(x)}{\sigma(x)} \frac{G_\alpha\varphi(x)}{\varphi(x)} + \frac{\tilde{\sigma}(x)}{\sigma^2(x)} \right] \chi(x) = 0. \quad (2.3)$$

The equation above can be reduced by expressing the coefficients of $G_\alpha\chi(x)$ and $\chi(x)$ in terms of some newly defined functions. To this end, the coefficient of $G_\alpha\chi(x)$ is taken as

$$2\frac{G_\alpha\varphi(x)}{\varphi(x)} + \frac{\tilde{\tau}(x)}{\sigma(x)} = \frac{\tau(x)}{\sigma(x)}, \quad (2.4)$$

or in the more compact form

$$\frac{G_\alpha \varphi(x)}{\varphi(x)} = \frac{\pi(x)}{\sigma(x)}, \quad (2.5)$$

where

$$\pi(x) = \frac{1}{2}[\tau x - \tilde{\tau}(x)] \quad (2.6)$$

and $\tau(x)$ are functions of degree at most α . The term $G_\alpha^{(2)}\varphi(x)/\varphi(x)$ in the coefficient of $\chi(x)$ can be written as

$$\frac{G_\alpha^{(2)}\varphi(x)}{\varphi(x)} = G_\alpha \left(\frac{G_\alpha \varphi(x)}{\varphi(x)} \right) + \left(\frac{G_\alpha \varphi(x)}{\varphi(x)} \right)^2 = G_\alpha \left(\frac{\pi(x)}{\sigma(x)} \right) + \left(\frac{\pi(x)}{\sigma(x)} \right)^2. \quad (2.7)$$

With the aid of (2.5), the coefficient of $\chi(x)$ reduces to the more compact form;

$$\frac{G_\alpha^{(2)}\varphi(x)}{\varphi(x)} + \frac{\tilde{\tau}(x)}{\sigma(x)} \frac{G_\alpha \varphi(x)}{\varphi(x)} + \frac{\tilde{\sigma}(x)}{\sigma^2(x)} = \frac{\tilde{\sigma}(x)}{\sigma^2(x)}, \quad (2.8)$$

where

$$\tilde{\sigma}(x) = \tilde{\sigma}(x) + \pi^2(x) + \pi(x)[\tilde{\tau}(x) - G_\alpha \sigma(x)] + \sigma(x)G_\alpha \pi(x). \quad (2.9)$$

Consequently, (2.3) reduces to the hypergeometric-type equation

$$G_\alpha^{(2)}\chi(x) + \frac{\tau(x)}{\sigma(x)}G_\alpha\chi(x) + \frac{\tilde{\sigma}(x)}{\sigma^2(x)}\chi(x) = 0. \quad (2.10)$$

If $\tilde{\sigma}(x)$ is divisible by $\sigma(x)$, i.e.,

$$\tilde{\sigma}(x) = \lambda\sigma(x), \quad (2.11)$$

we rewrite (2.10) as

$$\sigma(x)G_\alpha^{(2)}\chi(x) + \tau(x)G_\alpha\chi(x) + \lambda\chi(x) = 0, \quad (2.12)$$

where λ is a constant.

The function $\pi(x)$ is determined by comparing (2.9) with (2.11), and then a quadratic equation for $\pi(x)$ is obtained as follows,

$$\pi^2(x) + [\tilde{\tau}(x) - G_\alpha \sigma(x)]\pi(x) + \tilde{\sigma}(x) - k\sigma(x) = 0, \quad (2.13)$$

where

$$k = \lambda - G_\alpha \pi(x). \quad (2.14)$$

Its roots are given by

$$\pi(x) = \frac{G_\alpha \sigma(x) - \tilde{\tau}(x)}{2} \pm \sqrt{\left(\frac{G_\alpha \sigma(x) - \tilde{\tau}(x)}{2} \right)^2 - \tilde{\sigma}(x) + k\sigma(x)}. \quad (2.15)$$

For $\pi(x)$ to have a maximum first degree, the expression under the radical must have a zero discriminant. By setting the discriminant equal to zero, we obtain a quadratic equation for k , which can be solved algebraically to get the possible values of k . Following

the determination of k , we determine $\pi(x)$, $\tau(x)$ and λ by using (2.15), (2.6), and (2.14), respectively.

For the generalized solutions, we differentiate (2.12) n times in the Gohar fractional sense to obtain a recurrence relation via induction. To this end, we G_α differentiate (2.12) to get

$$\sigma(x)G_\alpha^{(2)}\nu_1(x) + \tau_1(x)G_\alpha\nu_1(x) + \mu_1\nu_1(x) = 0, \quad (2.16)$$

where $G_\alpha\chi(x) = \nu_1(x)$, $\tau_1(x) = G_\alpha\sigma(x) + \tau(x)$ and $\mu_1 = G_\alpha\tau(x) + \lambda$. $\tau_1(x)$ is a function of maximum α degree and μ_1 is a parameter that does not depend on x . By means of induction, using $\nu_n(x) = G_\alpha \dots G_\alpha\chi(x) = G_\alpha^{(n)}\chi(x)$, we have;

$$\sigma(x)G_\alpha^{(2)}\nu_n(x) + \tau_n(x)G_\alpha\nu_n(x) + \mu_n\nu_n(x) = 0, \quad (2.17)$$

while the recurrence relations for $\tau_n(x)$ and μ_n are

$$\tau_n(x) = nG_\alpha\sigma(x) + \tau(x), \quad (2.18)$$

$$\mu_n = \frac{n(n-1)}{2}G_\alpha^{(2)}\sigma(x) + nG_\alpha\tau(x) + \lambda. \quad (2.19)$$

When $\mu_n = 0$, (2.19) becomes

$$\lambda_n = -\frac{n(n-1)}{2}G_\alpha^{(2)}\sigma(x) - nG_\alpha\tau(x), \quad (2.20)$$

and then (2.12) has a particular solution of the form $\chi(x) = \chi_{(n,\alpha)}(x)$ which is a function of degree $n\alpha$. The eigenvalues of (2.12) are obtained by equating (2.14) and (2.20), and the eigenfunctions $\chi_{(n,\alpha)}(x)$ are obtained by multiplying (2.12) and (2.17) by the appropriate weight functions $\rho(x)$ and $\rho_n(x)$, respectively, thus they can be rewritten as

$$G_\alpha[\rho(x)\sigma(x)G_\alpha\chi(x)] + \lambda\rho(x)\chi(x) = 0, \quad (2.21)$$

$$G_\alpha[\rho(x)\sigma(x)G_\alpha\nu_n(x)] + \mu_n\rho_n(x)\nu_n(x) = 0, \quad (2.22)$$

where the weight functions $\rho(x)$ and $\rho_n(x)$ obey the differential equations

$$G_\alpha(\rho(x)\sigma(x)) = \rho(x)\tau(x), \quad (2.23)$$

$$G_\alpha(\rho_n(x)\sigma(x)) = \rho_n(x)\tau_n(x). \quad (2.24)$$

If χ is a function of degree $n\alpha$, that is, $\chi = \chi_{n,\alpha}(x)$, we have

$$\nu_m(x) = G_\alpha^{(m)}\chi_{n,\alpha}(x), \quad (2.25)$$

$$\nu_n(x) = G_\alpha^{(n)}\chi_{n,\alpha}(x) = \text{const.} \quad (2.26)$$

Finally, the eigenfunctions $\chi_{n,\alpha}(x)$ are obtained explicitly by the fractional Rodrigues formula

$$\chi_{n,\alpha}(x) = \frac{\Lambda_n}{\rho(x)}G_\alpha^{(n)}(\rho_n(x)) = \frac{\Lambda_n}{\rho(x)}G_\alpha^{(n)}(\sigma^n(x)\rho(x)), \quad n = 0, 1, 2, \dots, \quad (2.27)$$

where Λ_n is a normalization constant.

3. Analytical solutions of the hyper-radial SE with KP and MKP via GFNU method

The Hyper-radial SE with a given spherically symmetric potential $V(r)$ is of the form

$$\frac{d^2\psi(r)}{dr^2} + \frac{N-1}{r} \frac{d\psi(r)}{dr} + \left[\frac{2\mu}{\hbar^2} (E - V(r)) - \frac{\ell(\ell + N - 2)}{r^2} \right] \psi(r) = 0, \quad (3.1)$$

where n is the radial (vibrational) quantum number, ℓ is the orbital angular momentum (rotational) quantum number, r is the inter-nuclear distance, $V(r)$ is the central potential energy function, E denotes the energy spectrum, μ , \hbar , N are the reduced mass, the reduced planck's constant, and the dimensionality, respectively.

The fractional form of the hyper-radial SE is given by changing integer orders with fractional orders in (3.1) as follows

$$G_\alpha^{(2)}\psi(r) + \frac{N-1}{r^\alpha} G_\alpha\psi(r) + \left[\frac{2\mu}{\hbar^2} (E - V(r)) - \frac{\ell(\ell + N - 2)}{r^{2\alpha}} \right] \psi(r) = 0. \quad (3.2)$$

A generalized form of the Kratzer potential is defined as

$$V(r) = \Omega_0 + \frac{\Omega_1}{r^{2\alpha}} - \frac{\Omega_2}{r^\alpha}, \quad \Omega_1 = \mathcal{D}_e r_e^{2\alpha}, \quad \Omega_2 = 2\mathcal{D}_e r_e^\alpha, \quad r \in (0, \infty), \quad (3.3)$$

where the KP is obtained for $\Omega_0 = 0$ and the MKP is obtained for $\Omega_0 = \mathcal{D}_e$. Substituting (3.3) into (3.2) gives

$$G_\alpha^{(2)}\psi(r) + \frac{N-1}{r^\alpha} G_\alpha\psi(r) + \frac{1}{r^{2\alpha}} [-Q_2 r^{2\alpha} + Q_1 r^\alpha - Q_0] \psi(r) = 0, \quad (3.4)$$

where

$$Q_2 = \frac{2\mu}{\hbar^2} (\Omega_0 - E), \quad Q_1 = \frac{2\mu}{\hbar^2} \Omega_2, \quad Q_0 = \frac{2\mu}{\hbar^2} \Omega_1 + \ell(\ell + N - 2). \quad (3.5)$$

By comparing (3.4) with (2.1), we obtain

$$\tilde{\tau}(r) = N - 1, \quad \sigma(r) = r^\alpha, \quad \tilde{\sigma}(r) = -Q_2 r^{2\alpha} + Q_1 r^\alpha - Q_0. \quad (3.6)$$

By means of (3.6) and (2.15), $\pi(r)$ is given by

$$\pi(r) = \frac{\alpha g(\alpha, \eta) - (N - 1)}{2} \pm \sqrt{Q_2 r^{2\alpha} + (k - Q_1) r^\alpha + \left(\frac{(\alpha g(\alpha, \eta) - (N - 1))^2}{4} + Q_0 \right)}, \quad (3.7)$$

By imposing the condition that the discriminant of the expression under the radical of (3.7) must be equal to zero, the two possible roots of k are determined to be

$$k_\pm = Q_1 \pm 2\sqrt{Q_2} \sqrt{\frac{(\alpha g(\alpha, \eta) - (N - 1))^2}{4} + Q_0}. \quad (3.8)$$

Inserting (3.8) into (3.7) gives

$$\pi(r) = \frac{\alpha g(\alpha, \eta) - (N - 1)}{2} \pm \left\{ \begin{array}{ll} \sqrt{Q_2} r^\alpha + \sqrt{\frac{(\alpha g(\alpha, \eta) - (N - 1))^2}{4} + Q_0} & k = k_+ \\ \sqrt{Q_2} r^\alpha - \sqrt{\frac{(\alpha g(\alpha, \eta) - (N - 1))^2}{4} + Q_0} & k = k_- \end{array} \right\}. \quad (3.9)$$

To obtain a physically valid solution, it is necessary to select $\pi(r)$ in such a way that $G_\alpha \tau(r) < 0$. Accordingly, the negative sign in (3.9) is selected, and the function $\pi(r)$ becomes

$$\pi(r) = \frac{\alpha g(\alpha, \eta) - (N - 1)}{2} - \left(\sqrt{Q_2} r^\alpha - \sqrt{\frac{(\alpha g(\alpha, \eta) - (N - 1))^2}{4} + Q_0} \right), k = k_-. \quad (3.10)$$

Therefore, the function $\tau(r)$ is defined as

$$\tau(r) = \left(\alpha g(\alpha, \eta) + \sqrt{(\alpha g(\alpha, \eta) - (N - 1))^2 + 4Q_0} \right) - 2\sqrt{Q_2} r^\alpha, \quad (3.11)$$

And the expressions for λ and λ_n are obtained to be

$$\lambda = Q_1 - \left(\alpha g(\alpha, \eta) + 2\sqrt{\frac{(\alpha g(\alpha, \eta) - (N - 1))^2}{4} + Q_0} \right) \sqrt{Q_2}, \quad (3.12)$$

$$\lambda_n = 2n\alpha g(\alpha, \eta) \sqrt{Q_2}. \quad (3.13)$$

Equating (3.12) and (3.13), the diatomic energy spectrum formula in the N -dimensional space takes the form

$$E_{n,l}^{\alpha,\eta,N} = \Omega_0 - \frac{2\mu}{\hbar^2} \left(\frac{\Omega_2}{(2n + 1)\alpha g(\alpha, \eta) + \sqrt{4\ell(\ell + N - 2) + (\alpha g(\alpha, \eta) - (N - 1))^2 + \frac{8\mu}{\hbar^2}\Omega_1}} \right)^2, \quad (3.14)$$

Now we determine the corresponding normalized hyper-radial wave functions $\psi(r)$ in terms of the orthogonal associated Laguerre polynomials by expressing $\psi(r)$ as

$$\psi(r) = \varphi(r)\chi(r). \quad (3.15)$$

Inserting the functions $\pi(r)$ and $\sigma(r)$ into (2.5), we obtain the fractional logarithmic derivative

$$\frac{G_\alpha \varphi(x)}{\varphi(x)} = \frac{1}{r^\alpha} \left[\frac{\alpha g(\alpha, \eta) - (N - 1)}{2} - \left(\sqrt{Q_2} r^\alpha - \sqrt{\frac{(\alpha g(\alpha, \eta) - (N - 1))^2}{4} + Q_0} \right) \right], \quad (3.16)$$

using the properties of the GFI, Definition 2.1.2 and Theorem 2.1.3, we have

$$\varphi(r) = \mathfrak{B} r^{\frac{1}{g(\alpha,\eta)}} \left(\frac{\alpha g(\alpha,\eta) - (N-1)}{2} + \sqrt{\frac{(\alpha g(\alpha,\eta) - (N-1))^2}{4} + \frac{2\mu}{\hbar^2}\Omega_1 + \ell(\ell + N - 2)} \right) e^{-\frac{\sqrt{\frac{2\mu}{\hbar^2}(\Omega_0 - E)} r^\alpha}{\alpha g(\alpha,\eta)}}. \quad (3.17)$$

The weight function $\rho(x)$ is obtained by means of (2.23) as

$$\rho(r) = r^{\frac{1}{g(\alpha,\eta)}} \sqrt{(\alpha g(\alpha,\eta) - (N-1))^2 + 4\left(\ell(\ell + N - 2) + \frac{2\mu}{\hbar^2}\Omega_1\right)} e^{-\frac{2\sqrt{\frac{2\mu}{\hbar^2}(\Omega_0 - E)} r^\alpha}{\alpha g(\alpha,\eta)}}. \quad (3.18)$$

Inserting (3.18) into (2.27), we obtain the function $\chi(x)$ as follows

$$\chi(r) = \Lambda_n r^{\frac{-1}{g(\alpha, \eta)}} \sqrt{(\alpha g(\alpha, \eta) - (N-1))^2 + 4\left(\ell(\ell + N - 2) + \frac{2\mu}{\hbar^2} \Omega_1\right)} e^{\frac{2\sqrt{\frac{2\mu}{\hbar^2}(\Omega_0 - E)}r^\alpha}{\alpha g(\alpha, \eta)}} \cdot G_\alpha^{(n)} \left(r^{\alpha n + \frac{1}{g(\alpha, \eta)}} \sqrt{(\alpha g(\alpha, \eta) - (N-1))^2 + 4\left(\ell(\ell + N - 2) + \frac{2\mu}{\hbar^2} \Omega_1\right)} e^{-\frac{2\sqrt{\frac{2\mu}{\hbar^2}(\Omega_0 - E)}r^\alpha}{\alpha g(\alpha, \eta)}} \right), \tag{3.19}$$

for $n = 0, 1, 2, 3, \dots$, where Λ_n are the normalization constants.

Comparing (3.19) with the fractional form of the Rodrigues formula for the orthogonal associated Laguerre polynomials [34]

$$L_n^\gamma(x) = \frac{x^{-\gamma} e^x}{n!} G_\alpha^{(n)}(x^{n+\gamma} e^{-x}). \tag{3.20}$$

With

$$\Lambda_n = \frac{1}{n!}, \quad x = \delta r^\alpha, \quad \delta = \frac{2}{\alpha g(\alpha, \eta)} \sqrt{\frac{2\mu}{\hbar^2}(\Omega_0 - E)}, \tag{3.21}$$

$$\gamma = \frac{1}{g(\alpha, \eta)} \sqrt{(\alpha g(\alpha, \eta) - (N-1))^2 + 4\left(\ell(\ell + N - 2) + \frac{2\mu}{\hbar^2} \Omega_1\right)} \tag{3.22}$$

$\chi(r)$ can be expressed in terms of the associated Laguerre polynomial as follows

$$\chi(r) = L_n^\gamma(\delta r^\alpha) \tag{3.23}$$

Inserting (3.17) and (3.23) into (3.15), $\psi(r)$ takes the form

$$\psi(r) = \mathfrak{P} r^{\frac{\omega + \alpha g(\alpha, \eta) - (N-1)}{2g(\alpha, \eta)}} e^{-\frac{\delta r^\alpha}{2}} L_n^\gamma(\delta r^\alpha) \tag{3.24}$$

where

$$\omega = \sqrt{4\ell(\ell + N - 2) + (\alpha g(\alpha, \eta) - (N-1))^2 + \frac{8\mu}{\hbar^2} \Omega_1}, \tag{3.25}$$

and \mathfrak{P} is the normalization constant to be determined by means of the fractional normalization condition

$$\frac{1}{g(\alpha, \eta)} \int_0^\infty r^{(N-1)\alpha} |\psi(r)|^2 \frac{dr}{r^{(1-\alpha)}} = 1. \tag{3.26}$$

or equivalently,

$$\int_0^\infty \rho^{(N-1)} |\psi(\rho)|^2 d\rho = \alpha g(\alpha, \eta) \delta^{\left(\frac{\omega + \alpha g(\alpha, \eta) - (N-1)}{\alpha g(\alpha, \eta)} + N\right)}, \quad \rho = \delta r^\alpha. \tag{3.27}$$

The normalization constant \mathfrak{P} is determined by the generalized Coulomb-like integral [35]

$$\begin{aligned} \mathcal{J}_{n, \nu}^\beta(x) &= \int_0^\infty e^{-x} x^{\nu+\beta} \left(L_n^{(\nu)}(x)\right)^2 dx \\ &= \frac{\Gamma(\nu + n + 1)}{\Gamma(n + 1)} \sum_{j=0}^n (-1)^j \frac{\Gamma(n - j - \beta) \Gamma(\nu + \beta + j + 1)}{\Gamma(-j - \beta) \Gamma(\nu + j + 1) \Gamma(j + 1) \Gamma(n - j + 1)}, \end{aligned} \tag{3.28}$$

where $\text{Re}(\nu + \beta + 1) > 0$.

For our purpose, the value of β is equal to 1, and $\nu = \mathcal{N} - 2 + \frac{\omega + \alpha g(\alpha, \eta) - (\mathcal{N} - 1)}{\alpha g(\alpha, \eta)}$. $\mathcal{J}_{n, \nu}^1$ is restricted to only two nonzero terms, (for $j = n - 1$ and $j = n$) in the summation (3.28) due to the presence of gamma functions with negative integers. Inserting the obtained value $\mathcal{J}_{n, \nu}^1(x) = \frac{(2n + \nu + 1)\Gamma(\nu + n + 1)}{\Gamma(n + 1)}$ into the normalization condition (3.27), the normalization constant \mathfrak{P} is obtained as

$$\mathfrak{P} = \sqrt{\frac{\alpha g(\alpha, \eta) \delta^{\mathcal{N}} \Gamma(n + 1)}{(2n + \nu + 1) \Gamma(n + \nu + 1)}}. \quad (3.29)$$

Therefore, the normalized hyper-radial wave functions for the generalized KP are defined by

$$\psi(\rho) = \sqrt{\frac{\alpha g(\alpha, \eta) \delta^{\mathcal{N}} \Gamma(n + 1)}{(2n + \nu + 1) \Gamma(n + \nu + 1)}} \rho^{\frac{\omega + \alpha g(\alpha, \eta) - (\mathcal{N} - 1)}{2\alpha g(\alpha, \eta)}} e^{-\frac{\rho}{2}} L_n^{\nu}(\rho), \quad (3.30)$$

4. Results and Discussion

In this section, we analyze the diatomic binding energies and wavefunctions in the KP and MKP models numerically and graphically under the effect of the fractional parameter α in \mathcal{N} -dimensional space.

Figure 1 illustrates the KP and MKP for various DMs. Their graphical behavior reveals the nature of the chemical bond and the molecular behavior at $r = r_e$, where the two atoms of the DM are in their stable configuration. As the distance separating the atomic nuclei decreases, the repulsive forces between them intensify, leading to an increase in the potential that approaches an infinitely large value. On the other hand, during the process of decomposition of the DM, the distance between nuclei increases towards infinity, leading to the elimination of the potential. Figures 2 demonstrates the effect of the fractional parameter α on the KP and MKP for the molecular Nitrogen. As the value of the fractional parameter α increases steadily, we detect a gradual decrease in the equilibrium inter-nuclear distance of the potential. Figure 3 demonstrates a similar effect of the fractional parameter α on the wavefunction, where the wavefunction's peak gradually shifts to the left as the fractional parameter's value increases. Figures 2 and 3 together uncover the "Gohar fractional effect" (GFE) on the diatomic structure, in which raising the value of the fractional parameter α creates an internal attractive force between the two atoms of the DM and increases its coherence.

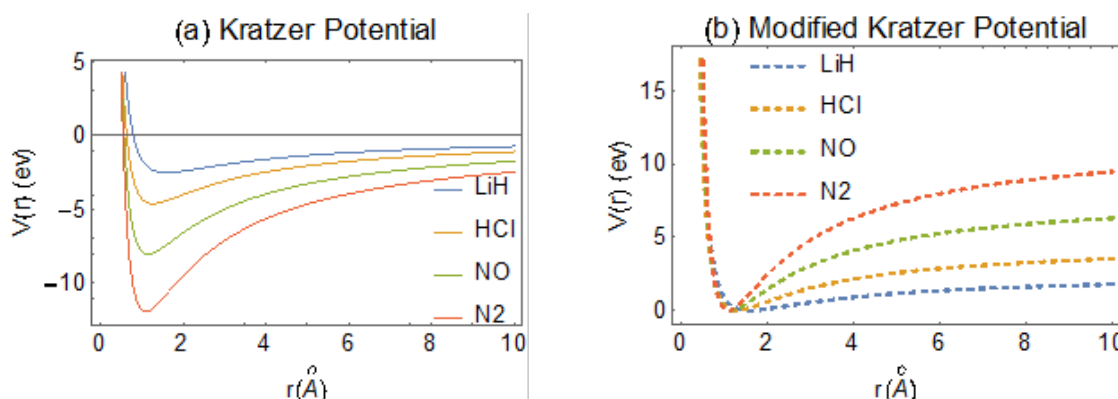


Figure 1: The KP and MKP for some DMs

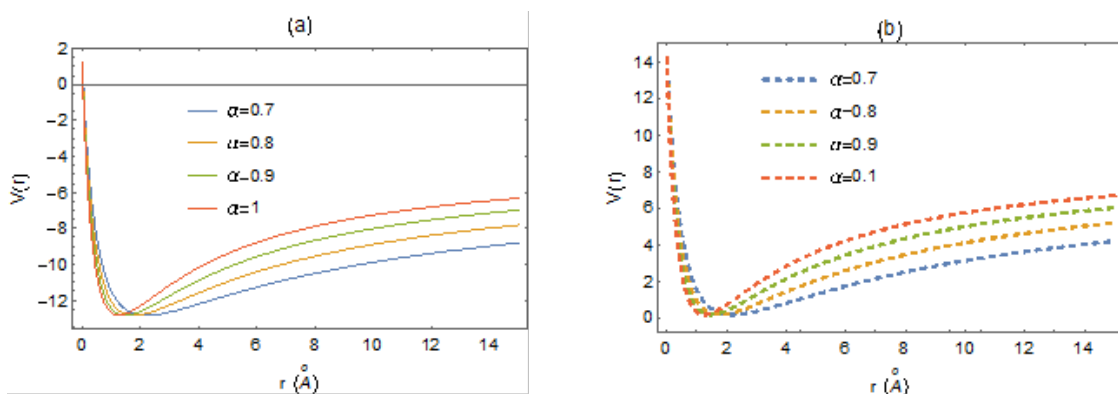


Figure 2: Gohar fractional effect on the KP in (a) and MKP in (b) for the molecular Nitrogen

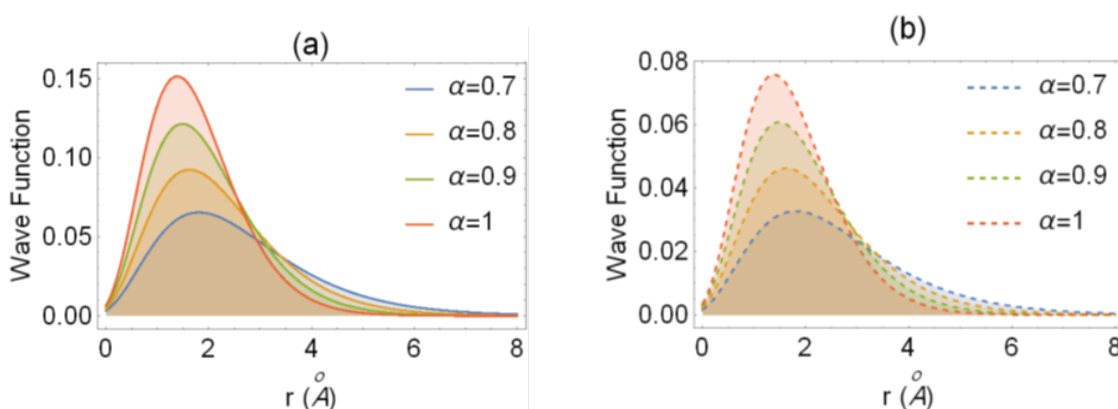


Figure 3: Gohar fractional effect on the wavefunction of the molecular Nitrogen modeled by the KP in (a) and MKP in (b) for $n = \ell = 0$

The energy levels' dependence on the quantum numbers n and ℓ is demonstrated in Figures 4 and 5, respectively. As the values of quantum numbers increase, there is a progressive rise in the diatomic energy spectra. Moreover, for a fixed value of n and ℓ , increasing the fractional parameter α causes a significant increase in the diatomic eigen-energies. Therefore, raising the fractional parameter enhances the internal coherence of the diatomic structure, and the DMs are more constrained in the classical case, where $\alpha = 1$, than in the fractional one, where $0 < \alpha < 1$. Figures 6 and 7 reveal the variation of the energy levels with the equilibrium inter-nuclear distance r_e and the reduced mass μ , respectively, for different values of the fractional parameter α . As r_e and μ assume larger values, we observe a corresponding reduction in the diatomic energy spectra. For a fixed value of r_e and μ , raising α augments the diatomic energy spectra.

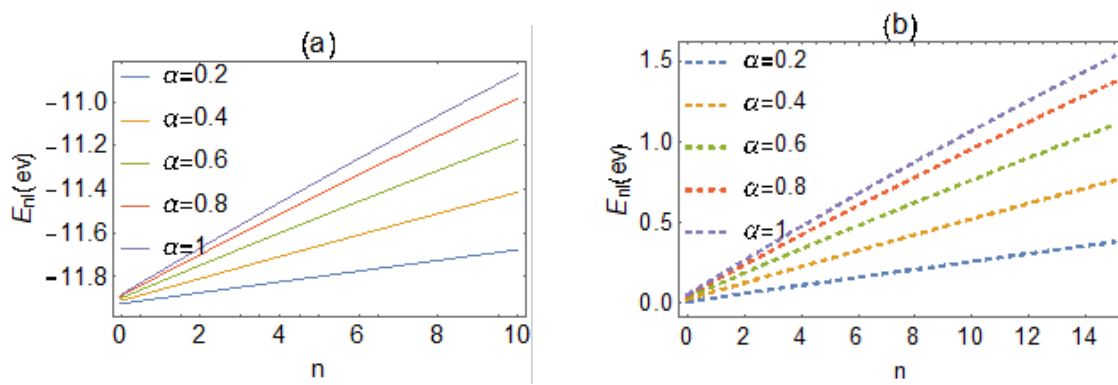


Figure 4: The variation of the Energy spectra of the molecular Nitrogen with n at various values of the fractional parameter α for KP in (a) and MKP in (b)

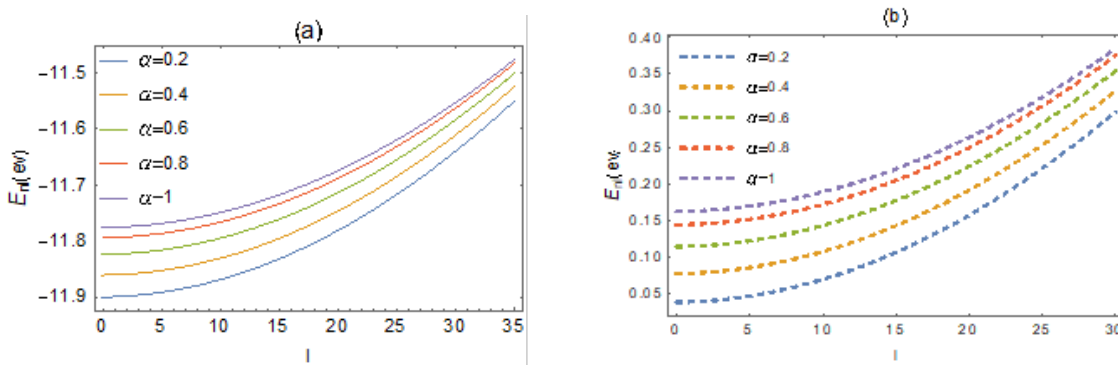


Figure 5: The variation of the Energy spectra of the molecular Nitrogen with ℓ at various values of the fractional parameter α for KP in (a) and MKP in (b)

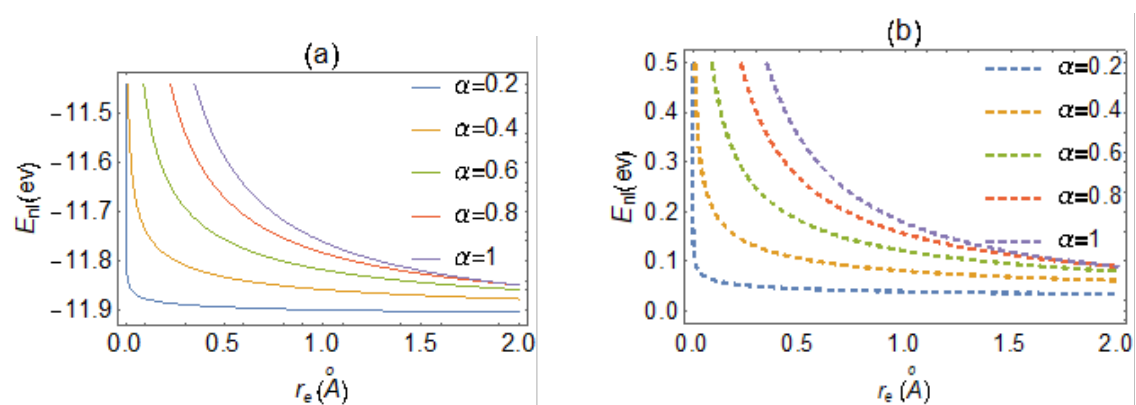


Figure 6: The variation of the Energy spectra of the molecular Nitrogen with the equilibrium bond length r_e at various values of the fractional parameter α for KP in (a) and MKP in (b)

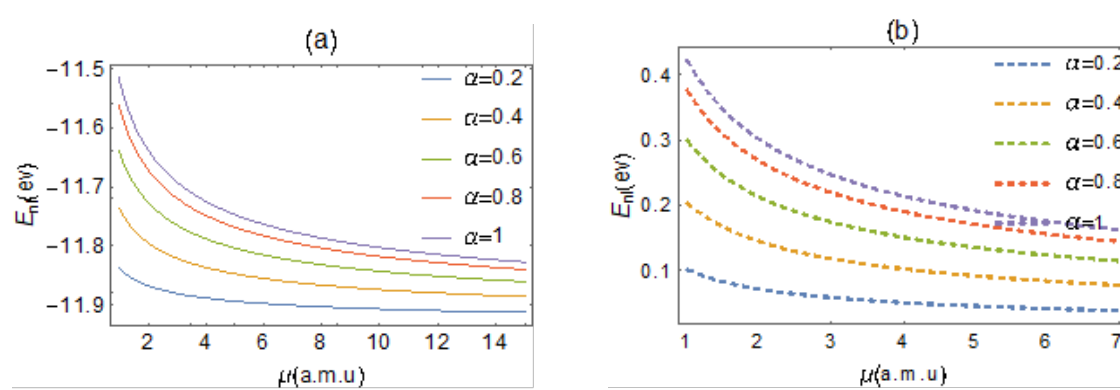


Figure 7: The variation of the Energy spectra of the molecular Nitrogen with the reduced mass μ at various values of the fractional parameter α for KP in (a) and MKP in (b)

Table 1 includes the spectroscopic parameters of the DMs. To validate the GFNU method, developed in this work, and study the effect of the dimensionality \mathcal{N} on the diatomic energy levels, the classical ro-vibrational energy spectra for NO and CO DMs, as modeled by KP, are obtained by setting $\alpha = 1$ and represented numerically in Tables 2 and 3, respectively, for different values of the dimensionality. For $\mathcal{N} = 3$, our results are compared to the corresponding results obtained by different analytical methods in the literature, such as the EQM [20] and AIM [21]; the remarkable consistency between our results and those previously reported in the literature demonstrates the validity and applicability of the GFNU method. As shown in Tables 2 and 3, increasing the dimensionality results in a corresponding decrease in the energy levels, as the multi-dimensional energy spectra are lower than their corresponding three-dimensional values.

Table 1: Spectroscopic parameters of various DMs [20, 21]

DM	$r_e \left(\overset{\circ}{\text{Å}} \right)$	$D_e(\text{eV})$	$\mu(\text{amu})$
HCl	1.2746	4.619061175	0.9801045
LiH	1.5956	2.515283695	0.8801221
ScH	1.7080	4.56	10.682771
NO	1.1508	8.043782568	7.468441
CO	1.1282	10.84507364	6.860586
H ₂	0.7416	4.7446	0.50391
O ₂	1.2080	5.156658828	7.997457504
I ₂	2.6620	1.581791864	63.452235
N ₂	1.0940	11.93827205	7.00335

Table 2: $E_{n,l}^{\alpha,\eta,\mathcal{N}}$ (eV) of NO molecule in the KP for $\alpha = 1$ and different values of the dimensional number $v\mathcal{N}$

		$\mathcal{N} = 3$					
n	l	GFNU	EQR [20]	AIM [21]	$\mathcal{N} = 4$	$\mathcal{N} = 5$	$\mathcal{N} = 6$
0	0	-8.002659243	-8.002659419	-8.002659417	-8.002501971	-8.002239863	-8.001872940
1	0	-7.921456323	-7.921456840	-7.921456839	-7.921301438	-7.921043309	-7.920681957
	1	-7.921043308	-7.921043829	-7.921043834	-7.920681957	-7.920217410	-7.919649704
2	0	-7.841483108	-7.841483958	-7.841483956	-7.841330563	-7.841076333	-7.840720439
	1	-7.841076333	-7.841077185	-7.841077188	-7.840720439	-7.840262909	-7.839703778
	2	-7.840262908	-7.840263768	-7.840263771	-7.839703778	-7.839043090	-7.838280896
3	0	-7.762714895	-7.762716067	-7.762716066	-7.762564643	-7.762314234	-7.761963689
	1	-7.762314233	-7.762315408	-7.762315413	-7.761963689	-7.761513035	-7.760962306
	2	-7.761513034	-7.761514215	-7.761514218	-7.760962306	-7.760311547	-7.759560807
	3	-7.760311547	-7.760312738	-7.760312744	-7.759560807	-7.758710145	-7.757759626

To the best of our knowledge, this study is the first to determine the ro-vibrational energy spectra for HCl, LiH, ScH, H₂, O₂, and I₂ DMs in the MKP model. With the aim of providing a comparative benchmark against which future studies can be compared, we have only included our numerical values for these DMs in Table 4. The molecules investigated in this work were selected due to their extensive applications in chemistry and molecular physics. In our calculations, we take $\eta = 1$, $\hbar c = 1973.29 \text{eV}\overset{\circ}{\text{Å}}$, and $1 \text{amu} = 931.494028 \text{MeV}/c^2$.

Table 3: $E_{n,\ell}^{\alpha,\eta,\mathcal{N}}$ (eV) of CO molecule in the KP for $\alpha = 1$ and different values of the dimensional number \mathcal{N}

n	l	$\mathcal{N} = 3$			$\mathcal{N} = 4$	$\mathcal{N} = 5$	$\mathcal{N} = 6$
		GFNU	EQR [20]	AIM [21]			
0	0	-10.794244204	-10.794315323	-10.79431532	-10.794065953	-10.793768882	-10.793353009
1	0	-10.693768716	-10.693839925	-10.69383992	-10.693592948	-10.693300014	-10.692889935
	1	-10.693300015	-10.693371229	-10.69337123	-10.692889935	-10.692362737	-10.691718454
2	0	-10.594689602	-10.594760890	-10.59476089	-10.594516271	-10.594227400	-10.593823006
	1	-10.594227400	-10.594298692	-10.59429869	-10.593823006	-10.593303117	-10.592667767
	2	-10.593303118	-10.593374417	-10.59337441	-10.592667767	-10.591916996	-10.591050856
3	0	-10.496981107	-10.497052462	-10.49705246	-10.496810168	-10.496525284	-10.496126471
	1	-10.496525284	-10.496596643	-10.49659664	-10.496126471	-10.495613757	-10.494987175
	2	-10.495613758	-10.495685124	-10.49568512	-10.494987175	-10.494246766	-10.493392578
	3	-10.494246766	-10.494318144	-10.49431814	-10.493392578	-10.492424666	-10.491343095

Table 4: $E_{n,\ell}^{\alpha,\eta,\mathcal{N}}$ (eV) for HCL, LiH, ScH, H₂, O₂, and I₂ DMs in the MKP model for $\alpha = 1$ and $\mathcal{N} = 3$.

n	l	HCL	LiH	ScH	H ₂	O ₂	I ₂
0	0	0.077213291515	0.047973594210	0.017454431185	0.185432876611	0.030300337196	0.002709298059
1	0	0.225334148907	0.139465053243	0.052031021007	0.521949955761	0.090018061581	0.008104747222
	1	0.227768274405	0.141176308997	0.052162862679	0.534573757990	0.090366889844	0.008113972715
2	0	0.366325536938	0.225960330363	0.086214327050	0.822538871353	0.148698340375	0.013472590593
	1	0.368643459152	0.227579006688	0.086344671973	0.833839937078	0.149041126287	0.013481768925
	2	0.373271652035	0.230809419789	0.086605338979	0.856243027720	0.149726556834	0.013500125265
3	0	0.500637769440	0.307816689241	0.120010291203	1.092137860359	0.206365065838	0.018813016179
	1	0.502846768819	0.309349345597	0.120139161948	1.102294716370	0.206701948152	0.018822147669
	2	0.507257561632	0.312408175247	0.120396880921	1.122434089221	0.207375574534	0.018840410330
	3	0.513855795085	0.316980281053	0.120783403098	1.152214844213	0.208385668635	0.018867803519
4	0	0.628686160049	0.385360021482	0.153424743565	1.334864984720	0.263041446378	0.024126210387
	1	0.630792955686	0.386812646528	0.153552162279	1.344027026860	0.263372559884	0.024135295355
	2	0.634999753900	0.389711832269	0.153806977505	1.362197675253	0.264034651600	0.024153464972
	3	0.641293023758	0.394045513847	0.154189144854	1.389076567943	0.265027451072	0.024180718601
	4	0.649652605983	0.399795752314	0.154698597763	1.424228919907	0.266350552966	0.024217055287
5	0	0.750854236603	0.458888095304	0.186463404953	1.554176326618	0.318750029899	0.029412358044
	1	0.752865037378	0.460266165482	0.186589393368	1.562469342699	0.319075505563	0.029421396804
	2	0.756880228920	0.463016626156	0.186841348308	1.578919731629	0.319726324465	0.029439474009
	3	0.762887042802	0.467128177136	0.187219226003	1.603261855385	0.320702221885	0.029466589024
	4	0.770866454582	0.472584014902	0.187722960823	1.635110936685	0.322002801084	0.029502740902
5	0.780793335481	0.479362005521	0.188352465304	1.673978294206	0.323627533705	0.029547928374	

5. Summary and Conclusions

In this work, the Gohar fractional calculus (GFC) is used to extend the scope of the “Nikiforov-Uvarov” (NU) analytical method into the domain of fractional calculus. The Gohar fractional NU (GFNU) method is applied to solve the hyper-radial Schrödinger equation (SE) with the molecular Kratzer potential (KP) and modified Kratzer potential (MKP) in \mathcal{N} -dimensional space for the bound state eigen-energies and their corresponding normalized hyper-radial eigen-states. The characteristic features of the KP and MKP are explored graphically, and the effect of the fractional parameter on them is investigated and discussed in detail. The binding ro-vibrational energy spectra for various well known diatomic molecules (DMs) are computed numerically and analyzed graphically. The effect of the fractional parameter and dimensionality on the obtained diatomic energy levels is investigated numerically and graphically. In the classic case $\alpha = 1$, our study provided entirely novel results that had not been previously reported in the literature, while the

remaining results are found to be perfectly compatible with those obtained via other analytical approaches. The remarkable consistency between our results and those in the literature demonstrates the accuracy and applicability of the GFNU method. Our work uncovered the "Gohar fractional effect,"(GFE), in which a progressive rise in the inter-nuclear attractive forces and binding ro-vibrational energy spectra of the DMs is observed upon increasing the Gohar fractional parameter α . The GFNU method opens the door to explore further diatomic interactions and molecular structures in the future.

Statements and Declarations

Author's contributions: **A. A. Gohar:** Conceptualization, Methodology, Writing-Original draft, Editing. **M. A. Abdel-Khalek:** Supervision, Software, Visualization, Validation, Data Curation. **A. SH. Yaqut:** Writing, Investigation, Visualization, Validation. **M. S. Younes:** Writing, Investigation, Visualization, Validation. **S. B. Doma:** Supervision, Formal analysis, Methodology, Writing- Review & Editing.

Declaration of competing interest: The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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