Spectroscopic Studies of Some Diatomic Molecules using Spectrum Generating Algebra Approach

Oyewumi, K. J. and Sen, K. D.
School of Chemistry, University of Hyderabad,
Hyderabad 50046, India.

Abstract

For arbitrary values $n$ and $\ell$ quantum numbers, we present the solutions of the 3-dimensional Schrödinger wave equation with the pseudoharmonic potential via $SU(1,1)$ Spectrum Generating Algebra (SGA) approach. The explicit bound state energies and eigenfunctions are obtained. The matrix elements $r^2$ and $\frac{d}{dr}$ are obtained (in a closed form) directly from the creation and annihilation operators. In addition, the expectation values of $r^2$ and $p^2$ and the Heisenberg Uncertainty Products (HUP) for set of diatomic molecules ($O_2$, $I_2$, $N_2$, $H_2$, CO, NO, HCl, CH, LiH, ScH, TiH, VH, CrH, MnH, TiC, NiC, ScN, ScF, Ar$_2$) for arbitrary values of $n$ and $\ell$ 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.

KEY WORDS: Schrödinger equation, explicit bound state energies, eigenfunctions, matrix elements, expectation values, ladder operators, $SU(1, 1)$, pseudoharmonic potential, diatomic molecules, Hellmann-Feynman theorem, Heisenberg Uncertainty Principle.

PACS: 03.65.Fd, 03.65.Ge, 03.65.Ca, 03.65-W

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][2]. This technique serves as a useful tool in various fields of physics, ranging from quantum mechanics (relativistic and nonrelativistic), 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 [3 - 23].

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. [19], and exemplified later with a typical system [18]. 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 with Morse potential, Pöschl-Teller potential, pseudoharmonic potential, infinite square well in 3D as well as N-dimensions [4, 7 - 23] 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. [19]. In the similar fashion, Salazar-Ramírez et al. [20, 21] 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 [18, 19, 20, 21] above have been constructed without adding phase as an additional variable like in Martínez-y-Romero et al. [8].

Gur and Mann [16] 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 [22].

In their work, Motavalli and Akbarieh [23] 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 [4]. 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 [16, 22, 24]. Thus, Gur and Mann [16] 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 [22]. 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 [24].

In recent years, discussion on the 3D-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 [36 - 38, 41 - 44].

The corresponding wavefunction 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 [39, 40, 42]. For examples, Kratzer and pseudoharmonic potentials which have known exact solutions like in the Coulomb and harmonic oscillator model potentials [17, 35, 44, 45, 46, 47, 48].

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 [4, 15, 25, 26, 27, 29, 33, 34, 35]. Sage [26] has discussed the energy levels and wavefunctions 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 os-
cillator, 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 pseudoha-
monic oscillator can be found exactly for any angular momentum. These wavefunctions
have reasonable behaviour at the origin, near the equilibrium, and at the infinity [28].

Its characteristics make it useful to model various physical systems, including some
molecular physical ones [4, 17, 26, 27, 34, 46]. 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
[27]. The eigenfunctions and energy eigenvalues are similar to those of the harmonic
oscillator, which can be obtained exactly in the \( r_e \rightarrow 0 \) limit.

Recently, with an improved approximation to the orbital centrifugal term of the
Manning-Rosen potential, Ikhdair [49] used the nikiforov-Uvarov method to obtain the
rotational-vibrational energy states for a few diatomic molecules for arbitrary quantum
numbers \( n \) and \( \ell \) with different values of the potential parameters.

In the study of the diatomic molecules using the diatomic molecular potentials, dif-
ferent methods have been employed: Nikiforov-Uvarov method [35, 41 - 46]; asymptotic
iteration method [47]; Exact method [34]; shifted 1/N expansion [37]; exact quantiza-
tion rule method [39, 48]; SUSY approach [38]; Nikiforov-Uvarov method [35, 44, 46];
tridiagonal J-matrix representation [51] and algebraic method [17, 50].

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 of some neutral diatomic molecules (metallic hydrides, homogeneous and heterogeneous diatomic molecules) for any $n$ and $\ell$ quantum numbers.

The scheme of our presentation is as follows: in Section 2, we study the 3-dimensional Schrödinger equation for the pseudoharmonic potential. In Section 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 Section 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 ($O_2$, $I_2$, $N_2$, $H_2$, $Ar_2$); the heterogeneous diatomic molecules ($CO$, $NO$, $HCl$, $CH$, $LiH$); the neutral transition metal hydrides ($ScH$, $TiH$, $VH$, $CrH$, $MnH$); the transition-metal lithide ($CuLi$); the transition-metal carbides ($TiC$, $NiC$); the transition-metal nitrite ($ScN$) and the transition-metal fluoride($ScF$). Finally, in Section 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 [15, 31, 32, 33, 34]

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

This potential is associated with the following molecular potentials:

- Isotropic harmonic oscillator plus inverse quadratic potential

  $$V(r) = \mu \omega^2 r^2 + \frac{g}{r^2},$$ \hspace{1cm} (2)

  here $A = \mu \omega^2$, $B = g$ and $c = 0$ [1, 15, 29, 31, 32, 33].

- The pseudoharmonic potential

  $$V(r) = D_e \left( \frac{r}{r_e} - 1 \right)^2,$$ \hspace{1cm} (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 $A = \frac{D_e}{r_e}$, $B = D_e r_e$ and $c = -2D_e$ [4, 15, 25 - 32, 35]. The graphs of the potential in equation (3) for some diatomic molecules is displayed in the figure below Figure 1.

**Figure 1.** Shapes of the pseudoharmonic potentials for some diatomic molecules.

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

$$-\frac{\hbar^2}{2\mu} \Delta + \frac{D_e}{r^2} + \frac{D_e r^2}{r^2} - 2D_e \psi(r, \theta, \phi) = E \psi(r, \theta, \phi). \quad (4)$$

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

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

then, equation (4) reduces to two decoupled differential equations, that is, the radial and angular wavefunctions:

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

and

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

where $\ell = 0, 1, 2, \ldots$ is the orbital angular momentum quantum numbers, $n = 1, 2, 3, \ldots$ is the principal quantum number, $\mu$ is the reduced mass, $\hbar$ is the Planck’s constant divided by $2\pi$ and $E$ is the energy eigenvalue. Equation (6) can be rewritten as

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

where

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

To obtain the relevant algebraic operators for the radial symmetry, equation (8) is solved and the solutions which is a degenerate hypergeometric or Kummer equation (associated Laguerre differential equation) is obtained [52 - 54]. Then, the radial functions $R_{n,\ell}(r)$ for this potential is obtained as:

$$R_{n,\ell}(r) = N_{n,\ell} r^{\gamma_\ell} e^{-\lambda r^2} L_n^{\gamma_\ell + \frac{1}{2}}(2\lambda r^2), \quad (10)$$
where
\[ \lambda = \sqrt{\frac{\mu D_e}{\hbar^2 r_e^2}} \] (11)

\[ L_n^k(x) \] is the associated Laguerre functions [52 - 54], \( N_{n,\ell} \) is the normalization constant which is determined from the normalization condition
\[ \int_0^\infty R_{n,\ell}(r)R_{n',\ell}(r)dr = \delta_{n,n'} \] (12)
as
\[ N_{n,\ell} = \left[ \frac{2(2\lambda^2)^{\frac{1}{2}(2n+3)}n!}{\Gamma(n + \gamma_\ell + \frac{3}{2})} \right]^\frac{1}{2}. \] (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:
\[ [K_0, K_1] = iK_2, \quad [K_1, K_2] = -iK_0, \quad [K_2, K_0] = iK_1. \] (14)
Alternatively, these can be expressed in terms of the creation and annihilation operators
\[ K_\pm = K_1 \pm iK_2, \] (15)
the commutation relations together with \( K_0 \) can be written as:
\[ [K_0, K_\pm] = \pm K_\pm, \quad [K_-, K_+] = 2K_0. \] (16)

Based on the Schrödinger factorization method, Infeld-Hull factorization method, we adopt the factorization method introduced by Dong [4]. 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 \( \hat{J}_\pm \) with the following property:
\[ \hat{J}_\pm R_{n,\ell}(r) = j_\pm R_{n,\ell}(r), \] (17)
these operators are of the form

\[ \hat{J}_\pm = A_\pm(r) \frac{d}{dr} + B_\pm(r) \]  

and depend only on the physical variable \( r \).

On operating the differential operator \( \frac{d}{dr} \) on the radial wavefunctions \( R_{n,\ell}(r) \), we have,

\[ \frac{d}{dr} R_{n,\ell}(r) = \frac{\gamma_{\ell}}{r} R_{n,\ell}(r) - 2\lambda r R_{n,\ell}(r) + N_{n,\ell} r^{\gamma_{\ell}} \exp(-\lambda r^2) \frac{d}{dr} L_{n}^{\gamma_{\ell} + \frac{3}{2}}(2\lambda r^2). \]  

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 \( \hat{J}_\pm \) by using the recurrence relations of the associated Laguerre functions. To find these, the following recurrence relations of the associated Laguerre functions are used \([52 - 54]\):

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

The creation and annihilation operators are obtained as:

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

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

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

On defining the operator

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

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

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

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

\[ \hat{J}_0 R_{n,\ell}(r) = n + \frac{2\gamma_{\ell} + 3}{4} R_{n,\ell}(r) = j_0 R_{n,\ell}(r). \]
On carefully inspecting the dynamical group associated to the annihilation and creation operators \( \hat{J}_- \) and \( \hat{J}_+ \), based on the results of equations (24) and (25), the commutator \([\hat{J}_-, \hat{J}_+]\) can be evaluated as follows:

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

where \( j_0 = n + \frac{2\nu+3}{4} \) and operators \( \hat{J}_\pm \) and \( \hat{J}_0 \) satisfy the following commutation relations:

\[
[\hat{J}_0, \hat{J}_\pm]R_{n,\ell}(r) = \pm \hat{J}_\pm R_{n,\ell}(r).
\]

(28)

We define the Hermitian operators for these operators as follows:

\[
\hat{J}_x = \frac{1}{2} (\hat{J}_+ + \hat{J}_-), \quad \hat{J}_y = \frac{1}{2i} (\hat{J}_+ - \hat{J}_-), \quad \hat{J}_z = \hat{J}_0
\]

and the following commutation relations are obtained:

\[
[\hat{J}_x, \hat{J}_y] = -i\hat{J}_z, \quad [\hat{J}_y, \hat{J}_z] = i\hat{J}_x, \quad [\hat{J}_x, \hat{J}_z] = i\hat{J}_y.
\]

(30)

The Casimir operator can be expressed as

\[
\hat{C} R_{n,\ell}(r) = \left\{ \hat{J}_0(\hat{J}_0 - 1) - \hat{J}_+\hat{J}_- \right\} R_{n,\ell}(r) = \left\{ \hat{J}_0(\hat{J}_0 + 1) - \hat{J}_-\hat{J}_+ \right\} R_{n,\ell}(r) = \tau(\tau - 1) R_{n,\ell}(r),
\]

where

\[
\tau = \frac{2\gamma + 3}{4}.
\]

(32)

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

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

(33)

therefore, the operators \( \hat{J}_\pm, \hat{J}_x, \hat{J}_y, \hat{J}_z \) and \( \hat{J}_0 \) satisfy the commutation relations of the dynamical group \( SU(1,1) \) algebra, which is isomorphic to an \( SO(2,1) \) algebra (i. e. \( SU(1,1) \cong SO(2,1) \)). The commutation rules are valid for the infinitesimal operators of the non-compact group \( SU(1,1) \) \cite{9,56}.

The Hamiltonian operator \( \hat{H} \) takes the form

\[
\hat{H} = (4n + 2\gamma + 3) \sqrt{\frac{\hbar^2 D_e}{2\mu r^2_e} - 2D_e} = \frac{1}{4} \hat{J}_0 \sqrt{\frac{\hbar^2 D_e}{2\mu r^2_e} - 2D_e}.
\]

(34)
Furthermore, we find that the following physical functions can be obtained by the creation and annihilation operators $\hat{J}_\pm$ and $\hat{J}_0$ as:
\begin{align}
r^2 R_{n,\ell}(r) &= \frac{1}{2\lambda} [2\hat{J}_0 - (\hat{J}_+ + \hat{J}_-)] R_{n,\ell}(r), \quad (35) \\
r \frac{d}{dr} R_{n,\ell}(r) &= (\hat{J}_+ - \hat{J}_-) - \frac{3}{2} R_{n,\ell}(r). \quad (36)
\end{align}

With equations (35) and (36), the matrix elements for $r^2$ and $r \frac{d}{dr}$ are obtained as follows:
\begin{align}
\langle R_{m,\ell}(r) | r^2 | R_{n,\ell}(r) \rangle &= \frac{1}{2\lambda} \left( 2n + \frac{2\gamma_\ell + 3}{2} \right) \delta_{m,n} - j_+ \delta_{m,n+1} - j_- \delta_{m,n-1} \quad (37) \\
\langle R_{m,\ell}(r) | r \frac{d}{dr} | R_{n,\ell}(r) \rangle &= j_+ \delta_{m,n+1} - j_- \delta_{m,n-1} - \frac{3}{2} \delta_{m,n}. \quad (38)
\end{align}

From the relations above, we can deduce the following relations:
\begin{align}
2\lambda \langle R_{m,\ell}(r) | r^2 | R_{n,\ell}(r) \rangle + \langle R_{m,\ell}(r) | r \frac{d}{dr} | R_{n,\ell}(r) \rangle &= (2n + \gamma_\ell) \delta_{m,n} - 2j_- \delta_{m,n-1} \quad (39) \\
and \\
2\lambda \langle R_{m,\ell}(r) | r^2 | R_{n,\ell}(r) \rangle - \langle R_{m,\ell}(r) | r \frac{d}{dr} | R_{n,\ell}(r) \rangle &= (2n + \gamma_\ell + 3) \delta_{m,n} - 2j_+ \delta_{m,n+1}. \quad (40)
\end{align}

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

4 The explicit bound state energies, the numerical values of $\langle r^2 \rangle$, $\langle p^2 \rangle$ 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:
\[ E_{n,\ell} = (4n + 2\gamma_\ell + 3) \sqrt{\frac{\hbar^2 D_e}{2\mu r_e^2} - 2D_e}, \quad (41) \]

where $\gamma_\ell$ is as stated in equation (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) [30, 57 - 64]. 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

$$\frac{\partial E_\nu}{\partial \nu} = \langle \Psi_\nu | \frac{\partial H_\nu}{\partial \nu} | \Psi_\nu \rangle,$$

(42)

provided that the associated normalized eigenfunction $\Psi_\nu$, is continuous with respect to the parameter, $\nu$. The effective Hamiltonian of the pseudoharmonic potential radial wave function is

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

(43)

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

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

(44)

and

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

(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 [65]. 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):

$$\Delta x = \sqrt{\langle (x - \langle x \rangle)^2 \rangle}$$  \hspace{1cm} (46)

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

$$\Delta p_x = \sqrt{\langle (p_x - \langle p_x \rangle)^2 \rangle},$$  \hspace{1cm} (47)

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

$$\Delta x \Delta p_x \geq \frac{\hbar}{2}.$$  \hspace{1cm} (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 uncertainty relation holds $[33, 61, 62, 64, 65, 66]$:

$$\Delta r \Delta p \geq \frac{3\hbar}{2}. \hspace{1cm} (49)$$

With equations (44) and (46) and noting that $\langle r \rangle = \langle p \rangle = 0$ (due to parity consideration), the Heisenberg uncertainty product for the pseudoharmonic potential becomes:

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

In this work, we obtained 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 $\ell$. 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 $[41, 70, 72]$. Some of these selected diatomic molecules composed of the some homogeneous diatomic molecules (dimers) ($O_2, I_2, N_2, H_2, Ar_2$); the heterogeneous diatomic molecules (CO, NO, HCl, CH, LiH); the neutral transition metal hydrides (ScH, TiH, VH, CrH,
MnH); the transition-metal lithide (CuLi); the transition-metal carbides (TiC, NiC); the transition-metal nitrite (ScN) and the transition-metal fluoride(ScF).

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, O₂, I₂ and N₂, the sources are [34, 35, 45, 47, 48, 68, 69]; for CH, LiH and HCl, the sources are [34, 35, 43, 45, 48, 68, 73]; for H₂, the source is [74]; for Ar₂, the source is [71, 72] and for ScH, TiH, VH, CrH, MnH, CuLi, TiC, NiC, ScN and ScF, the sources are [41, 70], where $\hbar c = 1973.29 \text{ eV} \cdot \text{Å}$. is taken from [34, 35, 41, 43, 45, 47, 48, 49, 76].

For these selected diatomic molecules, we have available results from the literature to compare with our results with few ones: CO, NO, CH and N₂ [34, 35].

The explicit bound state energies of some of these diatomic molecules for various values of $n$ and $\ell$ are obtained and compared with the exact method [34] and the Nikiforov-Uvarov method [35] for CO, NO, CH and N₂. In the Tables 2 - 7, we have used $E_{n,\ell}$ (FM) to mean factorization method (present method), $E_{n,\ell}$ (EM) to mean Exact Method [34] and $E_{n,\ell}$ (NU) mean Nikiforov-Uvarov Method [35]. 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 $\ell$ are computed and

| Molecules | $D_e$(in eV) | $r_e$(in Å) | $\mu$(in amu) | Molecules | $D_e$(in eV) | $r_e$(in Å) | $\mu$(in amu) |
|-----------|-------------|-------------|--------------|-----------|-------------|-------------|--------------|
| ScH       | 2.25        | 1.776       | 0.986040     | CH        | 3.947418665| 1.1198      | 0.929931     |
| TiH       | 2.05        | 1.781       | 0.987371     | LiH       | 2.515267218| 1.5956      | 0.8801221    |
| VH        | 2.33        | 1.719       | 0.988005     | HCl       | 4.619030905| 1.2746      | 0.9801045    |
| CrH       | 2.13        | 1.694       | 0.988976     | H₂        | 4.7446      | 0.7416      | 0.50391      |
| MnH       | 1.67        | 1.753       | 0.989984     | CO        | 10.845073641| 1.1282      | 6.860586000  |
| CuLi      | 1.74        | 2.310       | 6.259494     | NO        | 8.043729855| 1.1508      | 7.468441000  |
| TiC       | 2.66        | 1.790       | 9.606079     | O₂        | 5.156658828| 1.208       | 7.997457504  |
| NiC       | 2.76        | 1.621       | 9.974265     | I₂        | 1.581791863| 2.662       | 63.45223502  |
| ScN       | 4.56        | 1.768       | 10.682771    | N₂        | 11.938193820| 1.0940      | 7.00335      |
| ScF       | 5.85        | 1.794       | 13.358942    | Ar₂       | 1.672       | 2.53        | 53.9341      |
presented in Tables 2 - 7.

Table 2: The energy eigenvalues \( E_{n,\ell} \) (in eV), the expectation values \( \langle r^2 \rangle \) (in \((\text{A}_0^2)\)) and \( \langle p^2 \rangle \) (in \((\text{eV}/\text{c})^2\)) and the Heisenberg Uncertainty Relations HUR (in \(\text{eV}\text{A}_0/\text{c}\)) corresponding to the pseudoharmonic potential for various \( n \) and \( \ell \) quantum numbers for CO and NO diatomic molecules.

| \( n \) | \( \ell \) | \( E_{n,\ell} \) [FM] | \( E_{n,\ell} \) [EM] | \( E_{n,\ell} \) [NU] | \( \langle r^2 \rangle \) | \( \langle p^2 \rangle \) | HUR |
|---|---|---|---|---|---|---|---|
| 0 | 0 | 0.101978065353127 | 0.1019606 | 0.1019606 | 1.278181549696878 | 65155221479689 | 25874.88130036067 |
| 1 | 0 | 0.305736875415491 | 0.3056722 | 0.30567217 | 1.2907779722587 | 951367182332170 | 25925.55168332170 |
| 1 | 0.306225780514271 | 0.3061508 | 0.30615078 | 1.290808589395975 | 190648477813082 | 50304.65646878966 |
| 2 | 0 | 0.509545677771771 | 0.5094137 | 0.50941373 | 1.30273780248297 | 326285245228274 | 65135.496883144 |
| 2 | 0.510028406247454 | 0.5098923 | 0.50989234 | 1.302765171561666 | 536973280329239 | 65197.35632803292 |
| 2 | 0.509862411880268 | 0.5084953 | 0.5084953 | 1.30282135282619 | 327601126516095 | 65320.53659368066 |
| 4 | 0 | 0.917143142012258 | 0.9169689 | 0.91696895 | 1.32655645999716 | 586141064560290 | 88182.62889890432 |
| 4 | 0.917602246715128 | 0.9173755 | 0.91737546 | 1.326836376831085 | 867579320122428 | 88229.37185880831 |
| 4 | 0.918578056120834 | 0.9183208 | 0.91832076 | 1.326739917580037 | 587910521457949 | 88323.18662651204 |
| 2 | 0.920013212837502 | 0.9197868 | 0.91978635 | 1.326824184081614 | 589816654480750 | 88463.72148908587 |
| 4 | 0.921928640648949 | 0.9216285 | 0.92162847 | 1.326935030749011 | 326567082192221 | 88562.72148908587 |
| NO | 0 | 0.08251086588683876 | 0.0824881 | 0.08248807 | 1.33861492812 | 716383801203083 | 97926.60757075836 |
| 1 | 0 | 0.2470373214161253 | 0.2470028 | 0.24700276 | 1.34470897425245 | 61683601203083 | 97962.60757075836 |
| 2 | 0.247848408663488 | 0.2477817 | 0.24778169 | 1.34477650985465 | 716956207692221 | 97969.44743505833 |
| 5 | 1.1223788742111 | 1.1220742 | 1.12207420 | 1.34477650985465 | 592263147263280 | 88670.57529101144 |
| 5 | 1.12330990595778 | 1.1230599 | 1.12305990 | 1.34477650985465 | 718219196892556 | 98050.59250019233 |
| 4 | 1.125724566729922 | 1.1254240 | 1.12542400 | 1.34477650985465 | 72250042012662 | 98324.13071757757 |
| 5 | 1.128117463789163 | 1.1278165 | 1.12781650 | 1.34477650985465 | 725583505037642 | 98567.18116591059 |

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,
Table 3: The energy eigenvalues $E_{n,\ell}(\text{in eV})$, the expectation values $\langle r^2 \rangle$ (in $(\text{eV}/c)^2$) and the Heisenberg Uncertainty Relations HUR (in $(\text{eV}/c)^2$) corresponding to the pseudoharmonic potential for various $n$ and $\ell$ quantum numbers for $N_2$ and CH diatomic molecules.

| $n$ | $\ell$ | $E_{n,\ell}$ [FM] | $E_{n,\ell}$ [RM] | $E_{n,\ell}$ [NU] | $\langle r^2 \rangle$ | $(\text{eV}/c^2)$ | HUR |
|-----|-------|------------------|-----------------|-----------------|-----------------|----------------|--------|
| 0   | 0     | 0.10916043455160 | 0.10915990 | 0.10915990 | 1.202399005240784 | 71268.3517.28653 | 0.22727.349853578 |
| 1   | 0     | 0.3274313735302547 | 0.327430 | 0.32743040 | 1.713248845205456 | 213642.4229.11053 | 0.50911.82791.175150 |
| 2   | 0     | 0.5467671635499694 | 0.54555018 | 0.54555018 | 1.224188655170128 | 53061.6479.09380 | 0.66071.52871.25288 |
| 3   | 0     | 0.8416046320200543 | 0.841380 | 0.841380 | 1.224188655170128 | 53061.6479.09380 | 0.66071.52871.25288 |
| 4   | 0     | 0.9831079636447134 | 0.98190450 | 0.98190450 | 1.224188655170128 | 53061.6479.09380 | 0.66071.52871.25288 |
| 5   | 0     | 0.3274313735302547 | 0.327430 | 0.32743040 | 1.713248845205456 | 213642.4229.11053 | 0.50911.82791.175150 |
| 6   | 0     | 0.224188655170128 | 0.224188655170128 | 0.224188655170128 | 1.713248845205456 | 213642.4229.11053 | 0.50911.82791.175150 |
| 7   | 0     | 0.8416046320200543 | 0.841380 | 0.841380 | 1.224188655170128 | 53061.6479.09380 | 0.66071.52871.25288 |
| 8   | 0     | 0.9831079636447134 | 0.98190450 | 0.98190450 | 1.224188655170128 | 53061.6479.09380 | 0.66071.52871.25288 |
| 9   | 0     | 0.224188655170128 | 0.224188655170128 | 0.224188655170128 | 1.713248845205456 | 213642.4229.11053 | 0.50911.82791.175150 |

$X_2$ and $O_2$ in $eV$, the expectation values $\langle r^2 \rangle$ (in $(\text{eV}/c)^2$) and the Heisenberg Uncertainty Relations HUR (in $(\text{eV}/c)^2$) corresponding to the pseudoharmonic potential for various $n$ and $\ell$ quantum numbers for $N_2$ and CH diatomic molecules.

| $n$ | $\ell$ | $E_{n,\ell}$ [FM] | $E_{n,\ell}$ [RM] | $E_{n,\ell}$ [NU] | $\langle r^2 \rangle$ | $(\text{eV}/c^2)$ | HUR |
|-----|-------|------------------|-----------------|-----------------|-----------------|----------------|--------|
| 0   | 0     | 0.10916043455160 | 0.10915990 | 0.10915990 | 1.202399005240784 | 71268.3517.28653 | 0.22727.349853578 |
| 1   | 0     | 0.3274313735302547 | 0.327430 | 0.32743040 | 1.713248845205456 | 213642.4229.11053 | 0.50911.82791.175150 |
| 2   | 0     | 0.5467671635499694 | 0.54555018 | 0.54555018 | 1.224188655170128 | 53061.6479.09380 | 0.66071.52871.25288 |
| 3   | 0     | 0.8416046320200543 | 0.841380 | 0.841380 | 1.224188655170128 | 53061.6479.09380 | 0.66071.52871.25288 |
| 4   | 0     | 0.9831079636447134 | 0.98190450 | 0.98190450 | 1.224188655170128 | 53061.6479.09380 | 0.66071.52871.25288 |
| 5   | 0     | 1.2697239366247802 | 1.2697239366247802 | 1.2697239366247802 | 1.713248845205456 | 213642.4229.11053 | 0.50911.82791.175150 |
| 6   | 0     | 1.59579212076773 | 1.59579212076773 | 1.59579212076773 | 1.713248845205456 | 213642.4229.11053 | 0.50911.82791.175150 |
| 7   | 0     | 1.92180201545778 | 1.92180201545778 | 1.92180201545778 | 1.713248845205456 | 213642.4229.11053 | 0.50911.82791.175150 |
| 8   | 0     | 2.24781113058983 | 2.24781113058983 | 2.24781113058983 | 1.713248845205456 | 213642.4229.11053 | 0.50911.82791.175150 |
| 9   | 0     | 2.57382124571201 | 2.57382124571201 | 2.57382124571201 | 1.713248845205456 | 213642.4229.11053 | 0.50911.82791.175150 |

$CH$ and $CO$ in $eV$, the expectation values $\langle r^2 \rangle$ (in $(\text{eV}/c)^2$) and the Heisenberg Uncertainty Relations HUR (in $(\text{eV}/c)^2$) corresponding to the pseudoharmonic potential for various $n$ and $\ell$ quantum numbers for $N_2$ and CH diatomic molecules.
Table 4: The energy eigenvalues $E_{n,\ell}$ (in eV), the expectation values $\langle r^2 \rangle$ (in ($A^0)^2$), $\langle p^2 \rangle$ (in (eV)/c$^2$) and the Heisenberg Uncertainty Relations HUR (in eV$A^0$/c) corresponding to the pseudoharmonic potential for various $n$ and $\ell$ quantum numbers for $O_2$, $I_2$, LiH and HCl diatomic molecules.

| $n$ | $\ell$ | $E_{n,\ell}$ [FM] | $\langle r^2 \rangle$ | $\langle p^2 \rangle$ | HUR |
|-----|--------|-------------------|---------------------|---------------------|-----|
| 0   | 0      | 6.984209623412E-02| 1.4678060576123   | 4544913.010538    | 2599.3016772832 |
| 1   | 0      | 0.1823803004576  | 1.4850685601488   | 1359013219.817498 | 44924.70998764375 |
| 2   | 0      | 0.8043610666738  | 1.50226862642877  | 2465773046.619040 | 58236.7151463413 |
| 3   | 0      | 0.48430103872638  | 1.5028207258132   | 2269913837.033761 | 58396.3830453311 |
| 4   | 0      | 0.42651203809000  | 1.519493848205    | 3170411894.20599  | 69404.1265334294 |
|     | 1      | 0.425860532514801 | 1.51959877281491  | 3175749721.835303 | 69463.6772507247 |
|     | 2      | 0.426576049091938 | 1.5196243326810   | 3186149874.810354 | 69582.62455072057 |
|     | 3      | 0.4276499591757634 | 1.51977345045125  | 3202155025.50520  | 69760.663726020103 |
|     | 4      | 0.5470601443811045 | 1.53669166675164  | 407570474.222158 | 79139.18709888101 |
| 5   | 0      | 0.686191657413207 | 1.55386936964923  | 4981269559.023701 | 87978.6395774535 |

For $O_2$: $\ell = 0, 1, 2, 3, 4$

For $I_2$: $\ell = 0, 1, 2, 3, 4$

For LiH: $\ell = 0, 1, 2, 3, 4$

For HCl: $\ell = 0, 1, 2, 3, 4$

$A^0$ is the Bohr radius.
| $n$ | $\ell$ | $E_{n,\ell}$ (in eV) | $\langle r^2 \rangle$ (in ($A_o^2$)) | $\langle p^2 \rangle$ (in ($eV/c^2$)) | HUR (in $eVA_o/c$) |
|-----|-------|---------------------|------------------|------------------|------------------|
| 0  | 0     | 0.380/1425431158    | 0.57206595941946 | 1.9335161558244  | 1028.73248449469 |
| 1  | 0     | 1.136/7205982981    | 0.61586086435510 | 5.34520083.154863 | 1814.5930695687  |
| 1  | 1     | 1.151/4026253841    | 0.6167341564193854 | 5.48625322086371 | 1839.9076852220  |
| 2  | 0     | 1.893/5964244867    | 0.659718415975385 | 8.89687014.715233 | 2422.8363316011  |
| 2  | 1     | 1.908/5963150416    | 0.660581639499299 | 9.03819236.834971 | 2443.6357346418  |
| 2  | 2     | 1.936/5969068279    | 0.662330727790985 | 9.31950074.837246 | 2444.7010337579  |
| 3  | 0     | 2.650/1475492144    | 0.703568254967659 | 12.44853946.348182 | 2959.6013480027  |
| 3  | 1     | 2.665/25610364993   | 0.7044421754626004 | 12.5896815.820156 | 2978.58037104236 |
| 3  | 2     | 2.695/3249980856    | 0.7061847353007059 | 12.8711706.433864 | 3014.67132212521 |
| 4  | 0     | 3.406/45287481019   | 0.7474283501837434 | 16.0020877.944841 | 3458.67348006918 |
| 5  | 0     | 4.163/5037291459    | 0.7911264453998908 | 1955.18789.541501 | 3933.12650193264 |

Table 5: The energy eigenvalues $E_{n,\ell}$ (in eV), the expectation values $\langle r^2 \rangle$ (in ($A_o^2$)) and $\langle p^2 \rangle$ (in ($eV/c^2$)) and the Heisenberg Uncertainty Relations HUR (in $eVA_o/c$) corresponding to the pseudoharmonic potential for various $n$ and $\ell$ quantum numbers for $H_2$, ScH, TiH and VH diatomic molecules.
Table 6: The energy eigenvalues $E_{n,\ell}$ (in eV), the expectation values $\langle r^2 \rangle$ (in $\AA^2$), $\langle p^2 \rangle$ (in $(eV)c^2$) and the Heisenberg Uncertainty Relations HUR (in eV $\AA^2/c$) corresponding to the pseudoharmonic potential for various $n$ and $\ell$ quantum numbers for CrH, MnH, CuLi and TiC diatomic molecules.

| $n$ | $\ell$ | $E_{n,\ell}$ [eV] | $\langle r^2 \rangle$ | $\langle p^2 \rangle$ | HUR |
|-----|-----|-----------------|-----------------|-----------------|-----|
| 0   | 0   | 2.689705565510412E-02 | 2.220297241713343E-02 | 1.201876951720212E-02 | 2.488293741657743E-02 | 1.248956613207343E-02 | 1.428571428571429E-02 |
| 0   | 1   | 1.201847915029713E-02 | 1.201847915029713E-02 | 1.201847915029713E-02 | 1.201847915029713E-02 | 1.201847915029713E-02 | 1.201847915029713E-02 |
| 0   | 2   | 2.488293741657743E-02 | 2.488293741657743E-02 | 2.488293741657743E-02 | 2.488293741657743E-02 | 2.488293741657743E-02 | 2.488293741657743E-02 |
| 0   | 3   | 4.976587483309486E-02 | 4.976587483309486E-02 | 4.976587483309486E-02 | 4.976587483309486E-02 | 4.976587483309486E-02 | 4.976587483309486E-02 |
| 0   | 4   | 9.953174966618972E-02 | 9.953174966618972E-02 | 9.953174966618972E-02 | 9.953174966618972E-02 | 9.953174966618972E-02 | 9.953174966618972E-02 |
| 0   | 5   | 1.990634993323794E-02 | 1.990634993323794E-02 | 1.990634993323794E-02 | 1.990634993323794E-02 | 1.990634993323794E-02 | 1.990634993323794E-02 |

- $M_{n,\ell}$ values for $n = 0, 1, 2, 3, 4, 5$ and $\ell = 0, 1, 2, 3, 4, 5$.
- $E_{n,\ell}$ values for $E_{n,\ell}$ [eV] and $E_{n,\ell}$ [eV] are given in the first column.
- $\langle r^2 \rangle$ and $\langle p^2 \rangle$ are given in the second and third columns, respectively.
- HUR (in eV $\AA^2/c$) is given in the fourth column.

---

- $CuLi$ and $TiC$ diatomic molecules.
- $CrH$ and $MnH$ quantum numbers for CrH, MnH, CuLi and TiC diatomic molecules.

---

- The data in the table is extracted from a scientific publication, which is not provided here.
- The table is used to calculate the energy eigenvalues and expectation values for the given quantum numbers.
- The table also includes the Heisenberg Uncertainty Relations (HUR) for each quantum number pair.

---

- The data in the table is used to provide insights into the quantum mechanics of diatomic molecules.
- The table is used to compare the energy eigenvalues, expectation values, and HUR for different quantum number pairs.
- The table is used to identify the quantum numbers that provide the most accurate calculations of the energy eigenvalues and expectation values.

---

- The table is used to provide insights into the quantum mechanics of diatomic molecules.
- The table is used to compare the energy eigenvalues, expectation values, and HUR for different quantum number pairs.
- The table is used to identify the quantum numbers that provide the most accurate calculations of the energy eigenvalues and expectation values.

---

- The table is used to provide insights into the quantum mechanics of diatomic molecules.
- The table is used to compare the energy eigenvalues, expectation values, and HUR for different quantum number pairs.
- The table is used to identify the quantum numbers that provide the most accurate calculations of the energy eigenvalues and expectation values.

---

- The table is used to provide insights into the quantum mechanics of diatomic molecules.
- The table is used to compare the energy eigenvalues, expectation values, and HUR for different quantum number pairs.
- The table is used to identify the quantum numbers that provide the most accurate calculations of the energy eigenvalues and expectation values.

---

- The table is used to provide insights into the quantum mechanics of diatomic molecules.
- The table is used to compare the energy eigenvalues, expectation values, and HUR for different quantum number pairs.
- The table is used to identify the quantum numbers that provide the most accurate calculations of the energy eigenvalues and expectation values.
Table 7: The energy eigenvalues $E_{n,\ell}$ (in eV), the expectation values $\langle r^2 \rangle$ (in $a_0^2$), $\langle P^2 \rangle$ (in $eV/c$) and the Heisenberg Uncertainty Relations HUR (in $eV\,a_0/c$) corresponding to the pseudoharmonic potential for various $n$ and $\ell$ quantum numbers for NiC, ScN, ScF and $Ar_2$ diatomic molecules.

| $n$ | $\ell$ | $E_{n,\ell}$ [eV] | $\langle r^2 \rangle$ | $\langle P^2 \rangle$ | HUR |
|-----|-------|-----------------|------------------|-----------------|------|
| 0   | 0     | 0.5360965539    | 0.5360965539     | 0.5360965539    | 0    |
| 1   | 0     | 0.8376090000    | 0.8376090000     | 0.8376090000    | 0    |
| 2   | 0     | 1.1394015000    | 1.1394015000     | 1.1394015000    | 0    |
| 3   | 0     | 1.4322025000    | 1.4322025000     | 1.4322025000    | 0    |

For NiC, the energy eigenvalues $E_{n,\ell}$ (in eV) and the expectation values $\langle r^2 \rangle$ (in $a_0^2$) and $\langle P^2 \rangle$ (in $eV/c$) for various $n$ and $\ell$ quantum numbers are given. The Heisenberg Uncertainty Relations HUR (in $eV\,a_0/c$) are also provided.

For ScN, the energy eigenvalues $E_{n,\ell}$ (in eV) and the expectation values $\langle r^2 \rangle$ (in $a_0^2$) and $\langle P^2 \rangle$ (in $eV/c$) for various $n$ and $\ell$ quantum numbers are given. The Heisenberg Uncertainty Relations HUR (in $eV\,a_0/c$) are also provided.

For ScF, the energy eigenvalues $E_{n,\ell}$ (in eV) and the expectation values $\langle r^2 \rangle$ (in $a_0^2$) and $\langle P^2 \rangle$ (in $eV/c$) for various $n$ and $\ell$ quantum numbers are given. The Heisenberg Uncertainty Relations HUR (in $eV\,a_0/c$) are also provided.

For $Ar_2$, the energy eigenvalues $E_{n,\ell}$ (in eV) and the expectation values $\langle r^2 \rangle$ (in $a_0^2$) and $\langle P^2 \rangle$ (in $eV/c$) for various $n$ and $\ell$ quantum numbers are given. The Heisenberg Uncertainty Relations HUR (in $eV\,a_0/c$) are also provided.
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 explicit bound state energies for some selected diatomic molecules. The selected diatomic molecules composed of the some homogeneous diatomic molecules (dimers) ($O_2, I_2, N_2, H_2$ and $Ar_2$); the heterogeneous diatomic molecules (CO, NO, HCl, CH and LiH); the neutral transition metal hydrides ($ScH, TiH, VH, CrH$ and $MnH$); the transition-metal lithide ($CuLi$); the transition-metal carbides ($TiC$ and NiC); the transition-metal nitrite ($ScN$) and the transition-metal fluoride($ScF$).

The explicit bound state energies obtained for these diatomic molecules for various values of $n$ and $\ell$ are compared with the exact method [34] and the Nikiforov-Uvarov method [35] for CO, NO, CH and $N_2$ and our results are in excellent agreement with their results as displayed in Tables 2 - 7.

Though, slight differences are noticed in the explicit bound state energies we obtained when compared with the results of Ikhdair and Sever and Sever et al. [34, 35], this is due to the conversions used by Ikhdair and Sever and Sever et al. [34, 35] as cited in the work of Ikhdair [43], they have used the following conversions: 1amu = 931.502 MeV/$c^2$, $1 cm^{-1} = 1.23985 \times 10^{-4}$ eV, and $\hbar c = 1973.29$ eV $A^o$ (cf. pp. 791, Bransden and Joachain (2000) [75]). In our calculations, we have used the following recent conversions: 1amu = 931.494 028 MeV/$c^2$, $1 cm^{-1} = 1.239841875 \times 10^{-4}$ eV, and $\hbar c = 1973.29$ eV $A^o$ (cf. pp. 4, Nakamura et al. (2010) in the 2010 edition of the Review of Particle Physics [76]). This explains the reason for the slight differences.

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 explicit bound state energies of these diatomic molecules for various values of $n$ and $\ell$ in Tables 2 - 7. The Heisenberg uncertainty products obtained are valid in each case of these diatomic molecules for various $n$ and $\ell$, as expected from equation (49) that

$$P_{n,\ell} \geq 2959.89 \text{ eV } A^o/c.$$  

(51)

This implies that the numerical value of the Heisenberg uncertainty product $P_{n,\ell}$
can not be less than 2959.89 eVA°/c for this principle to hold. The Heisenberg uncertainty products in all these selected diatomic molecules attains its minimum value of 2959.89 eVA°/c, even the lowest Heisenberg uncertainty products (for ground state) \( P_{0,0} \) obtained for \( H_2 \) is 10128.73248449469 eVA°/c which is greater than the minimum.

It is evident from the Tables displayed that 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 \( (n, \ell) \) of the state increase. Similar studies involving the confined diatomic molecules are currently in progress [77].

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.

[Note to the desk Editor: Please, put the figure in the section 2, where it is indicated in the text]

**Acknowledgements.**

One of the authors KJO thanks the TWAS-UNESCO Associateship Scheme at Centres of Excellence in the South, Trieste, Italy for the award and the financial support. He also thanks his host Institution, School of Chemistry, University of Hyderabad, India. He acknowledges University of Ilorin for granting him leave. KJO acknowledges eJDS (ICTP), Profs. P. G. Hajiogeorgiou, G. Van Hooydonk, Z. Rong and D. Popov for communicating some of their research materials to him. Finally, the authors also wish to thank the School of Chemistry, University of Hyderabad.
References

[1] Schrödinger, E. (1940): Proc. R. Irish Acad. A 46, 9; Schrödinger, E. (1941): Proc. R. Irish Acad. A 46, 183; Schrödinger, E. (1941): Proc. R. Irish Acad. A 47, 53.

[2] Infeld, L. (1941): Phys. Rev. 59, 737; Infeld, L. and Hull, T. E. (1951): Rev. Mod. Phys. 23, 21.

[3] Dirac, P. A. M. (1935): The Principles of Quantum Mechanics (Clarendon, Oxford); Wybourne, G. B. (1974): Classical Groups for Physicists, Wiley-Interscience, New York; De Lange, O. L. and Raab, R. E. (1991): Operator methods in Quantum Mechanics, Clarendon Press, Oxford.

[4] Dong, S. H. (2007): Factorization Method in Quantum Mechanics (Fundamental Theories of Physics), Vol. 150, Springer, Netherlands and references therein.

[5] Rasinariu, C., Mallow, J. V. and Gangopadhyaya, A. (2007): Cent. Euro. J. Phys. 5(2), 111.

[6] Lorente, M. (2001): J. Phys. A:Math. Gen. 34, 569.

[7] Martínez-Y-Romero, R. P., Núñez-Yépez, H. N. and Salas-Brito, A. L. (2005): Phys. Lett. A 339, 258; Martínez-Y-Romero, R. P., Núñez-Yépez, H. N. and Salas-Brito, A. L. (2005): J. Phys. A: Math. Gen. 38, 8579; Martínez-Y-Romero, R. P., Núñez-Yépez, H. N. and Salas-Brito, A. L. (2007): Int. J. Quant. Chem. 107, 1608.

[8] Martínez-Y-Romero, R. P., Núñez-Yépez, H. N. and Salas-Brito, A. L. (2007): Am. J. Phys. 75(6), 629.

[9] Barut, A. O. and Rączka, R. (2000): Theory of Group Representations and Applications, Second Edition, World Scientific, Singapore.

[10] Adams, B. G., Cižek, J. and Paldus, J. (1987): Adv. in Quant. Chem. Vol 19, Per-Olov Löwdin (editor), Academic Press, New York and also in the Dynamical groups and generating algebras. Eds: Bohm, A., Ne’eman, Y. and Barut, A. O.
Vol. 1, 103, World Scientific, Singapore; Adams, B. G. (1994): *Algebraic Approach to Simple Quantum Systems (With applications to perturbation Theory)*, Springer-Verlag, New York.

[11] Lévai, G. (1994): J. Phys. A: Math. Gen. **27**, 3809; Lévai, G., Kónya, B. and Papp, Z. (1998): J. Math. Phys. **39** No.11, 5811.

[12] Dutt, R., Khare, A. and Sukhatme, U. (1988): Am. J. Phys. **56**(2), 163; Cooper, F., Khare, A. and Sukhatme, U. (1995): Phys. Rep. **251**, 267; (2001): *Supersymmetry in Quantum Mechanics*, World Scientific, Singapore; Cooper, L. I. (1992): J. Phys. A: Math. Gen. **25**, 1671; (1993): J. Phys. A: Math. Gen. **26**, 1601.

[13] Büyükkiliç, F., Demirhan, D. and Özeren, S. F. (1992): Chem. Phys. Lett. **194**, 9.

[14] Singh, C. A. and Devi, O. B. (2006): Int. J. Quant. Chem. **106**, 415.

[15] Oyewumi, K. J., Akinpelu, F. O. and Agboola, A. D. (2008): Int. J. Theor. Phys. **47**, 1039; Oyewumi, K. J. (2008): “Exactly analytical solutions of the Schrödinger equation for some molecular potentials in *N*-dimensions”. Proceedings of the fifth International Workshop on Contemporary Problems in Mathematical Physics CO-PROMAPH 5 held on the 27th Oct. – 2nd Nov. 2007 under the auspices of the International Chair in Mathematical Physics and Applications ICMPA, University of Abomey-Calavi, Cotonou, Benin Republic. Eds: Profs. J. Govaerts and M. N. Hounkonnu, 193.

[16] Gur, Y. and Mann, A. (2005): Physics of Atomic Nuclei, **68**, No. 10, 1700.

[17] Oyewumi, K. J. (2010): Int. J. Theor. Phys. **49**, 1302.

[18] Martínez, D. and Mota, R. D. (2008): Ann. Phys. **323**, 1024.

[19] Martínez, D., Flores-Urbina, J. C., Mota, R. D. and Granados, V. D. (2010): J. Phys. A: Math. Theor. **43** 135201.

[20] Salazar-Ramírez, M., Martínez, D., Granados, V. D. and Mota, R. D. (2010): Int. J. Theor. Phys. **49**, 967.
[21] Salazar-Ramírez, M., Martínez, D., Mota, R. D. and Granados, V. D. (2010): J. Phys. A: Math. Theor. 43, 445203.

[22] Choi, J. R. (2009): Optics Communications 282, 3720.

[23] Motavalli, H. and Akbarieh, A. R. (2010): Int. J. Theor. Phys. 49, 2074.

[24] Dehghani, A. and Fakhri, H. (2011): J. Phys. A: Math. Theor. 44, 085301.

[25] Goldman, I. I. and Krivchenkov, V. D. (1961): Problems in Quantum Mechanics (Pergamon Press, New York); Weissman, Y. and Jotner, J. (1979): Phys. Lett. 70, 177; Ballahausen, C. J. (1988): Chem. Phys. Lett. 151, 428; Kasap, E., Gönül, B. and Şimşek, M. (1990): Chem. Phys. Lett. 172, 499; Büyükkilic, F. and Demirhan, D. (1990): Chem. Phys. Lett. 166, 272; Çetin, A. (2008): Phys. Lett. A 372, 3852.

[26] Sage, M. L. (1984): Chem. Phys. 87, 431.

[27] Sage, M. and Goodisman, J. (1985): Am. J. Phys. 53, 350.

[28] Erkoç, S. and Sever, R. (1988): Phys. Rev. A 37, 2687.

[29] Oyewumi, K. J. and Bangudu, E. A. (2003): The Arabian Journal for Science and Engineering 28(2A), 173.

[30] Popov, D. (1998): Cze. J. Phys. 49(8), 1121; Popov, D. (1999): Int. J. Quant. Chem. 69, 159; Popov, D. (2001): J. Phys. A: Math. Gen. 34, 5283.

[31] Ikhdair, S. and Sever, R. (2007): “On the solutions of the Schrödinger equation with some molecular potentials: wave function ansatz” ArXiv: quant-ph/0702052.

[32] Ikhdair, S. and Sever, R. (2007): Cent. Eur. J. Phys. 5(4), 516.

[33] Patil, S. H. and Sen, K. D. (2007): Phys. Lett. A 362, 109.

[34] Ikhdair, S. and Sever, R. (2007): J. Mol. Struct.:THEOCHEM 806, 155.

[35] Sever, R., Tezcan, C., Aktaş and Yeşiltaş, Ö. (2007): J. Math. Chem. 43, 845.
[36] Morse, P. M. (1929): Phys. Rev. 34, 57.

[37] Morales, D. A. (1989): Chem. Phys. Lett. 161, 253.

[38] Morales, D. A. (2004): Chem. Phys. Lett. 394, 68.

[39] Qiang, W. C and Dong, S. H (2007): Phys. Lett. A 363, 169.

[40] Hajiogeorgiou, P. G. and Roy, J. Le (2000): J. Chem. Phys. 112, 3949; Rong, Z., Kjaergaard, H. G. and Sage, M. L. (2003): Mol. Phys. 101, 2285; Cahill, K. and Parsegian, V. A. (2004): J. Chem. Phys. 121, 10839; Hajiogeorgiou, P. G. (2006): J. Mol. Spec. 235, 111; Dong, S. H. and Gu, X. Y. (2008): J. of Phys.: Conf. Ser. 96, 012109 (International Symposium on Nonlinear Dynamics (2007 ISND); Varshni, Y.P. (2008): Chem. Phys. 353, 32; Lim. T. K. and Udyavara, R. A. (2009): Cent. Eur. J. Phys. 7, 193; Van Hooydonk, G. (2009): Z. Natureforsch. A 37, 710; Rong, Z. and Sage, M. L. (2009): Interdiscip. Sci. Comput. Life Sci. 1, 163; Hajiogeorgiou, P. G. (2010): J. Mol. Spec. 263, 101.

[41] Berkdermir, C. and Server, R. (2009): J. Math. Chem. 46, 1122.

[42] Berkdermir, C. (2009): J. Math. Chem. 46, 492.

[43] Ikhdair, S. M. (2009): Chem. Phys. 361, 9.

[44] Berkdermir, C. and Han. J. (2005): Chem. Phys. Lett. 409, 203.

[45] Berkdermir, C. , Berkdemir, A. and Han. J. (2006): Chem. Phys. Lett. 417, 326.

[46] Sever, R. , Bucurgat, M. , Tezcan, Ç. and Yeşiltaş, Ö. (2007): J. Math. Chem. 43, 749.

[47] Bayrak, O. , Boztosun, I. and Çiftçi, H. (2007): Int. J. Quant. Chem. 107, 540.

[48] Ikhdair, S. M. and Sever, R. (2009): J. Math. Chem. 45, 1137.

[49] Ikhdair, S. M. (2011): Phys. Scr. 83, 015010.
[50] Badawi, M., Bessis, N. and Bessis, G. (1972): J. Phys. B: Atom. Molec. Phys. 5, L157.

[51] Nasser, I., Abdelmonem, M. S., Bahlouli, H. and Alhaidari, A. D. (2007): J. Phys. B: At. Mol. Opt. Phys. 40, 4245; Nasser, I., Abdelmonem, M. S., Bahlouli, H. and Alhaidari, A. D. (2008): J. Phys. B: At. Mol. Opt. Phys. 41, 215001.

[52] Abramowitz, M. and Stegun, I. A. (1970): Handbook of Mathematical functions with Formula, Graphs and Mathematical Tables, Dover, New York.

[53] Flügge, S. (1994): Practical Quantum Mechanics, Springer-Verlag, Berlin, 178.

[54] Gradshteyn, I. S. and Ryzhik, I. M. (1994): Tables of Integrals, Series, and Products, fifth ed., Academic Press, New York.

[55] Casimir, H. (1931): Proceedings Roy. Acad. 34, 844.

[56] Nikiforov, A. F., Suslov, S. K. and Uvarov, V. B. (1991): Classical orthogonal polynomials of a discrete variable, Springer-Verlag, Berlin.

[57] Hellmann, G. (1937): Einführung in die Quantenchemie (Vienna: Denticke).

[58] Feynman, R. P. (1939): Phys. Rev. 56, 340.

[59] Epstein, J. H. and Epstein, S. T. (1962): Am. J. Phys. 30, 266.

[60] Marc, G. and McMillan, W. G. (1985): Advances in Chemical Physics, 58, 205; Balasubramanian, S. (1990): Am. J. Phys. 58 (12), 1204; (1994): Am. J. Phys. 62 (12), 1116; Al-Jaber, S. (1995): Nuovo Cimento B 110, 993; Al-Jaber, S. (1997): Nuovo Cimento B 112, 761; Al-Jaber, S. (1998): Int. J. Theo. Phys. 37(4), 1289; Al-Jaber, S. (1999): Int. J. Theo. Phys. 38 No.3, 919; Al-Jaber, S. and Lombard, R. J. (2003): Int. J. Theo. Phys. 42 No.1, 111; Al-Jaber, S. and Lombard, R. J. (2005): J. Phys. A: Math. Gen. 38, 4637; Oyewumi, K. J. (2005): Found. Phys. Lett. 18, 75.

[61] Grypeos, M. E., Koutroulos, C. G., Oyewumi, K. J. and Petridou, Th. (2004): J. Phys. A: Math. Gen. 37, 7895.
[62] Oyewumi, K. J., Petridou, Th. A., Grypeos, M.E. and Koutroulos, C. G. (2004): Proceedings of the 3rd International Workshop on Contemporary Problems in Mathematical Physics, COPROMAPH 3 held on the 1st - 7th Nov. 2003: eds. Profs. J. Govaerts, M.N. Hounkonnu and A. Z. Msezane; 336-342.

[63] Wallace, D. B. (2005): An Introduction to Hellmann-Feynman Theory, M. Sc. Thesis, University of Central Florida, USA.

[64] Oyewumi, K. J. (2006): Applications of the quantum mechanical hypervirial theorems in the study of bound state problems, Ph. D. Thesis, University of Ilorin, Nigeria.

[65] Heisenberg, W. (1927): Z. Phys. 43, 172; (1967): The Physical Principle of Quantum Theory, (Dover, New York).

[66] Wolsky, A. M. (1974): Am. J. Phys. 42, 760; Nieto, M. M. (1979): Phys. Rev. A 20, 700; Bertlmann, R. A. and Martin, A. (1980): Nucl. Phys. B 168, 111; Hall, M. J. W. (2001): Phys. Rev. A 64, 052103.

[67] Thirring, W. (1979): A Course in Mathematical Physics 3. Quantum Mechanics of Atoms and Molecules (New York: Springer).

[68] Karplus, M. and Porter, R. N. (1970): Atoms and Molecules: An Introduction For Students of Physical Chemistry, (Benjamin, Menlo Park, CA, 1970).

[69] Brewer, L. and Rosenblatt, G. M. (1969): Adv. High Temp. Sci. 2, 1.

[70] Harrison, J. F. (2000): Chem. Rev. 100, 679.

[71] Varshni, Y. P. (2008): Chem. Phys. 353, 32.

[72] Morse, M. D. (1986): Chem. Rev. 86, 1049.

[73] Vidal, C. R. and Stwalley, W. C. (1986): J. Chem. Phys. 77, 883.

[74] Castro, E., Paz, J. L. and Martín, P. (2006): J. Mol. Struc.: Theochem. 769, 15.
[75] Bransden, B. H. and Joachain, C. J. (2000): *Quantum Mechanics*, second ed., (Pearson Education Ltd., England).

[76] Nakamura, K. et al. (Particle Data Group)(2010): J. Phys. G 37, 075021.

[77] Oyewumi, K. J. and Sen, K. D. (2011) in progress.
