REVIEW

Exact solutions of the Schrödinger equation for the pseudoharmonic potential: an application to some diatomic molecules

K. J. Oyewumi · K. D. Sen

Abstract For arbitrary values n and ℓ quantum numbers, we present the solutions of the 3-dimensional Schrödinger wave equation with the pseudoharmonic potential via the $SU(1, 1)$ Spectrum Generating Algebra (SGA) approach. The explicit bound state energies and eigenfunctions are obtained. The matrix elements r^2 and $r\frac{d}{dr}$ are obtained (in a closed form) directly from the creation and annihilation operators. In addition, by applying the Hellmann–Feynman theorem, the expectation values of r^2 and p^2 are obtained. The energy states, the expectation values of r^2 and p^2 and the Heisenberg uncertainty products (HUP) for set of diatomic molecules (CO, NO, O_2, N_2, CH, H_2, ScH) for arbitrary values of n and ℓ quantum numbers are obtained. The results obtained are in excellent agreement with the available results in the literature. It is also shown that the HUP is obeyed for all diatomic molecules considered.

Keywords Bound state solutions · Expectation values · Spectrum generating algebra · Pseudoharmonic potential · Diatomic molecules · Heisenberg uncertainty principle

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1 Introduction

The spectrum generating algebra (SGA) methods have been playing an important role in solving some quantum mechanical problems, since its introduction by Schrödinger, Infeld, Infeld and Hull [1–5]. This technique serves as a useful tool in various fields of physics, ranging from quantum mechanics (relativistic and non relativistic), mathematical physics, optics, solid state physics, nuclear physics to chemical physics. This can be achieved through the construction of the ladder operators (creation and annihilation operators) or raising and lowering operators. From these ladder operators, the compact dynamical algebraic groups (a suitable Lie algebra) that such system belongs can be easily realized [6–37].

It should be noted that, Schrödinger factorization method has been less frequently applied to physical systems than Infeld-Hull factorization method, as it has been analyzed in detail by Martínez et al. [33], and exemplified later with a typical system [32]. Martínez and Mota presented a systematic procedure of using the factorization method to construct the generators for hidden and dynamical symmetries, and applied this study to 2D problems of hydrogen atom, the isotropic harmonic and other radial potential of interest.

This algebraic approach has been successfully applied to a set of model potentials such as the Morse potential, Pöschl-Teller potential, pseudoharmonic potential, infinite square well in 3D as well as N-dimensions [9,12–37] and their energy spectrum and the eigenfunctions have been studied.

The $SU(1, 1)$ dynamical algebra from the Schrödinger ladder operators for hydrogen atom, Mie-type potential, harmonic oscillator and pseudoharmonic oscillator for N-dimensional systems have been extensively discussed by Martínez et al. [33]. In a similar fashion, Salazar-Ramírez et al. [34,35] have applied the factorization method to construct the generators of the dynamical algebra $SU(1, 1)$ for the radial equation of the non-relativistic and relativistic generalized MICZ-Kepler problem. It should be noted that the generators in the examples [32–35] above have been constructed without adding phase as an additional variable like in Martínez-y-Romero et al. [15].

Gur and Mann [30] have used the $SU(1, 1)$ SGA method to construct the associated radial Barut-Girardello coherent states for the isotropic harmonic oscillator in arbitrary dimension and these states have been mapped into the Sturm-Coulomb radial coherent states. The dynamics of the $SU(1, 1)$ coherent states for the time-dependent quadratic Hamiltonian system has been discussed by Choi [36].

In their work, Motavalli and Akbarieh [37] presented a general construction for the ladder operators for special orthogonal functions based on the Nikiforov-Uvarov formalism and generated a list of creation and annihilation operators for some well known special functions.

In the present study, we have followed the approach introduced by Dong [9]. This is done by using the recursion relations for the generalized Laguerre polynomials and the explicit form of the eigenfunctions, the $SU(1, 1)$ dynamical algebra generators for some quantum mechanical systems can therefore be obtained.

Apart from generating the eigenvalues and eigenfunctions, this approach offers the additional advantages in that it can be used to find the matrix elements in a simple way, and it is also very useful in constructing coherent states of a given Hamiltonian

system [30,36,38]. Thus, Gur and Mann [30] used SGA approach to construct the radial Barut-Girardello coherent states for the isotropic harmonic oscillator in arbitrary dimension and mapped these states into Sturm-Coulomb radial coherent state; the dynamics of SU(1, 1) coherent states are investigated for the time-dependent quadratic Hamiltonian system by Choi [36]. Very recently, the second lowest and second highest bases of the discrete positive and negative irreducible representations of $SU(1, 1)$ Lie algebra via spherical harmonics are used to construct generalized coherent states by Dehghani and Fakhri [38].

In recent years, discussion on the 3-dimensional anharmonic oscillators has been receiving considerable attention in chemical physics. This is due to their usefulness in studying the dynamical variables of diatomic molecules. The Morse potential has been one of the most popular model potential which is employed in the study of molecular spectra [39–45].

The corresponding wave function does not vanish at the origin, and the exact solutions for any angular momentum ($\ell \neq 0$) are as yet unknown. Several other potentials are been used as alternatives and their performances have been compared with the Morse potential [43,46–56]. For examples, Kratzer and pseudoharmonic potentials which have known exact solutions like in the Coulomb and harmonic oscillator model potentials [31,45,57–61].

For the purpose of this study, we consider pseudoharmonic potential. This potential has been very useful in the area of physical sciences and it has been extensively used to describe interaction of some diatomic molecules since its introduction [9,28,29, 57,62–72]. Sage [68] has studied the energy levels and wave functions of a rotating diatomic molecule using a three-parameter model potential called the pseudogaussian (pseudoharmonic) potential and he found that the potential is reasonably behaved for both small and large internuclear separations.

Obviously, the pseudoharmonic oscillator behaves asymptotically as a harmonic oscillator, but has a minimum at $r = r_e$ and exhibits a repulsive inverse-square-type singularity at $r = 0$. The energy eigenvalues and the eigenfunctions of the pseudo-harmonic oscillator can be found exactly for any angular momentum. These wave functions have reasonable behaviour at the origin, near the equilibrium, and at the infinity [73].

Its characteristics make it useful to model various physical systems, including some molecular physical ones [9,31,59,68,69,72]. From the mathematical point of view, it resembles the harmonic oscillator, from which it deviates by two correction terms depending on the potential depth and the equilibrium distance parameter r_e: the first one is an energy shift and the second one is a modified centrifugal term. The latter can also be viewed as originating formally from a non-integer orbital angular momentum [69]. The eigenfunctions and energy eigenvalues are similar to those of the harmonic oscillator, which can be obtained exactly in the $r_e \to 0$ limit.

Recently, with an improved approximation to the orbital centrifugal term of the Manning-Rosen potential, Ikhdair [74] used the Nikiforov-Uvarov method to obtain the rotational-vibrational energy states for a few diatomic molecules for arbitrary quantum numbers n and ℓ with different values of the potential parameters.

In the study of the diatomic molecules using the diatomic molecular potentials, different methods have been employed: Nikiforov-Uvarov method [42–45,57–59];

asymptotic iteration method [60]; Exact method [72]; shifted $1/N$ expansion [40]; exact quantization rule method [46,61]; SUSY approach [41]; Nikiforov-Uvarov method [45,57,59]; tridiagonal J-matrix representation [75,76] and algebraic method [31,77].

The aim of this work is to realize the dynamical $SU(1,1)$ algebra generators for the pseudoharmonic potential to obtain the energy eigenvalues, eigenfunctions and the matrix elements of the pseudoharmonic potential. The results obtained are used to calculate the bound state energies, the expectation values and the HUP of some diatomic molecules (homogeneous and heterogeneous) for any n and ℓ quantum numbers.

The scheme of our presentation is as follows: in Sect. 2, we study the 3-dimensional Schrödinger equation for the pseudoharmonic potential. In Sect. 3, we present the formal solutions of the problem and describe the SGA method used in constructing the ladder operators for obtaining the energy eigenvalues, the eigenfunctions and the matrix elements for the pseudoharmonic potential. We present in Sect. 4, the explicit bound state energies, the numerical values of the expectation values of r^2 and p^2 and the Heisenberg uncertainty product for the pseudoharmonic potential for the homogeneous diatomic molecules (N_2 and H_2); the heterogeneous diatomic molecules (CO, NO and CH) and the neutral transition metal hydride (ScH). Finally, in Sect. 5, we discuss our conclusions.

2 The 3-dimensional Schrödinger equation for the pseudoharmonic potential

The pseudoharmonic-type potential can be written in the standard form as [9,28,29, 71,72,78,79]

$$V(r) = Ar^2 + \frac{B}{r^2} + c. \tag{1}$$

This potential is associated with the following molecular potentials:

- Isotropic harmonic oscillator plus inverse quadratic potential

$$V(r) = \mu\omega^2 \frac{r^2}{2} + \frac{g}{r^2}, \tag{2}$$

here $A = \mu\omega^2$, $B = g$ and $c = 0$ [9,28,29,70,71,78,79].

- The pseudoharmonic potential

$$V(r) = D_e \left(\frac{r}{r_e} - \frac{r_e}{r} \right)^2, \tag{3}$$

where D_e is the dissociation energy between two atoms in a solid and r_e is the equilibrium intermolecular separation. Here, we have $A = \frac{D_e}{r_e^2}$, $B = D_e r_e$ and $c = -2D_e$ [9,28,29,57,62–70,73,78–82].

The Schrödinger equation for the three-dimension for this potential is

$$\left[-\frac{\hbar^2}{2\mu}\Delta + \frac{D_e}{r_e^2}r^2 + \frac{D_e r_e^2}{r^2} - 2D_e \right]\psi(r,\theta,\phi) = E\psi(r,\theta,\phi). \tag{4}$$

If we propose $\psi_{n,\ell,m}(r,\theta,\phi)$ to have the form

$$\psi_{n,\ell,m}(r,\theta,\phi) = R_{n,\ell,m}(r)Y_{\ell,m}(\theta,\phi) \tag{5}$$

then, Eq. (4) reduces to two decoupled differential equations, that is, the radial and angular wave functions:

$$\left\{ \frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} + \left[\frac{2\mu}{\hbar^2}\left[E - \left(\frac{D_e}{r_e^2}r^2 + \frac{D_e r_e^2}{r^2} - 2D_e \right) \right] - \frac{\ell(\ell+1)}{r^2} \right] \right\} R_{n,\ell}(r) = 0 \tag{6}$$

and

$$L^2 Y_{\ell,m}(\theta,\phi) = \hbar^2 \ell(\ell+1)Y_{\ell,m}(\theta,\phi), \tag{7}$$

where $\ell = 0, 1, 2, \ldots$ is the orbital angular momentum quantum numbers, $n = 1, 2, 3, \ldots$ is the principal quantum number, μ is the reduced mass, $\hbar$ is the Planck's constant divided by 2π and E is the energy eigenvalue. With $K^2 = \frac{2\mu E}{\hbar^2}$, Eq. (6) can be re-written as

$$\left\{ \frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} + \left[K^2 + \frac{4\mu D_e}{\hbar^2} - \frac{2\mu D_e}{\hbar^2 r_e^2}r^2 - \frac{\gamma_\ell(\gamma_\ell+1)}{r^2} \right] \right\} R_{n,\ell}(r) = 0, \tag{8}$$

where

$$\gamma_\ell = \frac{1}{2}\left[-1 + \sqrt{(2\ell+1)^2 + \frac{8\mu D_e r_e^2}{\hbar^2}} \right]. \tag{9}$$

To obtain the relevant algebraic operators for the radial symmetry, Eq. (8) is solved and the solutions which is a degenerate hypergeometric or Kummer equation (associated Laguerre differential equation) is obtained [83–85]. Then, the radial functions $R_{n,\ell}(r)$ for this potential is obtained as:

$$R_{n,\ell}(r) = N_{n,\ell}\, r^{\gamma_\ell} e^{-\lambda r^2} L_n^{\gamma_\ell + \frac{1}{2}}(2\lambda r^2), \tag{10}$$

where

$$\lambda = \sqrt{\frac{\mu D_e}{2\hbar^2 r_e^2}}. \tag{11}$$

$L_n^k(x)$ is the associated Laguerre functions [83–85], $N_{n,\ell}$ is the normalization constant which is determined from the normalization condition

$$\int\limits_0^\infty R_{n,\ell}(r) R_{n',\ell}(r) dr = \delta_{n,n'} \tag{12}$$

as

$$N_{n,\ell} = \left[\frac{2(2\lambda^2)^{\frac{1}{4}(2\gamma_\ell+3)} n!}{\Gamma(n + \gamma_\ell + \frac{3}{2})} \right]^{\frac{1}{2}}. \tag{13}$$

3 The spectrum generating algebra (SGA)

In a brief introduction, the classical Lie algebra SU(1,1) can be generated by the elements K_0, K_1, K_2 which satisfies the following commutation relations:

$$[K_0, K_1] = i K_2, \quad [K_1, K_2] = -i K_0, \quad [K_2, K_0] = i K_1. \tag{14}$$

Alternatively, these can be expressed in terms of the creation and annihilation operators

$$K_\pm = K_1 \pm i K_2, \tag{15}$$

the commutation relations together with K_0 can be written as:

$$[K_0, K_\pm] = \pm K_\pm, \quad [K_-, K_+] = 2K_0. \tag{16}$$

Based on the Schrödinger factorization method, Infeld-Hull factorization method, we adopt the factorization method introduced by Dong [9]. This is done by construction of the creation and annihilation operators through the recursion relations of the Laguerre functions that evolved, and thereby construct a suitable Lie algebra in terms of these ladder operators.

In this case, we obtain the differential operators $\hat{\mathcal{J}}_\pm$ with the following property:

$$\hat{\mathcal{J}}_\pm R_{n_r,\ell}(r) = j_\pm R_{n_r\pm 1,\ell}(r), \tag{17}$$

these operators are of the form

$$\hat{\mathcal{J}}_\pm = A_\pm(r) \frac{d}{dr} + B_\pm(r) \tag{18}$$

and depend only on the physical variable r.

On operating the differential operator $\frac{d}{dr}$ on the radial wave functions (10), we have,

$$\frac{d}{dr} R_{n,\ell}(r) = \frac{\gamma_\ell}{r} R_{n,\ell}(r) - 2\lambda r R_{n,\ell}(r) + N_{n,\ell} \, r^{\gamma_\ell} \, \exp(-\lambda \, r^2) \frac{d}{dr} L_n^{\gamma_\ell+\frac{1}{2}}(2\lambda \, r^2).$$

(19)

In order to find the relationship between $R_{n,\ell}(r)$ and $R_{n+1,\ell}(r)$, the expression above is used to construct the ladder operators $\hat{\mathcal{J}}_\pm$ by using the recurrence relations of the associated Laguerre functions. To find these, the following recurrence relations of the associated Laguerre functions are used [83–85]:

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

(20)

The creation and annihilation operators are obtained as:

$$\hat{\mathcal{J}}_- = \frac{1}{2}\left[-r\frac{d}{dr} - 2\lambda r^2 + 2\hat{n} + \gamma_\ell\right]; \quad \hat{\mathcal{J}}_+ = \frac{1}{2}\left[r\frac{d}{dr} - 2\lambda r^2 + 2\hat{n} + \gamma_\ell + 3\right],$$

(21)

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

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

(22)

On defining the operator

$$\hat{\mathcal{J}}_0 = \frac{1}{4}\left[-\frac{d^2}{dr^2} - \frac{2}{r}\frac{d}{dr} + \frac{\gamma_\ell(\gamma_\ell+1)}{r^2} + \frac{2\mu D_e r^2}{\hbar^2 r_e^2}\right],$$

(23)

then, the operation of $\hat{\mathcal{J}}_\pm$ and $\hat{\mathcal{J}}_0$ on the radial wave functions $R_{n_r,\ell}(r)$ allows us to find the following properties:

$$\hat{\mathcal{J}}_+ \, R_{n,\ell}(r) = \sqrt{(n+1)\left(n+\gamma_\ell+\frac{3}{2}\right)} \, R_{n+1,\ell}(r) = j_+ \, R_{n+1,\ell}(r),$$

(24)

$$\hat{\mathcal{J}}_- \, R_{n,\ell}(r) = \sqrt{n\left(n+\gamma_\ell+\frac{1}{2}\right)} \, R_{n-1,\ell}(r) = j_- \, R_{n-1,\ell}(r),$$

(25)

$$\hat{\mathcal{J}}_0 \, R_{n,\ell}(r) = n + \frac{2\gamma_\ell+3}{4} \, R_{n,\ell}(r) = j_0 \, R_{n,\ell}(r).$$

(26)

On carefully inspecting the dynamical group associated to the annihilation and creation operators $\hat{\mathcal{J}}_-$ and $\hat{\mathcal{J}}_+$, based on the results of Eqs. (24) and (25), the commutator

$[\hat{\mathcal{J}}_-, \ \hat{\mathcal{J}}_+]$ can be evaluated as follows:

$$[\hat{\mathcal{J}}_-, \ \hat{\mathcal{J}}_+]R_{n,\ell}(r) = 2j_0 R_{n,\ell}(r), \tag{27}$$

where $j_0 = n + \frac{2\gamma_\ell + 3}{4}$ and operators $\hat{\mathcal{J}}_\mp$ and $\hat{\mathcal{J}}_0$ satisfy the following commutation relations:

$$[\hat{\mathcal{J}}_0, \ \hat{\mathcal{J}}_\mp]R_{\mu,\ell}(r) = \mp\hat{\mathcal{J}}_\mp R_{n,\ell}(r). \tag{28}$$

We define the Hermitian operators for these operators as follows:

$$\hat{\mathcal{J}}_x = \frac{1}{2}\left(\hat{\mathcal{J}}_+ + \hat{\mathcal{J}}_-\right), \quad \hat{\mathcal{J}}_y = \frac{1}{2i}\left(\hat{\mathcal{J}}_+ - \hat{\mathcal{J}}_-\right), \quad \hat{\mathcal{J}}_z = \hat{\mathcal{J}}_0 \tag{29}$$

and the following commutation relations are obtained:

$$[\hat{\mathcal{J}}_x, \ \hat{\mathcal{J}}_y] = -i\hat{\mathcal{J}}_z, \ \ [\hat{\mathcal{J}}_y, \ \hat{\mathcal{J}}_z] = i\hat{\mathcal{J}}_x, \ \ [\hat{\mathcal{J}}_z, \ \hat{\mathcal{J}}_x] = i\hat{\mathcal{J}}_y. \tag{30}$$

The Casimir operator can be expressed as [86]

$$\hat{\mathcal{C}}R_{n,\ell}(r) = \left\{\hat{\mathcal{J}}_0(\hat{\mathcal{J}}_0 - 1) - \hat{\mathcal{J}}_+\hat{\mathcal{J}}_-\right\}R_{n,\ell}(r) = \left\{\hat{\mathcal{J}}_0(\hat{\mathcal{J}}_0 + 1) - \hat{\mathcal{J}}_-\hat{\mathcal{J}}_+\right\}R_{n,\ell}(r)$$
$$= \left(\frac{2\gamma_\ell + 3}{4}\right)\left(\frac{2\gamma_\ell - 1}{4}\right)R_{n,\ell}(r) = \tau(\tau - 1)R_{n,\ell}(r), \tag{31}$$

where

$$\tau = \frac{2\gamma_\ell + 3}{4}. \tag{32}$$

Then, the Casimir operator $\hat{\mathcal{C}}$ now satisfies the following commutation relations:

$$[\hat{\mathcal{C}}, \hat{\mathcal{J}}_\pm] = [\hat{\mathcal{C}}, \hat{\mathcal{J}}_x] = [\hat{\mathcal{C}}, \hat{\mathcal{J}}_y] = [\hat{\mathcal{C}}, \hat{\mathcal{J}}_z] = 0, \tag{33}$$

therefore, the operators $\hat{\mathcal{J}}_\pm, \hat{\mathcal{J}}_x, \hat{\mathcal{J}}_y, \hat{\mathcal{J}}_z$ and $\hat{\mathcal{J}}_0$ 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 $SU(1, 1)$ [16,87].

The Hamiltonian operator $\hat{\mathcal{H}}$ takes the form

$$\hat{\mathcal{H}} = (4n + 2\gamma_\ell + 3)\sqrt{\frac{\hbar^2 D_e}{2\mu r_e^2}} - 2D_e = \frac{1}{4}\hat{\mathcal{J}}_0\sqrt{\frac{\hbar^2 D_e}{2\mu r_e^2}} - 2D_e. \tag{34}$$

Furthermore, we find that the following physical functions can be obtained by the creation and annihilation operators $\hat{\mathcal{J}}_{\mp}$ and $\hat{\mathcal{J}}_0$ as:

$$r^2 R_{n,\ell}(r) = \frac{1}{2\lambda}[2\hat{\mathcal{J}}_0 - (\hat{\mathcal{J}}_+ + \hat{\mathcal{J}}_-)]R_{n,\ell}(r), \tag{35}$$

$$r\frac{d}{dr}R_{n,\ell}(r) = (\hat{\mathcal{J}}_+ - \hat{\mathcal{J}}_-) - \frac{3}{2}R_{n,\ell}(r). \tag{36}$$

With Eqs. (35) and (36), the matrix elements for r^2 and $r\frac{d}{dr}$ are obtained as follows:

$$\langle R_{m,\ell}(r) \mid r^2 \mid R_{n,\ell}(r) \rangle$$
$$= \frac{1}{2\lambda}\left[\left(2n + \frac{2\gamma_\ell + 3}{2}\right)\delta_{m,n} - j_+\delta_{m,n+1} - j_-\delta_{m,n-1}\right] \tag{37}$$

and

$$\langle R_{m,\ell}(r) \mid r\frac{d}{dr} \mid R_{n,\ell}(r) \rangle = j_+\delta_{m,n+1} - j_-\delta_{m,n-1} - \frac{3}{2}\delta_{m,n}. \tag{38}$$

From the relations above, we can deduce the following relations:

$$2\lambda\langle R_{m,\ell}(r) \mid r^2 \mid R_{n,\ell}(r) \rangle + \langle R_{m,\ell}(r) \mid r\frac{d}{dr} \mid R_{n,\ell}(r) \rangle$$
$$= (2n + \gamma_\ell)\delta_{m,n} - 2j_-\delta_{m,n-1} \tag{39}$$

and

$$2\lambda\langle R_{m,\ell}(r) \mid r^2 \mid R_{n,\ell}(r) \rangle - \langle R_{m,\ell}(r) \mid r\frac{d}{dr} \mid R_{n,\ell}(r) \rangle$$
$$= (2n + \gamma_\ell + 3)\delta_{m,n} - 2j_+\delta_{m,n+1}. \tag{40}$$

These two relations form a useful link for finding the matrix elements from the creation and annihilator operators.

4 The numerical values of the explicit bound state energies, $\langle r^2 \rangle$, $\langle p^2 \rangle$ and the Heisenberg uncertainty products

4.1 The explicit bound state energies for the pseudoharmonic potential

The explicit bound state energies for the pseudoharmonic potential are obtained as :

$$E_{n,\ell} = (4n + 2\gamma_\ell + 3)\sqrt{\frac{\hbar^2 D_e}{2\mu r_e^2}} - 2D_e, \tag{41}$$

where γ_ℓ is as stated in Eq. (9).

4.2 The expectation values of r^2 and p^2 for the pseudoharmonic potential

The expectation values of r^2 and p^2 can be obtained by applying the Hellmann–Feynman theorem (HFT) [80–82, 88–104]. This theorem states that, a non-degenerate eigenvalue of a hermitian operator in a parameter dependent eigensystem varies with respect to the parameter according to the formula

$$\frac{\partial E_\nu}{\partial \nu} = \langle \Psi_\nu \mid \frac{\partial H_\nu}{\partial \nu} \mid \Psi_\nu \rangle, \tag{42}$$

provided that the associated normalized eigenfunction Ψ_ν, is continuous with respect to the parameter, ν. The effective Hamiltonian of the pseudoharmonic potential radial wave function is

$$\hat{\mathcal{H}} = \frac{-\hbar^2}{2\mu} \frac{d^2}{dr^2} + \frac{\hbar^2}{2\mu} \frac{\ell(\ell+1)}{r^2} + \frac{D_e}{r_e^2} r^2 + \frac{D_e r_e^2}{r^2} - 2D_e. \tag{43}$$

With $\nu = D_e$ and $\nu = \mu$, then, the following expectation values of r^2 and p^2 are obtained respectively as:

$$\langle r^2 \rangle = \left[2n + 1 + \frac{1}{2} \sqrt{(2\ell+1)^2 + \frac{8\mu D_e r_e^2}{\hbar^2}} \right] \sqrt{\frac{\hbar^2 r_e^2}{2\mu D_e}} \tag{44}$$

and

$$\langle p^2 \rangle = 2\mu D_e \left[2n + 1 + \frac{1}{2} \sqrt{(2\ell+1)^2 + \frac{8\mu D_e r_e^2}{\hbar^2}} \right] \sqrt{\frac{\hbar^2}{2\mu D_e r_e^2}}$$

$$- \frac{4\mu D_e}{\sqrt{(2\ell+1)^2 + \frac{8\mu D_e r_e^2}{\hbar^2}}} \sqrt{\frac{2\mu D_e r_e^2}{\hbar^2}} . \tag{45}$$

4.3 The Heisenberg uncertainty product for the pseudoharmonic potential

In 1927, Werner Heisenberg stated that certain physical quantities, like the position and momentum, cannot both have precise values at the same time, this is called the Heisenberg uncertainty principle [105, 106]. That is, the more precisely one property is measured, the less precisely the other can be measured. A mathematical statement of this principle is that every quantum state has the property that the root mean square (RMS) deviation of the position from its mean (the standard deviation of the x-distribution):

$$\Delta x = \sqrt{\langle (x - \langle x \rangle)^2 \rangle} \tag{46}$$

and the RMS deviation of the momentum from its mean (the standard deviation of p):

$$\Delta p_x = \sqrt{\langle (p_x - \langle p_x \rangle)^2 \rangle}, \tag{47}$$

the product of which can never be smaller than a fixed fraction of Planck's constant:

$$\Delta x \Delta p_x \geq \frac{\hbar}{2}. \tag{48}$$

This inequality is very important in physics, it has been pointed out that for a particle moving non-relativistically in a central potential V(r), the following 'uncertaintý6 relation holds [71,101,102,104–111]:

$$\Delta r \Delta p \geq \frac{3\hbar}{2}. \tag{49}$$

With Eqs. (44) and (45) and noting that $\langle r \rangle = \langle p \rangle = 0$ (due to parity consideration), the Heisenberg uncertainty product for the pseudoharmonic potential becomes:

$$P_{n,\ell} = \Delta r \Delta p = \left[2n + 1 + \frac{1}{2} \sqrt{(2\ell + 1)^2 + \frac{8\mu D_e r_e^2}{\hbar^2}} \right]^2 \hbar^2 \tag{50}$$

$$- \frac{4\mu D_e r_e^2}{\sqrt{(2\ell + 1)^2 + \frac{8\mu D_e r_e^2}{\hbar^2}}} \left[2n + 1 + \frac{1}{2} \sqrt{(2\ell + 1)^2 + \frac{8\mu D_e r_e^2}{\hbar^2}} \right].$$

In this work, we obtained the numerical values of the explicit bound state energies ($E_{n,\ell}$), the expectation values of r^2 and p^2 ($\langle r^2 \rangle$ and $\langle p^2 \rangle$) and the Heisenberg uncertainty product $P_{n,\ell}$ of some diatomic molecules for various values of n and ℓ. In the case of this study, we have selected some diatomic molecules for the purposes which they serve in various aspect of chemical synthesis, nature of bonding, temperature stability and electronic transport properties in chemical physics [42,112–114].

Some of these selected diatomic molecules composed of the homogeneous diatomic molecules (dimers) (N_2 and H_2); the heterogeneous diatomic molecules (CO, NO and CH) and the neutral transition metal hydride (ScH).

The spectroscopic parameters and reduced masses for some selected diatomic molecules used in our study are shown in Table 1. The spectroscopic parameters listed in this table are obtained from the following cited sources: for CO, NO and N_2, the sources are [57,58,60,61,72,115,116]; for CH, the sources are [44,46,57,58,61,72,115,117]; for H_2, the source is [118] and for ScH, the sources are [42,112], where $\hbar c = 1973.29$ eVÅ is taken from [42,44,57,58,60,61,72,74,119].

For these selected diatomic molecules, we have available results from the literature to compare with our results with few ones: CO, NO, CH and N_2 [57,72].

The numerical values of the explicit bound state energies of some of these diatomic molecules for various values of n and ℓ are obtained and compared with the

Table 1 Model parameters for some diatomic molecules in our study

Molecules	D_e(in eV)	r_e(in Å)	μ(in amu)
CO	10.845073641	1.1283	6.860586000
NO	8.043729855	1.1508	7.468441000
N_2	11.938193820	1.0940	7.00335
CH	3.947418665	1.1198	0.929931
H_2	4.7446	0.7416	0.50391
ScH	2.25	1.776	0.986040

exact method [72] and the Nikiforov-Uvarov method [57] for CO, NO, CH and N_2. In the Tables 2, 3 and 4, we have used $E_{n,\ell}$ (FM) to mean factorization method (present method), $E_{n,\ell}$(EM) to mean Exact Method [72] and $E_{n,\ell}$ (NU) mean Nikiforov-Uvarov Method [57]. Also, the numerical results for the expectation values of r^2 and p^2 ($\langle r^2 \rangle$ and $\langle p^2 \rangle$) and the Heisenberg uncertainty product $P_{n,\ell}$ of some of these diatomic molecules for various values of n and ℓ are computed and presented in Tables 2, 3 and 4.

5 Conclusions

We have used $SU(1, 1)$ spectrum generating algebra approach to obtain the solutions of the 3-dimensional Schrödinger wave equation with pseudoharmonic molecular potential. The explicit bound state energies, the eigenfunctions and the radial matrix elements are obtained for this molecular potential. Furthermore, based upon the solutions obtained, by using Hellmann–Feynman theorem, the expectation values of r^2 and p^2 are obtained. The Heisenberg uncertainty products $P_{n,\ell}$ for this potential are obtained also.

The solutions obtained have been applied to compute the numerical values of the explicit bound state energies for these selected diatomic molecules. The numerical values of the explicit bound state energies obtained for these diatomic molecules for various values of n and ℓ are compared with the exact method [72] and the Nikiforov-Uvarov method [57] for CO, NO, CH and N_2 and our results are in excellent agreement with their results as displayed in Tables 2, 3 and 4.

Though, slight differences are noticed in the numerical values of the explicit bound state energies we obtained when compared with the results of Ikhdair and Sever and Sever et al. [57,72], this is due to the conversions used by Ikhdair and Sever and Sever et al. [57,72] as cited in the work of Ikhdair [44], they have used the following conversions: 1amu = 931.502MeV/c², 1 cm⁻¹ = 1.23985 × 10⁻⁴ eV, and ℏc = 1973.29 eVÅ (cf. pp. 791, Bransden and Joachain [120]). In our calculations, we have used the following recent conversions: 1amu = 931.494028MeV/c², 1 cm⁻¹ = 1.239841875 × 10⁻⁴ eV, and ℏc = 1973.29 eVÅ (cf. pp. 4, Nakamura et al. [119] in the 2010 edition of the Review of Particle Physics). This explains the reason for the slight differences.

Table 2 The energy eigenvalues $E_{n,\ell}$ (in eV), the expectation values $\langle r^2 \rangle$ (in (Å)²), $\langle p^2 \rangle$ (in (eV/c)²) and the Heisenberg uncertainty relations HUR (in eVÅ/c) corresponding to the pseudoharmonic potential for various n and ℓ quantum numbers for CO and NO diatomic molecules

n	ℓ	$E_{n,\ell}$ [FM]	$E_{n,\ell}$ [EM]	$E_{n,\ell}$ [NU]	$\langle r^2 \rangle$	$\langle p^2 \rangle$	HUR
CO							
0	0	0.1019578053531127	0.1019306	0.10193061	1.278818514996878	651953274.6811209	28874.38170030767
1	0	0.3057536875651401	0.3056722	0.30567217	1.290777797622587	1954330222.150913	50225.55186332170
	1	0.3062325780354271	0.3061508	0.30615078	1.290805888935957	1960448477.813082	50304.65624687896
2	0	0.5095495697771710	0.5094137	0.50941373	1.302737080248297	3256707169.620706	65135.49868831414
	1	0.5100284602474545	0.5098923	0.50989234	1.302765171561666	3262825425.282874	65197.35673280329
	2	0.5109862411880286	0.5108495	0.51084953	1.302821352328619	3275061126.516209	65320.89685396806
4	0	0.9171714133420122258	0.9168969	0.91689685	1.326553645499716	5861461064.560290	88182.42688980432
	1	0.9176202246715128	0.9173755	0.91737546	1.3266383736813085	5867579320.222428	88229.3718580831
	2	0.9185780056120834	0.9183327	0.91833265	1.326739917580037	5879815021.455794	88323.18663268512
	3	0.9200131221837502	0.9197684	0.91976835	1.326824184081614	5898166548.480750	88463.72148098587
	4	0.9219286840648948	0.9216825	0.92168247	1.326936530740917	5922631472.632870	88650.75329151144
5	0	1.120937216413253	1.1206384	1.12063840	1.338614928125425	7163838012.030083	97926.60775078365
	1	1.121416106883540	1.1211170	1.12111700	1.338643019438795	7169956267.692221	97969.44374358583
	2	1.1223738887824111	1.1220742	1.12207420	1.338699200205747	7182191968.925556	98055.05925001923
	3	1.123809004395778	1.1235099	1.12350990	1.338783466707324	7200543495.950542	98183.34168119120
	4	1.125724566276922	1.1254240	1.12542400	1.338895813366626	7225008420.102662	98354.12307175575
	5	1.128117463789163	1.1278165	1.12781650	1.339036232750661	7255583505.037642	98567.18116591059
NO							
0	0	0.0825108658683876	0.0824883	0.08248827	1.331132968244588	574375573.8664465	27650.86368502856
1	0	0.2474257254889523	0.2473592	0.24735916	1.344708974060483	1721656608.599298	48115.76760100594
	1	0.2478484808663488	0.2477817	0.24778171	1.344743765885460	1727536886.807932	48198.49021361709

Table 2 Continued

n	ℓ	$E_{n,\ell}$ [FM]	$E_{n,\ell}$ [EM]	$E_{n,\ell}$ [NU]	$\langle r^2\rangle$	$\langle p^2\rangle$	HUR
2	0	0.4123405850910657	0.4122301	0.41223005	1.358284979876379	2868937643.332150	62424.63383264652
	1	0.4127633404684623	0.4126526	0.41265260	1.358319771701355	2874817921.540784	62489.37527988453
	2	0.4136075930227321	0.4134977	0.41349768	1.358389352609480	2886577551.185603	62618.65705212839
4	0	0.7421703042952892	0.7419718	0.74197183	1.385436991508170	5163499712.797879	84579.56909178477
	1	0.7425930596726857	0.7423944	0.74239438	1.385471783333147	5169379991.006488	84628.77829005003
	2	0.7434347312269555	0.7432395	0.74323946	1.385541364241271	5181139620.651306	84727.11052739678
	3	0.7447055783591487	0.7445070	0.74450700	1.385645728749967	5198776748.734846	84874.39423412152
	4	0.7463953416682116	0.7461969	0.74619689	1.385784868638066	5222288597.129426	85070.37391220915
5	0	0.9070851638974027	0.9068427	0.90684272	1.399012997324066	6310780747.530731	93962.03642460064
	1	0.9075079192747992	0.9072653	0.90726527	1.399047789149042	6316661025.739365	94006.97124609737
	2	0.9083521718290690	0.9081104	0.90811035	1.399117370057167	6328420655.384158	94096.77605516852
	3	0.9096204379612622	0.9093779	0.90937789	1.399221734565862	6346057783.467698	94231.32164752261
	4	0.9111310201270325	0.9110678	0.91106778	1.399360874453962	6369569631.862278	94410.41536789360
	5	0.9134227199567881	0.9131799	0.91317990	1.399534778764948	6398952498.950474	94633.80247007970

Table 3 The energy eigenvalues $E_{n,\ell}$ (in eV), the expectation values $\langle r^2 \rangle$ (in $(\text{Å})^2$), $\langle p^2 \rangle$ (in $(\text{eV}/c)^2$) and the Heisenberg uncertainty relations HUR (in $e\text{VÅ}/c$) corresponding to the pseudoharmonic potential for various n and ℓ quantum numbers for N$_2$ and CH diatomic molecules

n	ℓ	$E_{n,\ell}$ [FM]	$E_{n,\ell}$ [EM]	$E_{n,\ell}$ [NU]	$\langle r^2 \rangle$	$\langle p^2 \rangle$	HUR
N$_2$							
0	0	0.10918603434345160	0.1091559	0.10915590	1.20230900240784	7126283651.7236753	29272.27309853578
1	0	0.327431375502547	0.3273430	0.32734304	1.21324884205456	2136424222.911053	50911.82791175150
	1	0.32792932421378 36	0.3278417	0.32784167	1.21327384148512	2142930999.051733	50989.82379813161
2	0	0.54567671635499 69	0.5455302	0.54553018	1.22418685170128	3560164794.098396	66017.52387265288
	1	0.54617457521852 59	0.5460288	0.54602881	1.224213684113184	3566671570.239111	66078.49985452284
	2	0.54717195802539 11	0.5470260	0.54702603	1.224263680432900	3579684307.137500	66200.28311604151
4	0	0.98216739836447 43	0.9819045	0.98190446	1.246068365099471	6407645936.473118	89355.27346607656
	1	0.98266525722800 32	0.9824031	0.98240309	1.246093364042527	6414152712.613832	89401.52756605153
	2	0.98366264003487 20	0.9834003	0.98340031	1.246143360362243	6427165449.512221	89493.96376772718
	3	0.98515954678508 07	0.9848961	0.98489606	1.246218350926318	6446682516.785655	89632.43863141369
	4	0.98715264731900 38	0.9868903	0.98689026	1.246318331037525	6472701469.817430	89816.73837969733
5	0	1.200412739369217	1.2000916	1.20009160	1.257008205064143	7831386507.660496	99217.52414345898
	1	1.200910598232742	1.2005902	1.20059020	1.257033204007199	7837893283.801210	99259.72046708141
	2	1.201907981039611	1.2015875	1.20158750	1.257083200326915	7850906020.699599	99344.05903710042
	3	1.20340404887789 819	1.2030832	1.20308320	1.257158190890989	7870423087.973033	99470.43204300891
	4	1.205397988323746	1.2050774	1.20507740	1.257258171002197	7896642041.004807	99638.67862380833
	5	1.207892277880820	1.2075699	1.20756990	1.257383134399858	7928959622.092161	99848.58587960149
CH							
0	0	0.16867963352224 18	0.1686344	0.16863440	1.280743635551838	146502414.5533975	13697.88432686745
1	0	0.50514213277114 81	0.5050072	0.50500718	1.334184611139168	437954691.1786194	24172.55487834748
	1	0.50872567196297 78	0.5085903	0.50859034	1.334753837042328	444161731.2395528	24348.44091598796

Table 3 Continued

n	ℓ	$E_{n,\ell}$ [FM]	$E_{n,\ell}$ [EM]	$E_{n,\ell}$ [NU]	$\langle r^2 \rangle$	$\langle p^2 \rangle$	HUR
2	0	0.8416046320200543	0.841380	0.84137996	1.3876255586726497	729406967.8038429	31814.20707264606
	1	0.8451881712118841	0.8449631	0.84496312	1.3881948126296657	735614007.8647747	31955.83749200750
	2	0.8523507573365272	0.8521246	0.85212458	1.3893324903411191	748011217.9336663	32237.18797002816
4	0	1.5145296305178 67	1.5141255	1.51412550	1.4945007537901155	1312311521.054287	44286.10911211507
	1	1.5181131697 09697	1.5177087	1.51770870	1.4950767638043 16	1318518561.115218	44399.17187705266
	2	1.5252757558343 40	1.5248701	1.52487010	1.4962144415158 50	1330915771.184110	44624.38119780340
	3	1.5360077626224 79	1.5356002	1.53560020	1.4979190280977 72	1349469582.659151	44959.93956517626
	4	1.5502950711545 778	1.5498843	1.54988430	1.5001882221892 07	1374130067.794166	45403.23494488982
5	0	1.8509921297667 73	1.8504983	1.85049830	1.5479485134884 84	1603763797.679508	49825.13207814547
	1	1.8545756689586 03	1.8540815	1.85408150	1.5485177393916 45	1609970837.740440	49930.63590766994
	2	1.8617382550832 46	1.8612429	1.86124290	1.5496554417103 179	1622368047.809332	50140.91576569818
	3	1.8724702618713 85	1.8719729	1.87197290	1.5513600003685 101	1640921859.284373	50454.53935639852
	4	1.8867575707946 84	1.8862571	1.88625710	1.5536291977775 36	1665582344.419388	50869.41479505201
	5	1.9045796458119 28	1.9040761	1.90407610	1.5564599550193 57	1696283716.548377	51382.85392189649

Table 4 The energy eigenvalues $E_{n,\ell}$(in eV), the expectation values $\langle r^2 \rangle$ (in (Å)^2), $\langle p^2 \rangle$ (in (eV/c)^2) and the Heisenberg uncertainty relations HUR (in eVÅ/c) corresponding to the pseudoharmonic potential for various n and ℓ quantum numbers for H$_2$ and ScH diatomic molecules

n	ℓ	$E_{n,\ell}$ [FM]	$\langle r^2 \rangle$	$\langle p^2 \rangle$	HUR
H$_2$					
0	0	0.3802143254317158	0.5720067969319436	179353151.5582044	10128.73248449469
1	0	1.136872065928291	0.6158608064535510	534520083.1548633	18143.59306965887
	1	1.151940622653841	0.6167341564193854	548652322.0868371	18394.90763852220
2	0	1.893529806424867	0.6597148159751585	889687014.7515233	24226.83853110614
	1	1.908598363150416	0.6605881659409929	903819253.6834971	24434.65373466418
	2	1.938664759306279	0.6623307257790985	931950074.8372046	24844.70103375790
3	0	2.650187546921444	0.7035688254967659	1244853946.348182	29594.60134800272
	1	2.665256103646993	0.7044421754626004	1258986185.280156	29780.58037104236
	2	2.695322499802856	0.7061847353007059	1287117006.433864	30148.67132212521
	3	2.740245300798563	0.7087883221856139	1328983795.005013	30691.50035878782
4	0	3.406845287418019	0.7474228350183734	1600020877.944841	34581.67348006918
5	0	4.163503027914595	0.7912768445399808	1955187809.541501	39333.12650193264
ScH					
0	0	7.793888021911055E-02	3.208805616306735	71740403.45470674	15172.37652846693
1	0	0.2334806033879131	3.317829166958441	214603976.5716611	26683.69038972540
	1	0.2348245288753450	3.318771086193946	217072082.5705855	26840.50206786684
2	0	0.3890223265567156	3.426852717610148	357467549.6886156	34999.83777259364
	1	0.3903662520441475	3.427794636845652	359935655.6875399	35125.28306185265
	2	0.3930526196575466	3.429677632258357	364867451.6219697	35374.81784500067
3	0	0.5445640497255191	3.535876268261853	500331122.8055699	42060.77678076121
	1	0.5459079752129510	3.536818187497358	502799228.8044953	42170.00660535145
	2	0.5485940461540562	3.538701182910063	507731024.7389241	42387.59698123697
	3	0.5526210758596637	3.541523572150610	515117708.0628493	42711.84268486642
4	0	0.7001057728943216	3.644899818913559	643194695.9225243	48418.80038470771
5	0	0.8556474960631242	3.753923369565265	786058269.0394796	54321.28962006814

In addition, we obtained the numerical values of the expectation values of r^2 and p^2, and the Heisenberg uncertainty product for these diatomic molecules. These results are displayed together with the numerical values of the explicit bound state energies of these diatomic molecules for various values of n and ℓ in Tables 2, 3 and 4. The Heisenberg uncertainty products obtained are valid in each case of these diatomic molecules for various n and ℓ, as expected from Eq. (49) that

$$P_{n,\ell} \geq 2959.89 \text{ eVÅ/c}. \tag{51}$$

This implies that the numerical value of the Heisenberg uncertainty product $P_{n,\ell}$ can not be less than 2959.89 eVÅ/c for this principle to hold. The Heisenberg uncertainty products in all these selected diatomic molecules attains its minimum value of

2959.89 eVÅ/c, even the lowest Heisenberg uncertainty products (for ground state) $P_{0,0}$ obtained for H_2 is 10128.73248449469 eVÅ/c which is greater than the minimum.

It is evident from the Tables displayed that the numerical values of the explicit bound state energies, the expectation values of r^2 and p^2 and the Heisenberg uncertainty products $P_{n,\ell}$ increase as the quantum numbers (n, ℓ) of the state increase. We only presented the results for few selected diatomic molecules for this paper. Other diatomic molecules studied in this work, but not shown in the Tables are: I_2, HCl, LiH, TiH, VH, CrH, MnH, TiC, NiC, ScN, ScF and Ar_2. Similar studies involving the confined diatomic molecules are currently in progress [121].

It should be noted that the advantage of this SGA method is that, it allows one to find the explicit bound state energies and the eigenfunctions directly in a simple and unique way. This method, as applied here to the diatomic molecules demonstrates that the values obtained are in excellent agreement with earlier results derived from the other methods. We have also demonstrated that the Heisenberg uncertainty product is validated by all the diatoms considered. Finally, the method serves as a very useful link for finding the matrix elements from the creation and annihilation operators in addition to allowing the construction of the coherent states.

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