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Realization of the Spectrum Generating Algebra for the Generalized Kratzer Potentials

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Abstract The dynamical symmetries of the Kratzer-type molecular potentials (generalized Kratzer molecular potentials) are studied by using the factorization method. The creation and annihilation (ladder) operators for the radial eigenfunctions satisfying quantum dynamical algebra $SU(1,1)$ are established. Factorization method is a very simple method of calculating the matrix elements from these ladder operators. The matrix elements of different functions of r, $r\frac{d}{dr}$, their sum Γ_1 and difference Γ_2 are evaluated in a closed form. The exact bound state energy eigenvalues $E_{n,\ell}$ and matrix elements of r, $r\frac{d}{dr}$, their sum Γ_1 and difference Γ_2 are calculated for various values of n and ℓ quantum numbers for CO and NO diatomic molecules for the two potentials. The results obtained are in very good agreement with those obtained by other methods.

Keywords Schrödinger equation · Exact solutions · Wavefunction · Ansatz · Ladder operators · $SU(1,1)$ · Kratzer potential · (Modified) Kratzer potential · Diatomic molecules

1 Introduction

Exactly solvable models in Physics have been generating a renewed interest, because of the fact that they can be solved in terms of creation and annihilation operators by means of factorization method [1–17]. In the year 2002, this present method was proposed in the two related works: the ladder operators for the modified Pöschl-Teller potential and the Morse potential were obtained [5, 6]. With factorization method, the ladder operators of a quantum mechanical system with some important potentials like Morse potential, Pöschl-Teller potential, the pseudoharmonic potential, the infinitely square-well potential and other

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quantum systems have been established [5–14]. For comprehensive review (see Dong and references therein [4]).

Algebraic methods underlying Lie symmetry and its associated algebra have been widely used to study many of these exactly solvable potentials. In 2007, Rasinariu et al. [15] gave a review of the progress made so far in solving exactly solvable problems in quantum mechanics, by connecting supersymmetry and spectrum generating algebras through the property of shape invariance. The solutions of exactly solvable models can be achieved by dynamical algebraic approaches [1–15, 18–21]. In 1991, De Lange and Raab [16] presented operator methods with shift operators (that is, raising and lowering operators) for the Hamiltonian of exactly solvable models.

For the factorization method, we are going to adopt Dong's approach [4] by finding the ladder operators $K^{\pm}$ with the following properties:

$$K_n^{\pm}\Phi_n(x) = k_n\Phi_{n+1}(x). \tag{1}$$

In this case, we are seeking for the ladder operators of the form

$$K_n^{\pm} = A_n^{\pm}(x)\frac{d}{dx} + B_n^{\pm}(x), \tag{2}$$

these ladder operators depend on the physical variable x, which is different for different quantum systems. With (1), the following expressions are obtained:

$$K_{n+1}^{-}K_n^{+}\Phi_n(x) = k_n^{+}K_{n+1}^{-}\Phi_n(x), \qquad K_n^{+}K_{n+1}^{-}\Phi_{n+1}(x) = k_n^{+}K_{n+1}^{-}\Phi_{n+1}(x), \tag{3}$$

from which we find that the products of the operators $K_{n+1}^{-}K_n^{+}$ and $K_{n+1}^{+}K_n^{-}$ acting on the given wavefunctions $\Phi_n(x)$ and $\Phi_{n+1}(x)$, respectively, have the same constant

$$c_n = k_n^{+}K_{n+1}^{-}. \tag{4}$$

The $SU(1,1)$ algebra has useful applications in Physics [4, 21–23]. The algebra of the group $SU(1,1)$ is used to generate the energy spectra while the representation matrices of the group could be used to calculate time dependent excitations of the bound states and the scattering states respectively.

For diatomic molecules, the generalized Kratzer potentials is considered as one of the molecular potentials. These potentials have the general features of the true interaction energy, interatomic, inter-molecular and dynamical properties, their wavefunctions do vanish at the origin like Morse potential. This added advantage make these potentials important in Molecular Physics, Chemical Physics, Solid State Physics. These potentials (Kratzer and modified Kratzer molecular potentials) that are being considered in the present work are important molecular potentials which describe the interaction between two atoms . These potentials have been used extensively to describe the molecular structure and interactions and have been receiving much attention in the history of quantum chemistry for some decades ago [24–30].

It is the purpose of this paper to study the dynamical symmetries of the Kratzer-type molecular potentials (generalized Kratzer molecular potentials) and to establish that the generators obtained are an $SU(1,1)$ dynamical group, and to obtain some numerical results for the energy eigenvalues and matrix elements for some diatomic molecules.

The paper is organized as follows. In Section 2, we study the exact solutions of the Kratzer-type molecular potentials. Section 3 contained the construction of the creation and annihilation operators, the commutation relations of some of these operators and the matrix elements of some related functions r and $r\frac{d}{dr}$. Also, in Section 4, the numerical calculations of the energy levels and matrix elements for some diatomic molecules for the Kratzer and modified Kratzer potentials are given. We conclude with Section 5.

2 Exact Solutions of the Kratzer-Type Molecular Potentials

Consider the molecular potential (the generalized Kratzer potential) of the form [23, 27, 31, 32]

$$V(r) = \frac{a}{r} + \frac{b}{r^2} + c. \tag{5}$$

This potential is of great interest because, it is a generalized form of the molecular potential which can be used to generate other forms of the Kratzer-type molecular potentials:

- Standard Morse or Kratzer-Fues potential

$$V(r) = -D_0\left(\frac{2r_0}{r} - \frac{r_0^2}{r^2}\right) \tag{6}$$

where D_0 is the dissociation energy between two atoms in a solid and r_0 is the equilibrium intermolecular separation. On comparing with (5), we have $a = -2D_0r_0, b = D_0r_0^2, c = 0$ and this potential has minimum value to be $-D_0$ at $r = r_0$ [4, 23–25, 27, 28, 31–34].

- Modified Kratzer potential

$$V(r) = -D_0\left(\frac{2r_0}{r} - \frac{r_0^2}{r^2}\right) + D_0 = D_0\left(\frac{r-r_0}{r}\right)^2, \tag{7}$$

where, $a = -2D_0r_0$, $b = D_0r_0^2$ and $c = D_0$. Modified Kratzer potential is Kratzer potential shifted by the amount D_0 [26, 27, 31, 32]. The graphs of the two potentials ((6) and (7)) are shown below in Fig. 1.

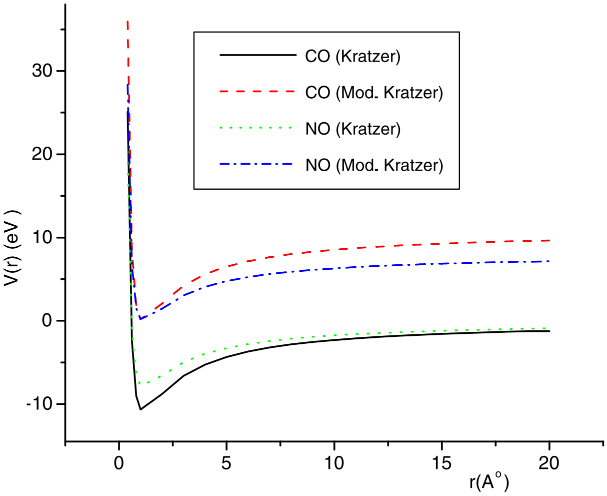

Fig. 1 Shapes of the Kratzer and modified Kratzer potentials for *CO* and *NO* diatomic molecules

Consider the motion of a particle in a spherically symmetric potential $V(r)$

$$-\frac{\hbar^2}{2\mu}\Delta\Psi(r,\theta,\phi)=[E-V(r)]\Psi(r,\theta,\phi) \tag{8}$$

where the potential $V(r)$ is taken as in (5). We seek for the wavefunctions of the form

$$\Psi_{n,\ell,m}(r,\theta,\phi)=R_{n,\ell}(r)Y_\ell^m(\theta,\phi) \tag{9}$$

which reduces (8) into the radial and angular wave functions as:

$$\frac{d^{\,2}R_{n,\ell}(r)}{dr^{\,2}}+\frac{2}{r}\frac{dR_{n,\ell}(r)}{dr}+\left\{\frac{2\mu}{\hbar^2}\left[E-\left(\frac{a}{r}+\frac{b}{r^2}+c\right)\right]-\frac{\ell\,(\ell+1)}{r^2}\right\}R_{n,\ell}(r)=0 \tag{10}$$

and

$$L^2Y_\ell^m(\theta,\phi)-\hbar^2\ell\,(\ell+1)Y_\ell^m(\theta,\phi)=0, \tag{11}$$

where $R_{n,\ell}(r)$ and $Y_\ell^m(\theta,\phi)$ are the radial and angular solutions of (10) and (11) respectively. For $\Psi_{n,\ell,m}\,(r,\theta,\phi)$ to be finite everywhere, $R_{n,\,\ell}(r)$ must vanish at $r=0$, that is, $R_{n,\ell}(0)=0$, then $R_{n,\ell}(r)$ is a real function.

For the bound state energy eigenvalues for this quantum system, the following dimensionless abbreviations are introduced:

$$\rho=\gamma^{\frac{1}{2}}r=\left[\frac{-8\mu}{\hbar^2}(E-c)\right]^{\frac{1}{2}}r; \tag{12a}$$

$$\alpha=\left(\frac{-\mu}{2\hbar^2(E-c)}\right)^{\frac{1}{2}}a; \tag{12b}$$

$$\beta_\ell(\beta_\ell+1)=\frac{2\mu b}{\hbar^2}+\ell\,(\ell+1). \tag{12c}$$

The above equations (12a) and (12b) are chosen in order that the acceptable bounds state solutions are obtained, this can only be possible if $E<0$ (otherwise, continuum state solutions will be obtained). β_ℓ in (12c) represents the usual centrifugal term, that is, $\beta_\ell(\beta_\ell+1)=\frac{2\mu b}{\hbar^2}+\ \ell\,(\ell+1)$, where ℓ is the angular momentum quantum number. These substitutions allow us to obtain the following hypergeometric-type equation.

$$\frac{d^2}{d\rho^2}R_{n,\ell}(\rho)+\frac{2}{\rho}\frac{d}{d\rho}R_{n,\ell}(\rho)+\left[-\frac{1}{4}+\frac{\alpha}{\rho}-\frac{\beta_\ell(\beta_\ell+1)}{\rho^2}\right]R_{n,\ell}(\rho)=0. \tag{13}$$

This differential equation has an irregular singularity as $\rho\to\infty$, where its normalized solutions in bound states behave like $\exp(\rho)$. It further has a singularity at $\rho\to 0$, where $R_{n,\ell}(\rho)\sim\rho^{\beta_\ell}$. Then, the ansatz for the wave functions which is a physically acceptable solution for $R_{n,\ell}(\rho)$ can be expressed in the form

$$R_{n,\ell}(\rho)=N_{n,\ell}e^{-\rho/2}\rho^{\beta_\ell}G(\rho) \tag{14}$$

and therefore, (13) becomes

$$\rho\frac{d^2G(\rho)}{d\rho^2}+[(2\beta_\ell+2)-\rho]\frac{dG(\rho)}{d\rho}-[\beta_\ell+1-\alpha]G(\rho)=0. \tag{15}$$

This is the associated Laguerre differential equation (Kummer equation) [25, 35], the solution of (15) which is regular at origin (regular at $r = 0$ or $\rho = 0$) is the degenerate hypergeometric function

$$G(\rho) = {}_1F_1(\beta_\ell + 1 - \alpha,\ 2\beta_\ell + 2; \rho). \tag{16}$$

For large values of ρ, this solution diverges as $\exp(\rho)$, thus preventing normalization, except for when

$$\beta_\ell + 1 - \alpha = -n_r = -n; \quad n_r = 1, 2, \ldots \tag{17}$$

becomes a polynomial.

Therefore, the solution for the radial equation for this generalized Kratzer-type molecular potential is

$$R_{n,\ell}(\rho) = N_{n,\ell} e^{-\rho/2} \rho^{\beta_\ell}\ {}_1F_1(-n, 2\beta_\ell + 2; \rho), \tag{18}$$

where the normalization $N_{n_r,\ell}$ is determined from the requirement that

$$\int_0^\infty |R_{n,\ell}(\rho)|^2 r^2 dr = 1. \tag{19}$$

By using the expression that relates the associated Laguerre functions with the confluent hypergeometric functions

$${}_1F_1(-\gamma,\ m + 1; z) = \frac{\gamma\ !m\ !}{(\gamma + m)\ !} L_\gamma^m(z) \tag{20}$$

together with the following important formular [25, 35]

$$\int_0^\infty e^{-x} x^a L_n^{a-1}(x) L_m^{a-1}(x) dx = \frac{(a + 2n)\Gamma(a + n)}{n\ !} \delta_{nm}, \tag{21}$$

and by substituting $\gamma = \xi^2$, the normalized radial wave function is obtained as

$$R_{n,\ell}(r) = N_{n,\ell} e^{-\frac{\xi r}{2}} r^{\beta_\ell} L_n^{2\beta_\ell + 1}(\xi r), \tag{22}$$

where

$$N_{n,\ell} = \left[\frac{\xi^{2\beta_\ell + 3}}{2} \frac{n!}{(n + \beta_\ell + 1)\Gamma(n + 2\beta_\ell + 2)}\right]^{\frac{1}{2}}. \tag{23}$$

The corresponding eigenvalues are:

$$E_{n,\ell} = \frac{-\mu a^2}{2\hbar^2 [n + \beta_\ell + 1]^2} + c, \tag{24}$$

where β_ℓ is obtained as the positive root of (12c) given as

$$\beta_\ell = \frac{1}{2}\left[-1 + \sqrt{(2\ell + 1)^2 + \frac{8\mu b}{\hbar^2}}\right]. \tag{25}$$

3 Construction of the Creation and Annihilation Operators

The ladder operators can be generated directly from the eigenfunction with the factorization method as shown in Dong [4] and references therein. We shall find the differential operators $\hat{L}_\pm$ with the following property:

$$\hat{L}_\pm R_{n,\ell}(r) = \ell_\pm R_{n\pm 1,\ell}(r), \tag{26}$$

the operators of the form

$$\hat{L}_\pm = A_\pm(r)\frac{d}{dr} + B_\pm(r) \tag{27}$$

which depend only on the physical variable r are to be obtained.

The action of the differential operator $\frac{d}{dr}$ on wave functions (22) gives:

$$\frac{d}{dr}R_{n,\ell}(r) = -\frac{\xi}{2}R_{n,\ell}(r) + \frac{\beta_\ell}{r}R_{n,\ell}(r) + N_{n,\ell}r^{\beta_\ell}\, e^{-\frac{\xi r}{2}}\frac{d}{dr}L_n^{2\beta_\ell+1}(\xi r). \tag{28}$$

The expression above is used to construct the ladder operators $\hat{L}_\pm$ by using the recurrence relations of the associated Laguerre functions in order to find the relation between $R_{n,\ell}(r)$ and $R_{n+1,\ell}(r)$. To find these, the following recurrence relations of the associated Laguerre functions are used [25, 35]:

$$x\frac{d}{dx}L_n^\alpha(x) = \begin{cases} nL_n^\alpha(x) - (n+\alpha)L_{n-1}^\alpha(x) \\ (n+1)L_{n+1}^\alpha(x) - (n+\alpha+1-x)L_n^\alpha(x) \end{cases} \tag{29}$$

and the creation and annihilation operators are obtained as:

$$\hat{\mathcal{L}}_- = -r\frac{d}{dr} - \frac{\xi r}{2} + \hat{n} + \beta_\ell, \qquad \hat{\mathcal{L}}_+ = r\frac{d}{dr} - \frac{\xi r}{2} + \hat{n} + \beta_\ell + 2, \tag{30}$$

where $\hat{n}$ is the number operator with the property

$$\hat{n}R_{n,\ell}(r) = nR_{n,\ell}(r). \tag{31}$$

The action of the creation and annihilation operators on the radial wavefunctions $R_{n,\ell}(r)$ gives the following properties

$$\hat{\mathcal{L}}_\pm R_{n,\ell}(r) = \ell_\pm R_{n\pm 1,\ell}(r), \tag{32}$$

where

$$\ell_- = \sqrt{\frac{n(n+\beta_\ell)(n+2\beta_\ell+1)}{(n+\beta_\ell+1)}}, \qquad \ell_+ = \sqrt{\frac{(n+1)(n+\beta_\ell+2)(n+2\beta_\ell+2)}{(n+\beta_\ell+1)}}\,. \tag{33}$$

On studying the dynamical group associated to the annihilation and creation operators $\hat{\mathcal{L}}_-$ and $\hat{\mathcal{L}}_+$ and based on the results of (32) and (33), we can evaluate the commutator $[\hat{\mathcal{L}}_-,\ \hat{\mathcal{L}}_+]$ as:

$$[\hat{\mathcal{L}}_-,\ \hat{\mathcal{L}}_+]R_{n,\ell}(r) = 2\ell_0 R_{n,\ell}(r), \tag{34}$$

where

$$\ell_0 = (n + \beta_\ell + 1) \tag{35}$$

and $\hat{\mathcal{L}}_0$ is defined as

$$\hat{\mathcal{L}}_0 = (\hat{n} + \beta_\ell + 1). \tag{36}$$

Thus, operators $\hat{\mathcal{L}}_\mp$ and $\hat{\mathcal{L}}_0$ satisfy the following commutation relations:

$$[\hat{\mathcal{L}}_0, \hat{\mathcal{L}}_\mp] R_{n,\ell}(r) = \mp \hat{\mathcal{L}}_\mp R_{n\mp 1,\ell}(r). \tag{37}$$

The action of $\hat{\mathcal{L}}_+$ on the radial wavefunction $R_{n,\ell}\ (r)$ gives

$$\begin{aligned}(\hat{\mathcal{L}}_0\hat{\mathcal{L}}_+ - \hat{\mathcal{L}}_+\hat{\mathcal{L}}_0) R_{n,\ell}(r) &= \hat{\mathcal{L}}_+ R_{n,\ell}(r) = \hat{\mathcal{L}}_0(\hat{\mathcal{L}}_+ R_{n,\ell}(r)) - \ell_0(\hat{\mathcal{L}}_+ R_{n,\ell}(r)) \\ &= (\ell_0 + 1)\hat{\mathcal{L}}_+ R_{n,\ell}(r).\end{aligned} \tag{38}$$

If $\hat{\mathcal{L}}_+ R_{n,\ \ell}(r)$ is non-zero, then, it is an eigenfunction of $\hat{\mathcal{L}}_0$ with eigenvalue $(\ell_0 + 1)$. Thus, the effect of $\hat{\mathcal{L}}_+$ is to raise the eigenvalue by one unit. Similarly, the action of $\hat{\mathcal{L}}_-$ on the radial wavefunction $R_{n,\ell}(r)$ gives

$$\begin{aligned}(\hat{\mathcal{L}}_0\hat{\mathcal{L}}_- - \hat{\mathcal{L}}_-\hat{\mathcal{L}}_0) R_{n,\ell}(r) &= -\hat{\mathcal{L}}_-\ R_{n,\ell}(r) = \hat{\mathcal{L}}_0(\hat{\mathcal{L}}_- R_{n,\ell}(r)) - \ell_0(\hat{\mathcal{L}}_-\ R_{n,\ell}(r)) \\ &= (\ell_0 - 1)\hat{\mathcal{L}}_- R_{n,\ell}(r),\end{aligned} \tag{39}$$

and if $\hat{\mathcal{L}}_+ R_{n,\ \ell}(r)$ is non-zero, then, it is an eigenfunction of $\hat{\mathcal{L}}_0$ with eigenvalue $(\ell_0 - 1)$ (this is the reason for calling $\hat{\mathcal{L}}_+$ and $\hat{\mathcal{L}}_-$ raising and lowering operators respectively).

For the Hermitian operators, we define the operators as follows:

$$\hat{\mathcal{L}}_x = \frac{1}{2}(\hat{\mathcal{L}}_+ + \hat{\mathcal{L}}_-), \qquad \hat{\mathcal{L}}_y = \frac{1}{2i}(\hat{\mathcal{L}}_+ - \hat{\mathcal{L}}_-), \qquad \hat{\mathcal{L}}_z = \hat{\mathcal{L}}_0, \tag{40}$$

we obtained the following commutation relations

$$[\hat{\mathcal{L}}_x, \hat{\mathcal{L}}_y] = -i\hat{\mathcal{L}}_z, \qquad [\hat{\mathcal{L}}_y, \hat{\mathcal{L}}_z] = i\hat{\mathcal{L}}_x, \qquad [\hat{\mathcal{L}}_z, \hat{\mathcal{L}}_x] = i\hat{\mathcal{L}}_y. \tag{41}$$

The Casimir operator [36] can be expressed as

$$\begin{aligned}\hat{\mathcal{C}} R_{n,\ell}(r) &= (\hat{\mathcal{L}}_0(\hat{\mathcal{L}}_0 - 1) - \hat{\mathcal{L}}_+\hat{\mathcal{L}}_-) R_{n,\ell}(r) \\ &= (\hat{\mathcal{L}}_0(\hat{\mathcal{L}}_0 + 1) - \hat{\mathcal{L}}_-\hat{\mathcal{L}}_+) R_{n,\ell}(r) = \beta_\ell(\beta_\ell + 1) R_{n,\ell}(r).\end{aligned}$$

The Casimir operator $\hat{\mathcal{C}}$ now satisfies

$$[\hat{\mathcal{C}}, \hat{\mathcal{L}}_\pm] = [\hat{\mathcal{C}}, \hat{\mathcal{L}}_x] = [\hat{\mathcal{C}}, \hat{\mathcal{L}}_y] = [\hat{\mathcal{C}}, \hat{\mathcal{L}}_z] = 0, \tag{43}$$

the operators $\hat{\mathcal{L}}_\pm$, $\hat{\mathcal{L}}_x$, $\hat{\mathcal{L}}_y$, $\hat{\mathcal{L}}_z$ and $\hat{\mathcal{L}}_0$ satisfy the commutation relations of the dynamical group $SU(1,1)$ algebra, which is isomorphic to an $SO(2,1)$ algebra (i.e. $SU(1,1) \sim SO(2,1)$). The commutation rules are valid for the infinitesimal operators of the non-compact group $SU(1,1)$ [20, 37].

These relations coincide with the formulas that define the action of the infinitesimal operators $\hat{\mathcal{L}}_\pm$ and $\hat{\mathcal{L}}_0$ of the dynamical group $SU(1,1)$ on a basis $|j,k\rangle$ of the irreducible representation $D^+(j)$ belonging to the discrete positive series in an abstract Hilbert space [4, 20, 21, 37]. The eigenvalues have the ground state and therefore, the representation of the dynamical group $SU(1,1)$ belongs to $D^+(j)$, using the Dirac notation $|j,k\rangle = R_{n,\ell}(r)$:

$$\begin{gathered}\hat{C}|j,k\rangle = j(j+1)|j,k\rangle \\ \hat{\mathcal{L}}_0|j,k\rangle = \ell_0|j,k\rangle = k|j,k\rangle \\ \hat{\mathcal{L}}_\pm|j,k\rangle = \left[\frac{k(k\pm 1)^2 - j(j+1)(k\pm 1)}{k}\right]^{\frac{1}{2}}|j,k\pm 1\rangle \\ k = -j+n,\ n = 1,2,\ \ldots,j<0.\end{gathered} \tag{44}$$

Furthermore, the following expressions can be easily obtained from the operators $\hat{\mathcal{L}}_\mp$ and $\hat{\mathcal{L}}_0$ as follows:

$$\begin{aligned} r &= \frac{1}{\xi}[2\hat{\mathcal{L}}_0 - (\hat{\mathcal{L}}_+ + \hat{\mathcal{L}}_-)] \\ r\frac{d}{dr} &= \frac{1}{2}(\hat{\mathcal{L}}_+ - \hat{\mathcal{L}}_-) - 1. \end{aligned} \tag{45}$$

With these, the matrix elements for r and $r\frac{d}{dr}$ are obtained as follows:

$$\langle R_{m,\ell}(r)|r|R_{n,\ell}(r)\rangle = \frac{1}{\xi}[(n+\beta_\ell+1)\delta_{m,n} - \ell_+\delta_{m,n+1} - \ell_-\delta_{m,n-1}] \tag{46}$$

and

$$\langle R_{m,\ell}(r)|r\frac{d}{dr}|R_{n,\ell}(r)\rangle = \frac{\ell_+}{2}\,\delta_{m,n+1} - \frac{\ell_-}{2}\,\delta_{m,n-1} - \delta_{m,n}. \tag{47}$$

From (46) and (47), We can deduce the following relations:

$$\begin{aligned} &\xi\langle R_{m,\ell}(r)|r|R_{n,\ell}(r)\rangle + \langle R_{m,\ell}(r)|r\frac{d}{dr}|R_{n,\ell}(r)\rangle \\ &\quad = (n+\beta_\ell)\delta_{m,n} - \frac{1}{2}\ell_+\delta_{m,n+1} - \frac{3\ell_-}{2}\delta_{m,n-1} \end{aligned} \tag{48}$$

and

$$\begin{aligned} &\xi\langle R_{m,\ell}(r)|r|R_{n,\ell}(r)\rangle - \langle R_{m,\ell}(r)|r\frac{d}{dr}|R_{n,\ell}(r)\rangle \\ &\quad = (n+\beta_\ell+1)\delta_{m,n} - \frac{3}{2}\ell_+\delta_{m,n+1} - \frac{\ell_-}{2}\delta_{m,n-1}, \end{aligned} \tag{49}$$

these relations form a useful link for finding the matrix elements from ladder operators.

4 Numerical Calculations of the Energy Levels and Matrix Elements

4.1 Energy Eigenvalues of the Kratzer and Modified Kratzer Potentials

The energy eigenvalues for the Kratzer and modified Kratzer potentials are obtained respectively, as:

$$E^{K}_{n,\ell} = -\frac{2\mu D_0^2 r_0^2}{\hbar^2[n+\beta_\ell+1]^2} \tag{50}$$

and

$$E^{MK}_{n,\ell} = -\frac{2\mu D_0^2 r_0^2}{2\hbar^2[n+\beta_\ell+1]^2} + D_0, \tag{51}$$

where

$$\beta_\ell = \frac{1}{2}\left[-1+\sqrt{(2\ell+1)^2+\frac{8\mu D_0 r_0^2}{\hbar^2}}\right]. \tag{52}$$

In this work, energy eigenvalues for *CO* and *NO* diatomic molecules for the various values of n and ℓ are obtained by means of the factorization method (FM) ((50) and (51)) with the parameters given in Table 1. The results obtained are compared with other results obtained by using: AIM method [24]; Nikiforov-Uvarov (NU) method [26] and Exact quantization rule (EQR) method [27].

Table 2 shows the exact bound state energy eigenvalues of the Kratzer potential for *CO* and *NO* diatomic molecules for various values of n and ℓ using (50) obtained by factorization method (FM) and other results obtained by using AIM [24] and EQR [27] methods. Similarly, Table 3 shows the exact bound state energy eigenvalues of the modified Kratzer potential for *CO* and *NO* diatomic molecules for various values of n and ℓ using (51) obtained by factorization method (FM) and other results obtained by using AIM [24] and NU [26] methods.

4.2 Matrix Elements of r and $r\frac{d}{dr}$ for the Two Potentials

The matrix elements for r and $r\frac{d}{dr}$ are given as:

$$\langle R_{n,\ell}(r)|r|R_{n,\ell}(r)\rangle = \frac{1}{\xi}\left[(n+\beta_\ell+1) - \sqrt{\frac{(n+2)(n+\beta_\ell+3)(n+2\beta_\ell+3)}{(n+\beta_\ell+2)}} - \sqrt{\frac{(n-1)(n+\beta_\ell-1)(n+2\beta_\ell)}{(n+\beta_\ell)}}\right] \tag{53}$$

Table 1 Reduced masses and spectroscopic properties of the *CO* and *NO* diatomic molecules in the ground electronic state. The data listed in this table are taken from [38, 39]

Parameters	*CO*	*NO*
D_o (in eV)	10.84514471	8.043782568
r_o (in Å)	1.1282	1.1508
μ (in amu)	6.860586000	7.468441000

Table 2 Comparison of the energy eigenvalues (in eV), corresponding to the Kratzer potential for various n and ℓ quantum numbers for *CO* and *NO* diatomic molecules, where $\hbar c = 1973.29$ eVÅ

n	ℓ	*CO* [FM]	*CO* [EQR]	*CO* [AIM]	*NO* [FM]	*NO* [EQR]	*NO* [AIM]
0	0	−10.79431534387622	−10.794315323	−10.79431532	−8.002658755212952	−8.002659419493	−8.002659417
1	0	−10.69383913769446	−10.693839925	−10.69383992	−7.921456003136883	−7.921456840689	−7.921456839
1	1	−10.69337109882925	−10.693371229	−10.69337123	−7.921042972272428	−7.921043829925	−7.921043834
2	0	−10.59476059512928	−10.594760890	−10.59476089	−7.841483226715529	−7.841483958093	−7.841483956
2	1	−10.59429734443464	−10.594298692	−10.59429869	−7.841075958492119	−7.841077185904	−7.841077188
2	2	−10.59337288634942	−10.593374417	−10.59337441	−7.840262393682968	−7.840263768523	−7.840263771
3	0	−10.49705105930509	−10.497052462	−10.49705246	−7.762714866929600	−7.762716067159	−7.762716066
3	1	−10.49659537021400	−10.496596643	−10.49659664	−7.762314093207729	−7.762315408528	−7.762315413
3	2	−10.49568316746262	−10.495685124	−10.49568512	−7.761512650377457	−7.761514215884	−7.761514218
3	3	−10.49431563207918	−10.494318144	−10.49431814	−7.760311623981464	−7.760312738370	−7.760312744
4	0	−10.40068823210378	−10.400689478	−10.40068947	−7.685127711083608	−7.685129080626	−7.685129079
4	1	−10.40023809235447	−10.400239921	−10.40023992	−7.684732464238659	−7.684734413653	−7.684734417
4	2	−10.39933885575065	−10.399340924	−10.39934092	−7.683942903888297	−7.683945202003	−7.683945203
4	3	−10.39798982948594	−10.397992722	−10.39799272	−7.682760084230797	−7.682761690175	−7.682761696
4	4	−10.39619321456787	−10.396195666	−10.39619567	−7.681181936089156	−7.681184244677	−7.681184246
5	0	−10.30564563709163	−10.305647347	−10.30564735	−7.608697429711712	−7.608699510108	−7.608699509
5	1	−10.30520186777971	−10.305203938	−10.30520394	−7.608308414224594	−7.608310715917	−7.608310719
5	2	−10.30431444380035	−10.304317236	−10.30431723	−7.607531297904489	−7.607533247563	−7.607533248
5	3	−10.30298450330134	−10.302987469	−10.30298747	−7.606365523492213	−7.606367345012	−7.606367349
5	4	−10.30121238898166	−10.301214985	−10.30121499	−7.604810653591787	−7.604813367976	−7.604813368
5	5	−10.29899764904374	−10.299000242	−10.29900024	−7.602869548627632	−7.602871795644	−7.602871795

Table 3 Comparison of the energy eigenvalues (in eV), corresponding to the modified Kratzer potential for various n and ℓ quantum numbers for *CO* and *NO* diatomic molecules, where $\hbar c = 1973.29$ eVÅ

n	ℓ	*CO* [FM]	*CO* [EQR]	*CO* [NU]	*NO* [FM]	*NO* [EQR]	*NO* [NU]
0	0	0.0508289279743650	0.050829386733	0.050823	0.0411234789789425 3	0.041123148507	0.041118
1	0	0.1513051341561269	0.151304784801	0.151287	0.1223262310550117	0.122325727312	0.122311
1	1	0.1517731730213381	0.151773481462	0.151755	0.1227392619194667	0.122738738076	0.122724
2	0	0.2503836767213095	0.250383819984	0.250354	0.2022990074763653	0.202298609907	0.202274
2	1	0.2508469274159442	0.250846018075	0.250816	0.2027062756997760	0.202705382097	0.202681
2	2	0.2517713855011650	0.251770292931	0.251744	0.2035198405089265	0.203518799478	0.203494
3	0	0.3480932125454999	0.348092247640	0.348051	0.2810673574989346	0.281066500842	0.281033
3	1	0.3485489016365868	0.348548066746	0.348507	0.2814681409841651	0.281467159473	0.281434
3	2	0.3494611043879683	0.349459585720	0.349418	0.2822695838144371	0.282268352117	0.282235
3	3	0.3508286397714091	0.350826566166	0.350785	0.2834706102104301	0.283469829631	0.283436
4	0	0.4444560397468020	0.444455232045	0.444403	0.3586545231082869	0.358653487375	0.358611
4	1	0.4449061794961153	0.444904789014	0.444852	0.3590497699532351	0.359048154348	0.359006
4	2	0.4458054160999403	0.445803785755	0.445751	0.3598393303035978	0.359837365998	0.359795
4	3	0.4471544423646421	0.447151987956	0.447099	0.3610221499610970	0.361020877826	0.360978
4	4	0.4489510572827147	0.448949044337	0.448895	0.3626002981027385	0.362598323324	0.362555
5	0	0.5394986347589601	0.539497362596	0.539434	0.4350848044801827	0.435083057893	0.435032
5	1	0.5399424040708798	0.539940771611	0.539877	0.4354738199673003	0.435471852084	0.435421
5	2	0.5408298280502333	0.540827474443	0.540764	0.4362509362874052	0.436249320438	0.436198
5	3	0.5421597685492472	0.542157240772	0.542093	0.4374167106996811	0.437415222989	0.437364
5	4	0.5439318828689306	0.543929725307	0.543865	0.4389715806001080	0.438969200025	0.438917
5	5	0.5461466228068463	0.546144468004	0.546082	0.4409126855642622	0.440910772357	0.440858

and

$$
\begin{aligned}
&\langle R_{n,\ell}(r)|r\frac{d}{dr}|R_{n,\ell}(r)\rangle \\
&\quad = \frac{1}{2}\sqrt{\frac{(n+2)(n+\beta_\ell+3)(n+2\beta_\ell+3)}{(n+\beta_\ell+2)}} - \frac{1}{2}\sqrt{\frac{(n-1)(n+\beta_\ell-1)(n+2\beta_\ell)}{(n+\beta_\ell)}} - 1,
\end{aligned}
\tag{54}
$$

where

$$
\xi = -\frac{4\mu D_0 r_0}{\hbar^2(n+\beta_\ell+1)}. \tag{55}
$$

With (53) and (54), we can deduce the following relations:

$$
\begin{aligned}
\Gamma_1 &= \xi\langle R_{n,\ell}(r)|r|R_{n,\ell}(r)\rangle + \langle R_{n,\ell}(r)|r\frac{d}{dr}|R_{n,\ell}(r)\rangle \\
&= (n+\beta_\ell) - \frac{1}{2}\sqrt{\frac{(n+2)(n+\beta_\ell+3)(n+2\beta_\ell+3)}{(n+\beta_\ell+2)}} \\
&\quad - \frac{3}{2}\sqrt{\frac{(n-1)(n+\beta_\ell-1)(n+2\beta_\ell)}{(n+\beta_\ell)}}
\end{aligned}
\tag{56}
$$

and

$$
\begin{aligned}
\Gamma_2 &= \xi\langle R_{n,\ell}(r)|r|R_{n,\ell}(r)\rangle - \langle R_{n,\ell}(r)|r\frac{d}{dr}|R_{n,\ell}(r)\rangle \\
&= (n+\beta_\ell+1) - \frac{1}{2}\sqrt{\frac{(n+2)(n+\beta_\ell+3)(n+2\beta_\ell+3)}{(n+\beta_\ell+2)}} \\
&\quad - \frac{3}{2}\sqrt{\frac{(n-1)(n+\beta_\ell-1)(n+2\beta_\ell)}{(n+\beta_\ell)}}.
\end{aligned}
\tag{57}
$$

In this case, the matrix elements for the two potentials (Kratzer and modified Kratzer potentials) give the same results, since these matrix elements depend on $b = D_0 r_0$ and $a = -2D_0 r_0$ only, and not on $c = D_0$. Hence, when the Kratzer potential is shifted by the amount D_0, (that is, the modified Krazter potential), it has no effect on the matrix elements. For the numerical results, see Tables 4 and 5.

5 Conclusions

In this paper, I have studied the eigenvalues, the eigenfunctions and the matrix elements of the Kratzer-type molecular potentials (generalized Kratzer molecular potentials). The ladder (creation and annihilation) operators for the radial wavefunctions are established. Also, the Hermitian operators of these ladder operators are obtained. These operators satisfy the commutation relations of an $SU(1,1)$ dynamical group, the action of $\hat{\mathcal{L}}_\pm$ on the wavefunctions that reveals the fact about the raising and lowering effect are established. The matrix elements of the different functions r and $r\frac{d}{dr}$ are also obtained from the ladder operators in a closed form.

Table 4 The values of the $\langle R_{n,\ell}|r|R_{n,\ell}\rangle$ (53), $\langle R_{n,\ell}|r\frac{d}{dr}|R_{n,\ell}\rangle$ (54), Γ_1 (56) and Γ_2 (57), corresponding to the Kratzer and modified Kratzer potentials for various n and ℓ quantum numbers for *CO* diatomic molecule, where $\hbar c = 1973.29$ eVÅ

n	ℓ	$\langle R_{n,\ell}\|r\|R_{n,\ell}\rangle$	$\langle R_{n,\ell}\|r\frac{d}{dr}\|R_{n,\ell}\rangle$	Γ_1	Γ_2
1	0	−0.4761490924054464	16.97323506451677	195.3895273866551	161.4430572576216
1	1	−0.4761710273791221	16.97343118040934	195.3940309777938	161.4471686169751
2	0	−0.4107558210705384	9.473123928272610	162.6714457007481	143.7251978442029
2	1	−0.4107755614421622	9.473236107448747	162.6755771602085	143.7291049453111
2	2	−0.4108150436563324	9.473460462197114	162.6838400978704	143.7369191734761
3	0	−0.3789129917968390	7.666855095230551	148.3356842660929	133.0019740756318
3	1	−0.3789316534237137	7.666946649417545	148.3396482090482	133.0057549102131
3	2	−0.3789689781099853	7.667129754891770	148.3475761191884	133.0133166094049
3	3	−0.3790249687207100	7.667404405854176	148.3594680449690	133.0246592332607
4	0	−0.3533372017343955	6.615793772861618	137.1863080576614	123.9547205119381
4	1	−0.3533549972979473	6.615873160774083	137.1901403213880	123.9583939998398
4	2	−0.3533905898264022	6.616031934119029	137.1978048773512	123.9657410091131
4	3	−0.3534439821224761	6.616270087936851	137.2093017825661	123.9767616066924
4	4	−0.3535151205980674	6.616587357061658	137.2246186798360	123.9914439657127
5	0	−0.3312181486228352	5.899103372782779	127.7353299114129	115.9371231658474
5	1	−0.3312351970446675	5.899174359294310	127.7390497423004	115.9407010237118
5	2	−0.3312692952626132	5.899316330129842	127.7464894362121	115.9478567759524
5	3	−0.3313204460252490	5.899529280914656	127.7576490574162	115.9585904955868
5	4	−0.3313885980893305	5.899812974634305	127.7725166245981	115.9728906753295
5	5	−0.3314738123034079	5.900167633018892	127.7911043436078	115.9907690775700

The solutions of the generalized Kratzer molecular potentials are obtained via an $SU(1,1)$ algebraic approach and the results can be generalized to other form of potentials in (5). The generalized Kratzer potential model proposed in this work [31, 32], allows one to obtain the eigenvalues, the matrix elements and the radial eigenfunctions for the two important molecular potentials simultaneously (that is, the Kratzer and modified Kratzer potentials).

This generalization covers the descriptions about the two potentials, the shapes of the two potentials for *CO* and *NO* diatomic molecules are also shown in figure 1. More importantly, the generalized Kratzer potential model used in this work generates results for the two molecular potentials. In addition, the numerical results are obtained for the eigenvalues for *CO* and *NO* diatomic molecules for the two molecular potentials. The results obtained are compared with other existing results (EQR, AIM and NU), and the results agree favourably with other results, see Tables 2 and 3.

Tables 4 and 5 show the matrix elements of r, $r\frac{d}{dr}$, their sum (Γ_1) and their difference (Γ_2) obtained for *CO* and *NO* diatomic molecules, the results obtained are the same results for the two molecular potentials. This is because, the matrix elements depend on $b = D_0 r_0$ and $a = -2D_0 r_0$ only, and not on $c = D_0$. Hence, the shifted amount D_0, (in the case of the modified Krazter potential) has no effect on the matrix elements.

The advantage of the present approach is that it enables one to find the energy eigenvalues, eigenfunctions and matrix elements in a simple way. The approach presented in this study is efficient and is a very useful link for finding the matrix elements from ladder oper-

Table 5 The values of the $\langle R_{n,\ell}|r|R_{n,\ell}\rangle$ (53), $\langle R_{n,\ell}|r\frac{d}{dr}|R_{n,\ell}\rangle$ (54), Γ_1 (56) and Γ_2 (57), corresponding to the Kratzer and modified Kratzer potentials for various n and ℓ quantum numbers for *NO* diatomic molecule, where $\hbar c = 1973.29$ eVÅ

n	ℓ	$\langle R_{n,\ell}\|r\|R_{n,\ell}\rangle$	$\langle R_{n,\ell}\|r\frac{d}{dr}\|R_{n,\ell}\rangle$	Γ_1	Γ_2
1	0	−0.4819553974463722	16.21611432627930	178.3853413621973	145.9531127096387
1	1	−0.4819818755489971	16.21633768030118	178.3902449613004	145.9575696006980
2	0	−0.4124035377598499	9.040224937878095	147.1042625831576	129.0238127074014
2	1	−0.4124272376527343	9.040352590403065	147.1087421492765	129.0280369684704
2	2	−0.4124746395526131	9.040607890585319	147.1177013069172	129.0364855257466
3	0	−0.3785773170199991	7.313655510582683	133.4152241892145	118.7879131680491
3	1	−0.3785996534470747	7.313759628367830	133.4195129653269	118.7919937085912
3	2	−0.3786443283574571	7.313967860029029	133.4280905503876	118.8001548303296
3	3	−0.3787112793749515	7.314279887895779	133.4409442456685	118.8123844698770
4	0	−0.3514058390444385	6.309618628486895	122.7741267465619	110.1548894895881
4	1	−0.3514270813879861	6.309708856787779	122.7782656025786	110.1588478890030
4	2	−0.3514695680843574	6.309889310052519	122.7865433532380	110.1667647331330
4	3	−0.3515332399199089	6.310159713089281	122.7989477575504	110.1786283313719
4	4	−0.3516182293790348	6.310520592939504	122.8155035676796	110.1944623818006
5	0	−0.3278978812775772	5.625407532078025	113.7570644421939	102.5062493780379
5	1	−0.3279181800627655	5.625488165029850	113.7610753342060	102.5100990041463
5	2	−0.3279587796016631	5.625649427995388	113.7690971617573	102.5177983057665
5	3	−0.3280196234075503	5.625891075135918	113.7811180744773	102.5293359242055
5	4	−0.3281008382258643	5.626213577576859	113.7971620775729	102.5447349224192
5	5	−0.3282023110716663	5.626616443662535	113.8172054699764	102.5639725826513

ators. This approach can be used to find the energy eigenvalues, eigenfunctions and radial matrix elements of the Schrödinger equation with a given exactly solvable molecular potentials for various diatomic molecules for any values of n and ℓ quantum numbers.

The ladder operators constructed in this study, are very useful tools in quantum-mechanical calculations of the various matrix elements based on the Kratzer molecular basis function. Furthermore, these operators can be used in constructing coherent states.

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