

Research Article

Investigating Some Diatomic Molecules Bounded by the Two-Dimensional Isotropic Oscillator plus Inverse Quadratic Potential in an External Magnetic Field

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We investigate the nonrelativistic magnetic effect on the energy spectra, expectation values of some quantum mechanical observables, and diamagnetic susceptibility for some diatomic molecules bounded by the isotropic oscillator plus inverse quadratic potential. The energy eigenvalues and normalized wave functions are obtained via the parametric Nikiforov-Uvarov method. The expectation values square of the position $\langle r^2 \rangle$, square of the momentum $\langle p^2 \rangle$, kinetic energy $\langle T \rangle$, and potential energy $\langle V \rangle$ are obtained by applying the Hellmann-Feynman theorem, and an expression for the diamagnetic susceptibility X is also derived. Using the spectroscopic data, the low rotational and low vibrational energy spectra, expectation values, and diamagnetic susceptibility X for a set of diatomic molecules (I_2 , H_2 , CO , and HCl) for arbitrary values, Larmor frequencies are calculated. The computed energy spectra, expectation values, and diamagnetic susceptibility X were found to be more influenced by the external magnetic field strength and inverse quadratic potential strength g than the vibrational frequencies and the masses of the selected molecules.

1. Introduction

Several studies in quantum mechanics, solid state physics, condensed matter physics, nuclear physics, chemical physics, molecular physics, and other related areas have proven to an outstanding degree that potential models are very important models for stimulating atomic and molecular interaction since it is capable of predicting and describing some behavior of atoms and molecules. It also provides an insight into the understanding of molecular spectra, vibrations and dynamics [1, 2], spin-orbit interaction, relativistic corrections and diamagnetic susceptibility [3, 4], optical properties [5, 6], interband light absorption and interband optical transitions [7, 8], energy and relativistic effects in weakly bound nuclei [9–11], external magnetic fields and/or Aharonov-Bohm flux fields [12–17], interactions between the magnetic and electric fields [18], thermal and/or thermo-

dynamic properties [19–23], spin and pseudospin symmetries [24], and two-body effects [25–28] among others.

One of the important potential models in this regard is the so-called isotropic oscillator plus inverse quadratic potential (IOPIQP) or anharmonic oscillator potential, which has been explored by some authors in both the relativistic and nonrelativistic domains of quantum mechanics [29–32], [33, 34]. An isotropic oscillator (three-dimensional harmonic oscillator) plus inverse quadratic potential may be defined [29–34] as

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

where g is the potential strength, μ represents the mass of the vibrating molecules, and ω is the angular frequency with which the molecules vibrate in the presence of a magnetic

field. Oyewumi [29] employed the hyperradial equation for the isotropic harmonic oscillator plus inverse quadratic potential and presented the normalized hyperradial and hyperangular solutions, and the solutions depend on the dimension as well as the potential parameters. The hidden symmetries and thermodynamic properties for a harmonic oscillator plus inverse square potential have been exposed by Dong et al. [30], while Arda and Sever reported the exact solutions of Schrödinger for this potential within the framework of the Laplace transform technique [31].

In the same vein, Abdelmadjid [32] also studied the exact nonrelativistic quantum spectrum systems for the isotropic harmonic oscillator plus inverse quadratic potential within the formalisms of both Boopp's shift method and standard perturbation theory in both noncommutativity of the two-dimensional real space and phase (NC-2D: RSP) and presented the exact corrections for the spectrum and the associated noncommutative anisotropic Hamiltonian. Again, due to the unflinching interest, Abdelmadjid [33] looked into the effect of both noncommutativity of the three-dimensional space and phase on the Schrödinger equation with an isotropic harmonic oscillator plus inverse quadratic potential and reported the exact degenerated spectrum associated for noncommutative space and phase.

Furthermore, Dianawati et al. [34] investigated the Schrödinger equation with quantum deformation for a three-dimensional harmonic oscillator plus inverse quadratic potential via the hypergeometric method. The energy spectra which were calculated and visualized by MATLAB R2013a were found to depend on the quantum deformation and quantum number.

It is in the light of the relevance of this potential model that we are motivated to examine the two-dimensional radial Schrödinger equation with the isotropic harmonic oscillator plus inverse quadratic potential in an external magnetic field via the parametric Nikiforov-Uvarov method, obtain the eigensolutions, and discuss the behavior of energy spectra, expectation values of some quantum mechanical observables, and diamagnetic susceptibility for some selected diatomic molecules bounded by this interaction potential model.

The sensitivity of the bounded molecules in an external magnetic field (using arbitrary values of Larmor frequencies), low rotational and vibrational levels, and inverse quadratic potential strength would be adequately investigated. The situation where Larmor frequency $\omega_L = 0$ implies the absence of an external magnetic field, whereas Larmor frequencies $\omega_L > 0$ indicate the presence of an external magnetic field. The case of the low vibrational energy level ($n = 0, 1, 2, 3$), low rotational energy level ($m = 0, +1$), and inverse quadratic potential strengths ($g = 0, 1$) would be examined.

Other methods that can be used to solve the aforementioned bound state problems include the wave function ansatz method [13], asymptotic iteration method [16], formula method [17], Euler-Maclaurin approximation [23], Laplace transform technique [31, 35], and supersymmetric approach [36], among others. In Section 2, we give a review of the parametric Nikiforov-Uvarov method. Section 3 contains nonrelativistic eigensolutions, expectation values of

some quantum mechanical observables, and diamagnetic susceptibility of the isotropic harmonic oscillator plus inverse quadratic potential in an external magnetic field. The results are discussed extensively in Section 4, while the concluding remarks are given in Section 5.

2. Review of the Parametric Nikiforov-Uvarov Method

The parametric Nikiforov-Uvarov method is a straightforward, consistent, and efficient analytical technique for analyzing second-order linear differential equations arising from bound state problems. The choice of this method is due to the fact that it has been proven to an outstanding degree and is well reported to give excellent results in comparison with other methods in the literature [12]. According to Nikiforov and Uvarov [37], the second-order linear differential equation reduces to the generalized equation of hypergeometric type [37, 38]. With an appropriate coordinate transformation $z = z(r)$, the equation takes the form

$$\psi_{nl}''(z) + \frac{\bar{\tau}(z)}{\sigma(z)}\psi_{nl}'(z) + \frac{\bar{\sigma}(z)}{\sigma^2(z)}\psi_{nl}(z) = 0, \quad (2)$$

where $\sigma(z)$ and $\bar{\sigma}(z)$ are polynomials, at most in the second degree, and $\bar{\tau}(z)$ is a first-degree polynomial.

To solve equation (2), one needs to break the wave function $\Psi(z)$ into parts as

$$\psi_{nl}(z) = \phi(z)y(z). \quad (3)$$

Therefore, equation (2) reduces to the hypergeometric-type equation:

$$\sigma(z)y''(z) + \tau(z)y'(z) + \lambda y(z) = 0, \quad (4)$$

where

$$\tau(z) = \bar{\tau}(z) + 2\pi(z), \quad (5)$$

satisfies the condition $\tau'(z) < 0$, has a negative derivative, and is related to the function $\phi(s)$ by

$$\pi(z) = \sigma(z) \frac{d}{dz} [\ln \phi(z)]. \quad (6)$$

The parameter λ is defined by

$$\lambda = \lambda_n = -n\tau'(z) - \left[\frac{n(n-1)}{2} \sigma'' \right] \quad (n = 0, 1, 2, \dots). \quad (7)$$

The energy eigenvalues can be calculated from equation (7). In order to calculate the energy eigenvalues, we need first to determine λ by using the first derivative of $\pi(z)$ and defining

$$\lambda = k + \pi'(z). \quad (8)$$

By solving the resulting quadratic equation for $\pi(z)$, we obtain the following expression:

$$\pi(z) = \left(\frac{\sigma' - \bar{\tau}}{2} \right) \pm \sqrt{\left(\frac{\sigma' - \bar{\tau}}{2} \right)^2 - \bar{\sigma} + k\sigma}. \quad (9)$$

Here, $\pi(z)$ is a polynomial with the parameter z and the prime denotes the first derivative of the functions $\sigma(z)$ and $\tau(z)$, respectively. The determination of k is the essential point in the calculation of $\pi(z)$. It can be obtained by setting the discriminant of the square root to zero [37]; therefore, a general quadratic expression for k can be obtained. On substitution of the values of k , $\pi'(z)$, $\tau'(z)$, and σ'' into equations (7) and (8) and equating (7) and (8), one can evaluate the energy equation for any potential. The wave function $\phi(s)$ in equation (2) satisfies the condition

$$\frac{\phi'(z)}{\phi(z)} = \frac{\pi(z)}{\sigma(z)}, \quad (10)$$

which can be evaluated using the Rodrigues relation. The polynomial solutions $y_n(z)$ are given by

$$y_n(z) = \frac{C_n}{\rho(z)} \frac{d^n}{dz^n} [\sigma^n(z)\rho(z)], \quad (11)$$

where C_n is a normalization constant and the weight function $\rho(z)$ satisfies the following relation:

$$\frac{d}{ds} [\sigma(z)\rho(z)] = \tau(z)\rho(z). \quad (12)$$

A more generalized form of equation (2) for any potential may be presented as [39]

$$\psi_{nl}''(z) + \left[\frac{\beta_1 - \beta_2 z}{z(1 - \beta_3 z)} \right] \psi_{nl}'(z) + \left[\frac{-\rho_2 z^2 + \rho_1 z - \rho_0}{z^2(1 - \beta_3)^2} \right] \psi_{nl}(z) = 0, \quad (13)$$

which satisfies the wave functions of equation (3). By comparing equation (2) with equation (13), we have the following polynomials:

$$\begin{aligned} \bar{\tau}(z) &= \beta_1 - \beta_2 z, \\ \sigma(z) &= z(1 - \beta_3 z), \\ \bar{\sigma}(z) &= -\rho_2 z^2 + \rho_1 z - \rho_0. \end{aligned} \quad (14)$$

Substituting equation (13) into equation (9), one obtains

$$\pi(z) = \beta_4 + \beta_5 z \pm \sqrt{(\beta_6 - k\beta_3)z^2 + (\beta_7 + k)z + \beta_8}, \quad (15)$$

with the following parametric constants:

$$\begin{aligned} \beta_4 &= \frac{1}{2}(1 - \beta_1), \\ \beta_5 &= \frac{1}{2}(\beta_2 - 2\beta_3), \\ \beta_6 &= \beta_5^2 + \rho_2, \\ \beta_7 &= 2\beta_4\beta_5 - \rho_1, \\ \beta_8 &= \beta_4^2 + \rho_0. \end{aligned} \quad (16)$$

According to the Nikiforov-Uvarov method, the discriminant of equation (15) must be set to zero so that the expression for k can be quadratically obtained as

$$k_{\pm} = -(\beta_7 + 2\beta_3\beta_8) \pm 2\sqrt{\beta_8\beta_9}, \quad \beta_9 = \beta_3(\beta_7 + \beta_3\beta_8) + \beta_6. \quad (17)$$

Since the negative value of k (that is k_-) gives the bound state solution, we consider

$$k_- = -(\beta_7 + 2\beta_3\beta_8) - 2\sqrt{\beta_8\beta_9}. \quad (18)$$

Inserting equation (18) into (15), we have

$$\pi(z) = \beta_4 + \beta_5 z - \left[\left(\sqrt{\beta_9} + \beta_3\sqrt{\beta_8} \right) z - \sqrt{\beta_8} \right], \quad (19)$$

having its first derivative as

$$\pi'(z) = \beta_5 - \left(\sqrt{\beta_9} + \beta_3\sqrt{\beta_8} \right). \quad (20)$$

Putting equations (14) and (15) into equation (5), one obtains

$$\tau(z) = \beta_1 + 2\beta_4 + (2\beta_5 - \beta_2)z - 2 \left[\left(\sqrt{\beta_9} + \beta_3\sqrt{\beta_8} \right) z - \sqrt{\beta_8} \right], \quad (21)$$

and its first derivative becomes

$$\tau'(z) = -(\beta_2 - 2\beta_5) - 2 \left[\left(\sqrt{\beta_9} + \beta_3\sqrt{\beta_8} \right) \right]. \quad (22)$$

By applying equation (16) to equation (22), we have

$$\tau'(z) = -2\beta_3 - 2 \left[\left(\sqrt{\beta_9} + \beta_3\sqrt{\beta_8} \right) \right] < 0. \quad (23)$$

By applying equations (18) and (20) in equation (8), we have

$$\lambda = -(\beta_7 + 2\beta_3\beta_8) - 2\sqrt{\beta_8\beta_9} + \beta_5 - \left(\sqrt{\beta_9} + \beta_3\sqrt{\beta_8}\right). \quad (24)$$

With equations (14) and (22), the parameter λ_n in equation (7) becomes

$$\lambda_n = \beta_2 n - 2n\beta_5 + 2n\left(\sqrt{\beta_9} + \beta_3\sqrt{\beta_8}\right) + n(n-1)\beta_3 \quad (n=0, 1, 2, \dots). \quad (25)$$

Equating equations (24) and (25), one obtains the bound state energy equation for any potential [37–40] as

$$\begin{aligned} &\beta_2 n - (2n+1)\beta_5 + (2n+1)\left(\sqrt{\beta_9} + \beta_3\sqrt{\beta_8}\right) \\ &+ n(n-1)\beta_3 + \beta_7 + 2\beta_3\beta_8 + 2\sqrt{\beta_8\beta_9} = 0. \end{aligned} \quad (26)$$

Using equations (10)–(12), the wave function parameters can be evaluated as

$$\begin{aligned} \rho(z) &= z^{\beta_{10}}(1 - \beta_3 z)^{\beta_{11}}, \\ \varphi(z) &= z^{\beta_{12}}(1 - \beta_3 z)^{\beta_{13}}, \quad \beta_{12} > 0, \beta_{13} > 0, \\ \gamma_{nl}(z) &= P_{nl}^{(\beta_{10}, \beta_{11})}(1 - 2\beta_3 z), \quad \beta_{10} > -1, \beta_{11} > -1, \end{aligned} \quad (27)$$

in such a way that the associated wave function in equation (3) becomes

$$\psi_{nl}(z) = N_{nl} z^{\beta_{12}} (1 - \beta_3 z)^{\beta_{13}} P_{nl}^{(\beta_{10}, \beta_{11})}(1 - 2\beta_3 z), \quad (28)$$

where $P_{nl}^{(\mu, \nu)}(x)$, $\mu > -1$, $\nu > -1$, and $x \in [-1, 1]$, are Jacobi polynomials with the following parametric constants:

$$\begin{aligned} \beta_{10} &= \beta_1 + 2\beta_4 + 2\sqrt{\beta_8} - 1 > -1, \\ \beta_{11} &= \beta_2 - 2\beta_5 + 2\left(\sqrt{\beta_9} + \beta_3\sqrt{\beta_8}\right) > -1, \beta_3 \neq 0, \\ \beta_{12} &= \beta_4 + \sqrt{\beta_8} > 0, \\ \beta_{13} &= \beta_5 - \left(\sqrt{\beta_9} - \beta_3\sqrt{\beta_8}\right), \beta_3 \neq 0. \end{aligned} \quad (29)$$

By considering a special case where $\beta_3 = 0$, then the associated wave function reduces to the form [39, 40]

$$\begin{aligned} \lim_{\beta_3 \rightarrow 0} P_{nl}^{(\beta_{10}, \beta_{11})}(1 - 2\beta_3 z) &= L_{nl}^{\beta_{10}}(\beta_{11} z), \\ \lim_{\beta_3 \rightarrow 0} (1 - \beta_3 z)^{\beta_{13}} &= e^{\beta_{13} z}, \end{aligned} \quad (30)$$

$$\psi_{nl}(z) = N_{nl} z^{\beta_{12}} e^{\beta_{13} z} L_{nl}^{\beta_{10}}(\beta_{11} z),$$

where $L_{nl}^{\beta_{10}}(z)$ is well known as a Laguerre polynomial.

3. Nonrelativistic Eigensolutions of the Isotropic Oscillator plus Inverse Quadratic Potential in an External Magnetic Field

For a charged particle moving in a uniform magnetic field, the Hamiltonian of the system may be defined ([16] and the references therein) as

$$H = \frac{1}{2\mu} \left(p + \frac{e}{c}A\right)^2 + V(r), \quad (31)$$

where m is the mass of the charged particle, e is the electronic charge, p is the momentum of the charged particle, $A = (1/2)B \times r$ is the vector potential in the symmetric gauge, c is the velocity of light, and $V(r)$ is the cylindrical potential representing the potential in equation (1). The Hamiltonian for this system can be evaluated, in the CGS system and in atomic units $\hbar = e = 1$, as

$$H = \frac{1}{2\mu} \left(-i\nabla + \frac{1}{2}B \times r\right)^2 + V(r), \quad (32)$$

and the Schrödinger equation yields

$$H\varphi = \frac{1}{2\mu} \left(-i\nabla + \frac{1}{2}B \times r\right)^2 \varphi + V(r)\varphi = i\partial_t \varphi = E\varphi. \quad (33)$$

Since this problem involves two dimensions, therefore, it is sufficient enough to study in polar coordinates (r, ϕ) within the plane and to employ the following ansatz for the eigenfunction:

$$\varphi(r, \phi) = \frac{e^{im\phi}}{\sqrt{2\pi}} \frac{R(r)}{\sqrt{r}}, \quad m = 0, \pm 1, \pm 2, \dots \quad (34)$$

Consequently, the radial wave function $R(r)$ must satisfy the following radial Schrödinger equation [16, 17]:

$$\frac{d^2 R(r)}{dr^2} + 2[E - V_{\text{eff}}(r)]R(r) = 0, \quad (35)$$

with the effective potential $V_{\text{eff}}(r)$ defined as

$$V_{\text{eff}}(r) = m\omega_L + \frac{1}{2}\omega_L^2 r^2 + \frac{m^2 - (1/4)}{2r^2} + V(r), \quad (36)$$

where $\omega_L = B/2c$, m , and E symbolize the Larmor frequency, the eigenvalue of the angular momentum, and the energy spectra of the vibrating molecules, respectively. By using the $V(r)$ as the isotropic oscillator plus inverse quadratic potential (IOPIQP), the effective potential influenced by an external magnetic field becomes

$$V_{\text{eff}}(r) = m\omega_L + \frac{((m^2 - (1/4))/2) + g}{r^2} + \frac{1}{2}[\omega_L^2 + \mu\omega^2]r^2, \quad (37)$$

where μ and ω represent the mass and angular frequency of the vibrating molecules bounded by the IOPIQP, and the molecular constants for the selected diatomic molecules in this study are displayed in Table 1. Inserting equation (37) into equation (35) and applying a variable $z = r^2$, equation (35) can be transformed as

$$R''(z) + \left(\frac{1}{2z}\right)R'(z) + \left(\frac{-\rho_1 z^2 + \rho_2 z - \rho_3}{z^2}\right)R(z) = 0. \quad (38)$$

Comparing equation (38) with equation (13), we obtain the following analytical expressions:

$$\begin{aligned} \beta_1 &= \frac{1}{2}, \\ \beta_2 &= \beta_3 = 0, \\ \rho_1 &= \frac{\omega_L^2 + \mu\omega^2}{4}, \\ \rho_2 &= \frac{E - m\omega_L}{2}, \\ \rho_3 &= \frac{m^2 + 2g - (1/4)}{4}. \end{aligned} \quad (39)$$

Using equations (16) and (29), other values of parametric constants $\beta_i (i = 4, 5, 6, \dots)$ and their analytical values required for the derivation of energy eigenvalues and eigenfunctions are obtained and displayed in Table 2.

Using the analytical values in Table 2 for the parametric constants $\beta_i (i = 1, 2, 3, \dots)$ in equations (26) and (30), the energy eigenvalues and the normalized radial eigenfunctions for the IOPIQP in the presence of an external magnetic field are obtained, respectively, as

$$E = m\omega_L + \sqrt{\omega_L^2 + \mu\omega^2} \left(2n + 1 + \sqrt{m^2 + 2g}\right), \quad (40)$$

$$R(r) = \left[\frac{2n! \gamma^{2\delta+2}}{(n + 2\delta + 1)!} \right]^{1/2} r^{2\delta+3/2} e^{-(1/2)\gamma r^2} L_n^{2\delta+1}(\gamma r^2), \quad (41)$$

where $\delta = -(1/2) + \sqrt{(m^2/4) + (g/2)}$, $\gamma = \sqrt{\omega_L^2 + \mu\omega^2}$, and $L_n^{2\delta+1}(\gamma r^2)$ is the associated Laguerre polynomial.

3.1. Expectation Values (r^{-2} , p^2 , T , and V) of the Isotropic Oscillator plus Inverse Quadratic Potential in an External Magnetic Field. The Hellmann-Feynman theorem (HFT) is one of the useful techniques for obtaining expectation values of some quantum mechanical observables for any arbitrary values of quantum numbers [41, 42]. Suppose that the Hamiltonian $H(\alpha)$ for a particular quantum mechanical system depends on parameter α such that $E_{nl}(\alpha)$ and $\psi_{nm}(\alpha)$ are the eigenvalues and the eigenfunctions, respectively. Therefore, the Hellmann-Feynman theorem (HFT) states that

$$\frac{\partial E_{nm}(\alpha)}{\partial \alpha} = \left\langle \psi_{nm}(\alpha) \left| \frac{\partial H(\alpha)}{\partial \alpha} \right| \psi_{nm}(\alpha) \right\rangle, \quad (42)$$

TABLE 1: Molecular parameters for this study [21].

Molecules	Vibrational frequencies $\omega \times 10^{13} \text{ s}^{-1}$	Mass μ in a.m.u.
CO	6.471	6.8606719
HCl	8.814	0.9801045
I ₂	0.642	63.45223502
H ₂	12.960	0.50391

TABLE 2: The values of parametric constants required for the derivation of energy eigenvalues and eigenfunctions.

Parametric constants	Analytical values
β_4	$\frac{1}{4}$
β_5	0
β_6	$\frac{\omega_L^2 + \mu\omega^2}{4}$
β_7	$\frac{m\omega_L - E}{2}$
β_8	$\frac{m^2 + 2g}{4}$
β_9	$\frac{\omega_L^2 + \mu\omega^2}{4}$
β_{10}	$\sqrt{m^2 + 2g} > -1$
β_{11}	$\sqrt{\omega_L^2 + \mu\omega^2}$
β_{12}	$\frac{1 + 2\sqrt{m^2 + 2g}}{4} > 0$
β_{13}	$-\sqrt{\frac{\omega_L^2 + \mu\omega^2}{4}}$

provided that the normalized eigenfunctions $\psi_{nm}(\alpha)$ are continuous, differentiable with respect to parameter α . The effective Hamiltonian of the isotropic oscillator plus inverse quadratic potential in an external magnetic field is given as

$$H = -\frac{1}{2} \frac{d^2}{dr^2} + m\omega_L + \frac{((m^2 - (1/4))/2) + g}{r^2} + \frac{1}{2} [\omega_L^2 + \mu\omega^2] r^2. \quad (43)$$

To find the expectation value of r^2 , we let $\alpha = \omega$ such that equation (42) becomes

$$\frac{\partial E_{nm}(\omega)}{\partial \omega} = \left\langle \psi_n(\omega) \left| \frac{\partial H(\omega)}{\partial \omega} \right| \psi_n(\omega) \right\rangle. \quad (44)$$

Taking the first derivative of the effective Hamiltonian $H(\omega)$ in equation (43) with respect to vibrational frequency ω , one obtains

$$\frac{\partial H(\omega)}{\partial \omega} = \mu\omega \langle r^2 \rangle. \quad (45)$$

TABLE 3: Energy spectra for CO molecules bounded by the isotropic oscillator plus inverse quadratic potential for arbitrary Larmor frequencies ω_L .

n	$m = 0, \omega_L = 0$	$m = 1, \omega_L = 0$	$m = 0, \omega_L = 5$	$m = 1, \omega_L = 5$	$m = 0, \omega_L = 10$	$m = 1, \omega_L = 10$
$g = 0$						
0	6.90572	13.8114	8.52578	22.0516	12.1527	34.3055
1	20.7172	27.6229	25.5773	39.1031	36.4582	58.6109
2	34.5286	41.4343	42.6289	56.1547	60.7637	82.9164
3	48.3488	55.2457	59.6805	73.2062	85.0691	107.222
$g = 1$						
0	16.6719	18.8668	20.5831	28.2929	29.3393	43.2019
1	30.4833	32.6782	37.6346	45.3444	53.6448	67.5074
2	44.2947	46.4896	54.6862	62.3960	77.9502	91.8128
3	58.1062	60.3011	71.7377	79.4475	102.256	116.118

TABLE 4: Energy spectra for HCl molecules bounded by the isotropic oscillator plus inverse quadratic potential for arbitrary Larmor frequencies ω_L .

n	$m = 0, \omega_L = 0$	$m = 1, \omega_L = 0$	$m = 0, \omega_L = 5$	$m = 1, \omega_L = 5$	$m = 0, \omega_L = 10$	$m = 1, \omega_L = 10$
$g = 0$						
0	3.55519	7.11039	6.1351	17.2702	10.6132	31.2263
1	10.6656	14.2208	18.4053	29.5404	31.8395	52.4527
2	17.7760	21.3312	30.6755	41.8106	53.0659	73.6790
3	24.8864	28.4416	42.9457	54.0808	74.2922	94.9054
$g = 1$						
0	8.5830	9.71297	14.8114	21.7614	25.6225	38.9957
1	15.6934	16.8234	27.0816	34.0316	46.8488	60.2221
2	22.8038	23.9337	39.3518	46.3018	68.0751	81.4484
3	29.9142	31.0441	51.6220	58.5720	89.3015	102.675

Taking the first derivative of the energy eigenvalues $E(\omega)$ in equation (40) with respect to vibrational frequency ω , we have

$$\frac{\partial E_{nm}(\omega)}{\partial \omega} = \frac{\mu\omega(2n+1+\sqrt{m^2+2g})}{\sqrt{\omega_L^2+\mu\omega^2}}. \quad (46)$$

With equations (45) and (46) in equation (44), it is easy for

one to evaluate $\langle r^2 \rangle$ as

$$\langle r^2 \rangle = \frac{(2n+1+\sqrt{m^2+2g})}{\sqrt{\omega_L^2+\mu\omega^2}}. \quad (47)$$

In principle and with $\alpha = \mu$ in equation (44), the expectation values of p^2 , T , and V can be obtained, respectively, as

$$\begin{aligned} \langle p^2 \rangle &= -\frac{\mu^2\omega^2(2n+1+\sqrt{m^2+2g})}{\sqrt{\omega_L^2+\mu\omega^2}}, \\ \langle T \rangle &= -\frac{\mu\omega^2(2n+1+\sqrt{m^2+2g})}{2\sqrt{\omega_L^2+\mu\omega^2}}, \\ \langle V \rangle &= \left[m\omega_L + \sqrt{\omega_L^2+\mu\omega^2}(2n+1+\sqrt{m^2+2g}) + \frac{(\mu\omega^2/2)(2n+1+\sqrt{m^2+2g})}{\sqrt{\omega_L^2+\mu\omega^2}} \right]. \end{aligned} \quad (48)$$

TABLE 5: Energy spectra for I_2 molecules bounded by the isotropic oscillator plus inverse quadratic potential for arbitrary Larmor frequencies ω_L .

n	$m = 0, \omega_L = 0$	$m = 1, \omega_L = 0$	$m = 0, \omega_L = 5$	$m = 1, \omega_L = 5$	$m = 0, \omega_L = 10$	$m = 1, \omega_L = 10$
$g = 0$						
0	2.08359	4.16718	5.41677	15.8335	10.2148	30.4295
1	6.25077	8.33437	16.2503	26.6671	30.6443	50.859
2	10.4180	12.5015	27.0838	37.5006	51.0738	71.2886
3	14.5851	16.6687	37.9174	48.3341	71.5033	91.7181
$g = 1$						
0	5.03023	5.69248	13.0772	19.7989	24.6606	37.9072
1	9.19742	9.85966	23.9108	30.6324	45.0901	58.3368
2	13.3646	14.0268	34.7443	41.4659	65.5197	78.7663
3	17.5318	18.1940	45.5778	52.2995	85.9492	99.1958

TABLE 6: Energy spectra for H_2 molecules bounded by the isotropic oscillator plus inverse quadratic potential for arbitrary Larmor frequencies ω_L .

n	$m = 0, \omega_L = 0$	$m = 1, \omega_L = 0$	$m = 0, \omega_L = 5$	$m = 1, \omega_L = 5$	$m = 0, \omega_L = 10$	$m = 1, \omega_L = 10$
$g = 0$						
0	3.74831	7.49662	6.24899	17.4980	10.6794	31.3588
1	11.2449	14.9932	18.7470	29.9959	32.0382	52.7176
2	18.7416	22.4899	31.2449	42.4939	53.3971	74.0765
3	26.2382	29.9865	43.7429	54.9919	74.7559	95.4353
$g = 1$						
0	9.04922	10.2406	15.0864	22.0725	25.7824	39.1767
1	16.5458	17.7372	27.5844	34.5705	47.1412	60.5355
2	24.0425	25.2338	40.0823	47.0685	68.5000	81.8943
3	31.5391	32.7304	52.5803	59.5665	89.8588	103.253

TABLE 7: Expectation values $\langle r^2 \rangle$ for CO, HCl, I_2 , and H_2 molecules bounded by the isotropic oscillator plus inverse quadratic potential for arbitrary Larmor frequencies ω_L with $g = m = 1$.

n	CO			HCl		
	$\omega_L = 0$	$\omega_L = 5$	$\omega_L = 10$	$\omega_L = 0$	$\omega_L = 5$	$\omega_L = 10$
0	0.395622	0.320446	0.224810	0.768467	0.445315	0.257421
1	0.685237	0.555028	0.389382	1.331020	0.771308	0.445866
2	0.974852	0.789611	0.553954	1.893580	1.097300	0.634311
3	1.264470	1.024190	0.718526	2.456140	1.423290	0.822756
I_2						
0	1.31122	0.504369	0.267461	0.728875	0.437199	0.255824
1	2.27110	0.873593	0.463256	1.262450	0.757251	0.443100
2	3.23098	1.242820	0.659051	1.796020	1.077300	0.630377
3	4.19087	1.612040	0.854846	2.329600	1.397350	0.817653

3.2. *Diamagnetic Susceptibility of the Isotropic Oscillator plus Inverse Quadratic Potential in an External Magnetic Field.* The diamagnetic susceptibility is given [3, 21] as

$$X = -\frac{Nze^2}{6\mu c^2} \langle r^2 \rangle, \quad (49)$$

where N is the Avogadro number, z is the atomic number, e is the electronic charge, c is the speed of light, and μ is the effective mass of the vibrating molecules in this study. It has been found that diamagnetism is a fundamental magnetic phenomenon that explains the tendency of electric charges to partially shield the interior of a body from an

TABLE 8: Expectation values $\langle \bar{p}^2 \rangle$ for CO, HCl, I₂, and H₂ molecules bounded by the isotropic oscillator plus inverse quadratic potential for arbitrary Larmor frequencies ω_L with $g = m = 1$.

n	CO			HCl		
	$\omega_L = 0$	$\omega_L = 5$	$\omega_L = 10$	$\omega_L = 0$	$\omega_L = 5$	$\omega_L = 10$
0	-2.14868e-25	-1.74039e-25	-1.22098e-25	-1.58027e-26	-9.15745e-27	-5.29359e-27
1	-3.72163e-25	-3.01445e-25	-2.11479e-25	-2.73712e-26	-1.58612e-26	-9.16877e-27
2	-5.29457e-25	-4.28850e-25	-3.00861e-25	-3.89396e-26	-2.25649e-26	-1.30440e-26
3	-6.86752e-25	-5.56256e-25	-3.90242e-25	-5.0508e-26	-2.92686e-26	-1.69191e-26
	I ₂			H ₂		
0	-5.99593e-25	-2.30637e-25	-1.22304e-25	-8.56614e-27	-5.13820e-27	-3.00659e-27
1	-1.03852e-24	-3.99475e-25	-2.11837e-25	-1.48370e-26	-8.89963e-27	-5.20756e-27
2	-1.47746e-24	-5.68313e-25	-3.01369e-25	-2.11078e-26	-1.26611e-26	-7.40853e-27
3	-1.91639e-24	-7.37151e-25	-3.90902e-25	-2.73787e-26	-1.64225e-26	-9.60951e-27

TABLE 9: Expectation values $\langle \bar{T} \rangle$ for CO, HCl, I₂, and H₂ molecules bounded by the isotropic oscillator plus inverse quadratic potential for arbitrary Larmor frequencies ω_L with $g = m = 1$.

n	CO			HCl		
	$\omega_L = 0$	$\omega_L = 5$	$\omega_L = 10$	$\omega_L = 0$	$\omega_L = 5$	$\omega_L = 10$
0	-9.43338	-7.64086	-5.36046	-4.85649	-2.81426	-1.62682
1	-16.3391	-13.2344	-9.28460	-8.41168	-4.87444	-2.81774
2	-23.2448	-18.8279	-13.2087	-11.9669	-6.93462	-4.00866
3	-30.1505	-24.4214	-17.1329	-15.5221	-8.99480	-5.19957
	I ₂			H ₂		
0	-2.84624	-1.09482	-0.580571	-5.12029	-3.07129	-1.79714
1	-4.92983	-1.89629	-1.00558	-8.86860	-5.31962	-3.11274
2	-7.01342	-2.69775	-1.43059	-12.6169	-7.56796	-4.42834
3	-9.09701	-3.49922	-1.85559	-16.3652	-9.81600	-5.74390

TABLE 10: Expectation values $\langle \bar{V} \rangle$ for CO, HCl, I₂, and H₂ molecules bounded by the isotropic oscillator plus inverse quadratic potential for arbitrary Larmor frequencies ω_L with $g = m = 1$.

n	CO			HCl		
	$\omega_L = 0$	$\omega_L = 5$	$\omega_L = 10$	$\omega_L = 0$	$\omega_L = 5$	$\omega_L = 10$
0	28.3002	35.9337	48.5623	14.5695	24.5757	40.6225
1	49.0173	58.5788	76.7919	25.2350	38.9060	63.0398
2	69.7345	81.2238	105.022	35.9006	53.2364	85.4571
3	90.4516	103.869	133.251	46.5662	67.5668	107.874
	I ₂			H ₂		
0	8.53872	20.8937	38.4878	15.3609	25.1438	40.9738
1	14.7895	32.5287	59.3423	26.6058	39.8901	63.6483
2	21.0403	44.1637	80.1969	37.8507	54.6365	86.3227
3	27.2910	55.7987	101.051	49.0957	69.3828	108.997

TABLE 11: Diamagnetic susceptibilities X for CO, HCl, I_2 , and H_2 molecules bounded by the isotropic oscillator plus inverse quadratic potential for arbitrary Larmor frequencies ω_L with $g = m = z = e = 1$.

n	CO			HCl		
	$\omega_L = 0$	$\omega_L = 5$	$\omega_L = 10$	$\omega_L = 0$	$\omega_L = 5$	$\omega_L = 10$
0	-3.87265e+31	-3.13677e+31	-2.20061e+31	-5.26560e+32	-3.05133e+32	-1.76387e+32
1	-6.70762e+31	-5.43304e+31	-3.81157e+31	-9.12028e+32	-5.28506e+32	-3.05511e+32
2	-9.54260e+31	-7.72932e+31	-5.42252e+31	-1.29750e+33	-7.51880e+32	-4.34635e+32
3	-1.23776e+32	-1.00256e+32	-7.03348e+31	-1.68297e+33	-9.75253e+32	-5.63759e+32
n	I_2			H_2		
	$\omega_L = 0$	$\omega_L = 5$	$\omega_L = 10$	$\omega_L = 0$	$\omega_L = 5$	$\omega_L = 10$
0	-1.38779e+31	-5.33822e+30	-2.83079e+30	-9.71393e+32	-5.82668e+32	-3.40944e+32
1	-2.40372e+31	-9.24607e+30	-4.90308e+30	-1.68250e+33	-1.00921e+33	-5.90532e+32
2	-3.41966e+31	-1.31539e+31	-6.97536e+30	-2.39361e+33	-1.43575e+33	-8.40121e+32
3	-4.43559e+31	-1.70618e+31	-9.04765e+30	-3.10472e+33	-1.86229e+33	-1.08971e+33

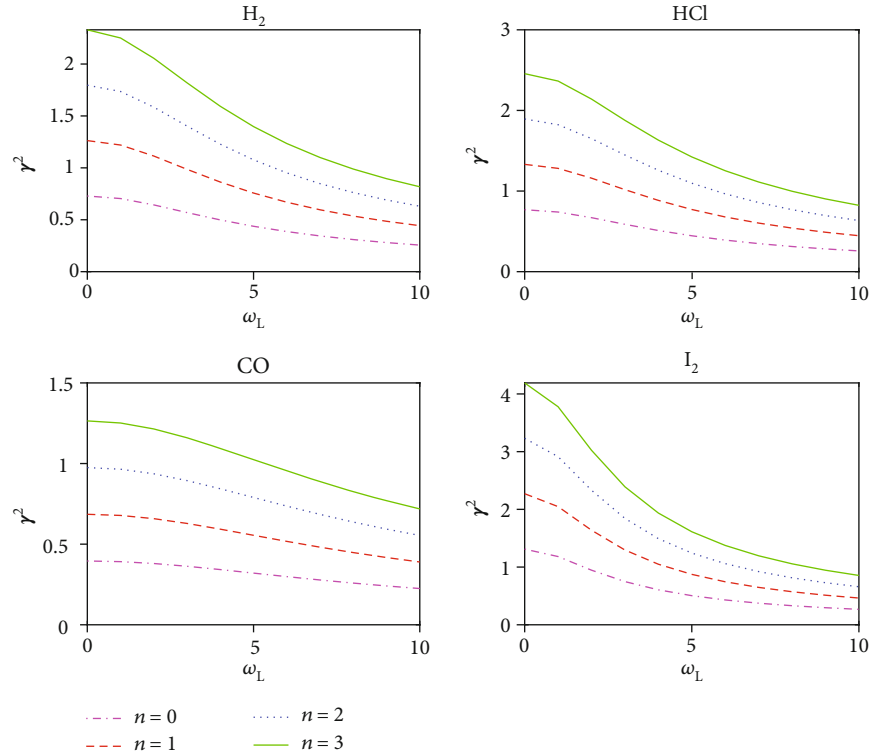


FIGURE 1: The expectation value of the square of the position r^2 as a function of Larmor frequencies ω_L for various numbers of states n with $g = m = 1$.

external magnetic field and that diamagnetic materials possess magnetic effects due to an external field that alters electron motion within the atoms [21]. Using equation (47) in (49) defines the diamagnetic susceptibility for the isotropic oscillator plus inverse quadratic potential in an external magnetic field as

$$\chi = -\frac{Nze^2}{6\mu c^2} \left[\frac{(2n+1 + \sqrt{m^2 + 2g})}{\sqrt{\omega_L^2 + \mu\omega^2}} \right], \quad (50)$$

where all the symbols have been explained accordingly. The corresponding magnetic moment μ_B can be expressed as

$$\mu_B = -\frac{e^2}{6\mu c^2} \langle r^2 \rangle B = -\frac{2e^2\omega_L}{6\mu c} \left[\frac{(2n+1 + \sqrt{m^2 + 2g})}{\sqrt{\omega_L^2 + \mu\omega^2}} \right]. \quad (51)$$

4. Results and Discussions

In order to verify the reliability, validity, and consistency of our results, using the molecular constants in Table 1 [21],

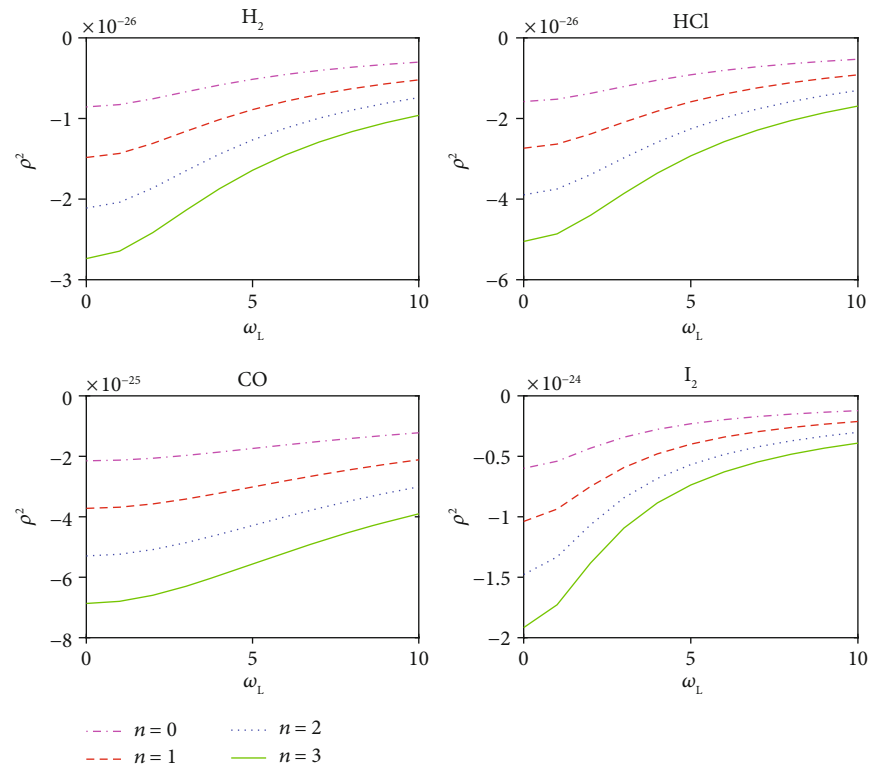


FIGURE 2: The expectation value of the square of the momentum p^2 as a function of Larmor frequencies ω_L for the molecules (H_2 , HCl, CO, and I_2) and for various numbers of states n with $g = m = 1$.

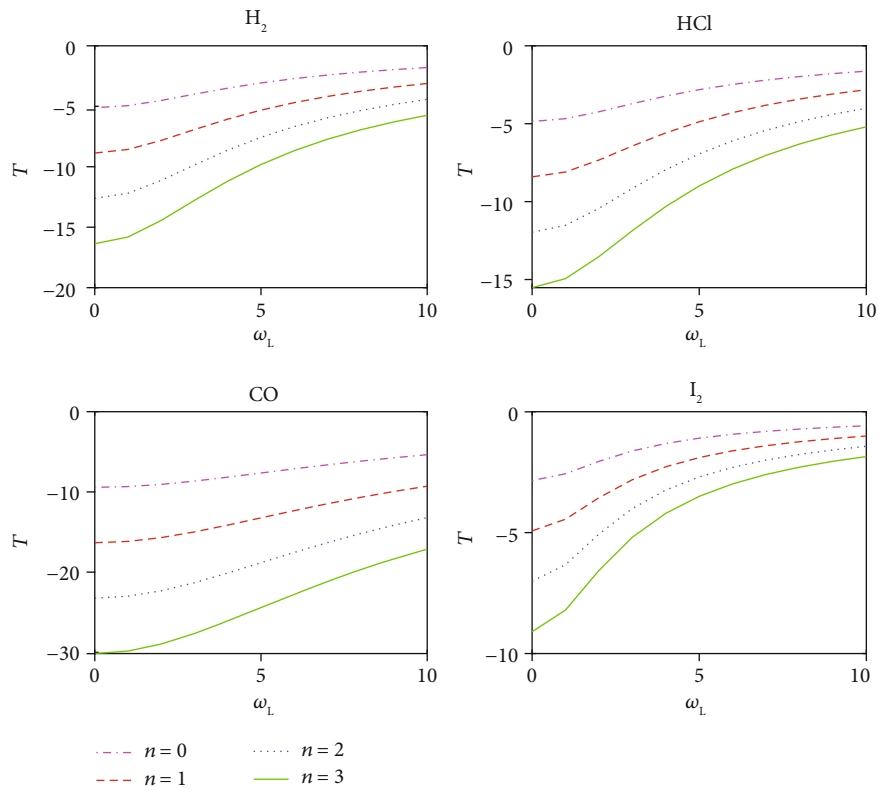


FIGURE 3: The expectation value of kinetic energy T as a function of Larmor frequencies ω_L for various numbers of states n with $g = m = 1$.

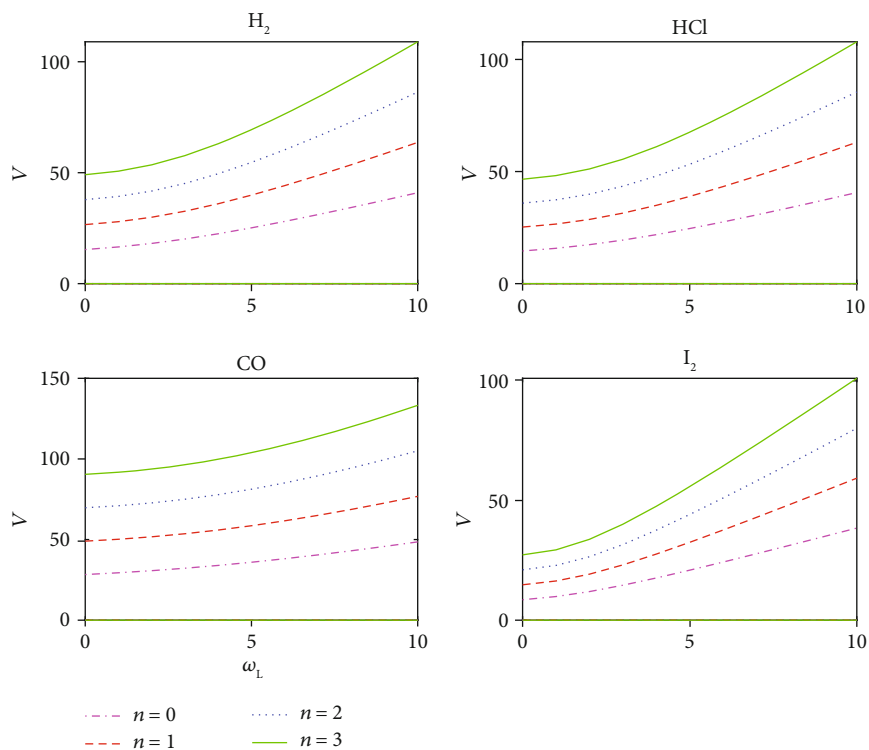


FIGURE 4: The expectation value of potential energy V as a function of Larmor frequencies ω_L for the molecules (H_2 , HCl , CO , and I_2) and for various numbers of states n with $g = m = 1$.

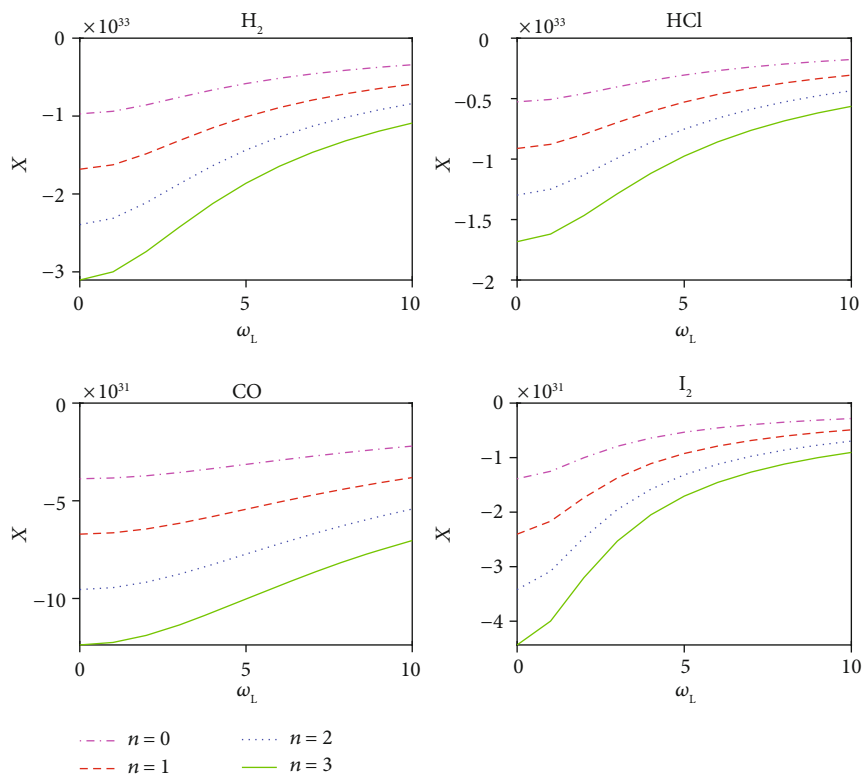


FIGURE 5: The diamagnetic susceptibilities X as a function of Larmor frequencies ω_L for the molecules (H_2 , HCl , CO , and I_2) and various numbers of states n with $g = m = z = e = 1$.

we present the computed results for the energy spectra, expectation values $\langle r^2 \rangle$, $\langle p^2 \rangle$, $\langle T \rangle$, and $\langle V \rangle$, and diamagnetic susceptibility X for the selected molecules bounded by the isotropic oscillator plus inverse quadratic potential with varying Larmor frequencies ω_L for the case of the low vibrational energy level ($n = 0, 1, 2, 3$), low rotational energy level ($m = 0, +1$), and inverse quadratic potential strength ($g = 0, 1$) in Tables 3–11. Figures 1–4 show the variation of expectation values for some quantum mechanical observables as a function of Larmor frequencies ω_L for various rotational energy levels ($n = 0, 1, 2, 3$) with $g = m = 1$ for the selected molecules in Table 2. Figure 5 shows the variation of diamagnetic susceptibility as a function of Larmor frequencies ω_L for various rotational energy levels n with $g = m = z = e = 1$ for the molecules in Table 1. In all the calculations, we have also employed the following recently used conversions: 1 a.m.u. = 1.66×10^{-27} kg, $c = 3.00 \times 10^8$ m/s, and $N = 6.02 \times 10^{23}$ moles. All our results are in their standard units.

It was observed that energy spectra increase with the increase in the magnetic field strength (Larmor frequency), vibrational level, and inverse quadratic potential strength g for all the selected molecules. See Tables 3–6. This observation suggests that the energy spectra of the selected molecules would be affected significantly by the external magnetic field. The expectation value $\langle r^2 \rangle$ which is positive increases with increasing rotational energy level n but decreases monotonically towards zero with the increase in magnetic field strengths for all the selected molecules for $g = m = 1$. See Table 7 and Figure 1. The expectation value $\langle p^2 \rangle$ which is negative decreases with increasing rotational energy level n but increases with the increase in magnetic field strengths and tends to converge at a very high magnetic field strength (Larmor frequencies $\omega_L > 10$) for all the selected molecules for $g = m = 1$. See Table 8 and Figure 2.

The expectation value $\langle T \rangle$ which is negative decreases with increasing rotational energy level n but increases monotonically with the increase in magnetic field strengths and tends to converge at a very high magnetic field strength (Larmor frequencies $\omega_L > 10$) for all the selected molecules for $g = m = 1$. See Table 9 and Figure 3. The expectation value $\langle V \rangle$ which is positive increases with increasing rotational energy level n as well as the magnetic field strength. A clear divergence is noticeable at all values of magnetic field strength for all the selected molecules for $g = m = 1$. See Table 10 and Figure 4.

The diamagnetic susceptibility X which is negative increases monotonically with increasing rotational energy level n as well as the magnetic field strength and tends to converge at any $\omega_L > 10$ for all the selected molecules for $g = m = z = e = 1$. See Table 11 and Figure 5.

5. Concluding Remarks

We have studied the two-dimensional radial Schrödinger equation with the isotropic harmonic oscillator plus inverse quadratic potential in an external magnetic field via the parametric Nikiforov-Uvarov method. The energy eigenvalue equation, normalized wave function, expressions for

expectation values square of the position $\langle r^2 \rangle$, square of the momentum $\langle p^2 \rangle$, kinetic energy $\langle T \rangle$, and potential energy $\langle V \rangle$, and diamagnetic susceptibility X for the interaction potential model have been obtained. The computed results for the energy spectra, expectation values $\langle r^2 \rangle$, $\langle p^2 \rangle$, $\langle T \rangle$, and $\langle V \rangle$, and diamagnetic susceptibility X for some diatomic molecules bounded by the isotropic harmonic oscillator plus inverse quadratic potential for low vibrational and rotational levels are found to have strong dependence on the magnetic field strengths as well as the inverse quadratic potential strength g .

The expectation values $\langle r^2 \rangle$, $\langle p^2 \rangle$, and $\langle T \rangle$ and diamagnetic susceptibility X as a function of Larmor frequencies ω_L for all the molecules tend to converge at a very high magnetic field strength ($\omega_L > 10$). This may signify a case where low vibrational and rotational energy levels cease to have any significant effect on the expectation values of $\langle r^2 \rangle$, $\langle p^2 \rangle$, and $\langle T \rangle$ and diamagnetic susceptibility X for all the molecules, despite the increasing magnetic field strength. A divergence is noticeable for the expectation value of potential energy $\langle V \rangle$ which signifies that the rotational and vibration energy levels will continue to have a meaningful effect as long as the magnetic field strength increases. Also, as the magnetic field strength increases, diamagnetic susceptibility X increases, which may likely increase the tendency of the magnetic field to shield or alter the vibrational motion of the molecules bounded by the potential model in this study.

Using the results obtained in this work, one can study the thermodynamic properties of the system, Shannon entropy, and Fisher information for the first and second excited states. And this would be our focus in the subsequent research work.

Data Availability

All the data used are included in this paper.

Consent

Consent is not applicable.

Conflicts of Interest

The authors declared that there are no competing interests regarding the paper.

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