

ALL ℓ -STATE EIGENSOLUTIONS OF THE NON-RELATIVISTIC SCHRÖDINGER EQUATION WITH GENERAL MOLECULAR OSCILLATOR

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Abstract

The approximate analytical bound state solutions of the Schrodinger equation for the general molecular oscillator (GMO) were obtained within the confines of the exact quantization rule (EQR). The Improved Pekeris-type approximation was used to deal with the spin-orbit term of the effective potential of the Schrodinger equation. Energy eigenvalues and corresponding wave-functions were obtained for different quantum numbers and some diatomic molecules. Special cases of the Morse and shifted Deng-fan oscillator were studied; their energy level values were compared with those in literature, results obtained by EQR are in good accord with those in literature.

Keywords: General molecular oscillator, exact quantization rule, Riccati equation.

1. Introduction

It is well known that exact solutions of Schrödinger equation play an important role in quantum mechanics since they contain all information regarding the quantum system under consideration [1-2]. The exact analytical solutions of the wave equations are possible for only few potentials of physical interest such as, the Coulombic potential and harmonic oscillator potential [3-4] for all quantum states n, ℓ where n is the vibrational quantum number and ℓ is the rotational quantum number [5], similarly, few other potential energy functions such as Eckart, Hulthén and Morse potentials give exact solution only for the s-wave ($\ell = 0$) state [6-7]. Most of the known potential energy functions have no exact solutions with the Schrödinger equation for all values of n and ℓ , for such potentials, approximate solutions (numerical or analytical) can be used in place of exact solutions [8]. In order to obtain approximate analytical solution, a very suitable approximation scheme [9-11] must be applied on the spin-orbit term of the effective potential, having applied the approximation model on the centrifugal term; a solution method must be adopted to solve the resulting equation. Over the last few decades a variety of analytical solution methods such as: ansatz method [12], generalized pseudospectral method [13], proper quantization rule [14], variational method [15], path integral approach [16], Laplace transform approach [4], Nikiforov-Uvarov method [17-18], asymptotic iteration method [19] have been developed to solve the wave equations exactly for physically interesting potentials. Recently an alternative method for solving radial Schrödinger equation for a given potential energy function was developed by Ma and Xu [20] which is called exact quantization rule (EQR) to find the exact energy eigenvalues for Coulombic and harmonic oscillator potentials. By employing this method Qiang *et al.* have solved the arbitrary ℓ -state approximate solutions of the Hulthén potential [21]. Moreover, Ikhdair and Sever applied the exact quantization rule to the Kratzer-type oscillator and obtained the energy eigenvalues for some diatomic molecule [22], their results show that the EQR is a powerful tool in finding the eigenvalues of all solvable quantum oscillators especially for large values of n and ℓ . In describing a suitable molecular potential for diatomic molecule, researchers have developed and used various forms of potential energy functions, Jia *et al.* have shown that improved Tietz potential is equivalent with the Wei potential for diatomic molecules [23], Wang *et al.* have defined an improved form of Manning-Rosen and Schiöberg potentials and proved that the Deng-Fan and the improved forms of Manning-Rosen and Schiöberg potentials they are same solvable potentials [24]. The answer to which potential is more successful in explaining experimental data, will depends on the examined molecule, for these reasons it can be said that none of these potentials are sufficiently successful on their own,

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thus in order to overcome this problem, Yanar *et al.* proposed the general molecular oscillator, to model all diatomic molecule, they used the GMO to model diatomic molecules and successfully computed the vibrational energies of some molecules which were consistent with RKR data, they also showed that the general molecular potential can be reduced to Rosen-Morse potential which gave outstanding results in explaining the vibration of nitrogen in ammonia molecule [25]. In previous study, Ikot *et al.* obtained the energy spectral of general molecular oscillator and used their results to explore the thermodynamic properties of this potential [26]. Motivated by the successes in the application of EQR as a solution method of the Schrodinger equation, in this letter, we are encouraged to solve the radial Schrodinger equation with the GMO, to obtain closed form expressions for bound state energy eigenvalues and radial wave-functions, to test the accuracy of our results we will deduce closed form expressions for the bound state energy eigenvalues of Morse and shifted Deng-fan oscillator which are special cases of the GMO and compare our results with the existing literature. To the best of our knowledge this approach of EQR on GMO was not done before.

2. Review of the concepts of exact quantization rule

Here we present a brief introduction of the exact quantization rule as proposed by Ma and Xu [20]. The EQR has been proposed to solve the one-dimensional Schrödinger equation:

$$\frac{d^2}{dx^2} \psi_{n\ell}(x) = -\frac{2\mu}{\hbar^2} [E_{n\ell} - V_{\text{eff}}(x)] \psi_{n\ell}(x) \quad (1)$$

Can be expressed as,

$$\frac{d}{dx} \varphi_{n\ell}(x) = -\frac{2\mu}{\hbar^2} [E_{n\ell} - V_{\text{eff}}(x)] \varphi_{n\ell}(x) - \varphi_{n\ell}(x)^2 \quad (2)$$

where $\varphi_{n\ell}(x)$ represent the logarithmic derivative of the wave function, given as:

$$\varphi_{n\ell}(x) = \psi'_{n\ell}(x) / \psi_{n\ell}(x) \quad (3)$$

$E_{n\ell}$ is the energy eigenvalue, μ is the reduced mass of the two interacting particle and the effective potential $V_{\text{eff}}(x)$ is a piecewise continuous real function of x and $\psi_{n\ell}(x)$ is the wave function. Due to Sturm-Liouville theorem, $\varphi_{n\ell}(x)$ decreases monotonically with respect to x between two turning points determined by the equation $E_{n\ell} \geq V_{\text{eff}}(x)$. Specifically, as x increases across a node of the wave function $\psi_{n\ell}(x)$, where $E_{n\ell} \geq V_{\text{eff}}(x)$, $\varphi_{n\ell}(x)$ decreases to $-\infty$ and jumps to $+\infty$ and then decreases again. In the usual notation, Eq. (2) is expressed as Riccati non linear differential form as

$$\varphi'_{n\ell}(x) + \varphi_{n\ell}^2(x) + k_{n\ell}^2(x) = 0 \quad (4)$$

where $k_{n\ell}(x) = \sqrt{\frac{2\mu}{\hbar^2} \{E_{n\ell} - V_{\text{eff}}(x)\}}$. After carefully studying the Schrödinger equation, the exact quantization rule was proposed (Ma and Xu, 2005) as:

$$\int_{x_{nA}}^{x_{nB}} k_{n\ell}(x) dx = N\pi + \int_{x_{nA}}^{x_{nB}} \varphi_{n\ell}(x) \left[\frac{d k_{n\ell}(x)}{dx} \right] \left[\frac{d \varphi_{n\ell}(x)}{dx} \right]^{-1} dx \quad (5)$$

where x_{nA} and x_{nB} are two turning points determined by letting $E_{n\ell} = V_{\text{eff}}(x)$ and $x_{nA} < x_{nB}$. N is the number of nodes of $\varphi_{n\ell}(x)$ in the neighborhood of $E_{n\ell} \geq V_{\text{eff}}(x)$ and it is larger by one than the number of nodes n of the wavefunction $\psi_{n\ell}(x)$, the term, $N\pi$ in Eq.(5) is the contribution from the nodes of the phase angle while the second term is the quantum correction, it is independent of n for all exactly solvable quantum systems, accordingly it can be evaluated at the ground state ($n = 0$), for a spherically symmetric potential Eq. (5) can be expressed as:

$$Q_c = \int_{x_{0A}}^{x_{0B}} \varphi_{0\ell}(x) \left[\frac{d k_{0\ell}(x)}{dx} \right] \left[\frac{d \varphi_{0\ell}(x)}{dx} \right]^{-1} dx \quad (6)$$

or

$$\int_{x_{0A}}^{x_{0B}} \varphi_{0\ell}(x) \left[\frac{d k_{0\ell}(x)}{dx} \right] \left[\frac{d \varphi_{0\ell}(x)}{dx} \right]^{-1} dx \quad (7)$$

Eq. (6) is equivalent to Eq. (7), where Q_c is the quantum correction term. The quantization rule Eq. (5) is generalized to the three dimensional Schrodinger equation with spherical symmetric potential as follows:

$$\int_{r_{n,A}}^{r_{n,B}} k_{n\ell}(r) dr = N\pi + \int_{r_{n,A}}^{r_{n,B}} \phi_{0\ell}(r) \left[\frac{dk_{0\ell}(r)}{dr} \right] \left[\frac{d\phi_{0\ell}(r)}{dr} \right]^{-1} dr \tag{8}$$

Explicitly, Eq. (6) can be written as:

$$I = N\pi + Q_c \tag{9}$$

where the momentum integral is given by:

$$I = \int_{r_{n,A}}^{r_{n,B}} k_{n\ell}(r) dr \tag{10}$$

and the quantum correction is:

$$Q_c = \int_{r_{n,A}}^{r_{n,B}} \phi_{0\ell}(r) \left[\frac{dk_{0\ell}(r)}{dr} \right] \left[\frac{d\phi_{0\ell}(r)}{dr} \right]^{-1} dr \tag{11}$$

The radial Schrödinger equation in three-dimensional spherical coordinates [4] is written as:

$$\frac{d^2\psi_{n\ell}(r)}{dr^2} + \frac{2\mu}{\hbar^2} \{E_{n\ell} - V_{eff}(r)\} \psi_{n\ell}(r) = 0 \tag{12}$$

$\psi_{n\ell}(r)$ is the radial wave function, r is the inter-nuclear separation and $V_{eff}(r)$ is the effective potential defined in terms of a spherically symmetric potential $V(r)$ and a parameter $L = \ell(\ell+1)$ by:

$$V_{eff}(r) = V(r) + \frac{L\hbar^2}{2\mu r^2} \tag{13}$$

3. The energy eigenvalues and eigenfunctions of the generalized molecular oscillator

The general molecular oscillator can be expressed in the form [25]:

$$V(r) = De \left\{ \frac{E + F e^{-\delta(r-r_e)} + G e^{-2\delta(r-r_e)}}{(1 - q e^{-\delta(r-r_e)})^2} \right\} \tag{14}$$

where E, F, G, δ are adjustable potential parameters, q is a dimensionless parameter and r_e is the equilibrium bond length. The effective potential is given by:

$$V(u) = De \left\{ \frac{E + F e^{-\alpha u} + G e^{-2\alpha u}}{(1 - q e^{-\alpha u})^2} \right\} + \frac{L\hbar^2}{2\mu r^2} \tag{15}$$

where $\alpha = \delta r_e, u = r/(r_e - 1), L = \ell(\ell + 1)$ and \hbar is the reduced Planck's constant

For a given value of parameters: E, F, G and q , Eqs. (15) and (12) have solution only for the pure vibrational state ($\ell = 0$). In order to obtain analytical solution for all states, an approximation scheme must be used on the spin-orbit or centrifugal term of Eq. (15), therefore, we invoke the Pekeris-type approximation model [27] given by:

$$\frac{1}{r^2} \approx \frac{1}{r_e^2} \left\{ c_0 + \frac{c_1}{e^{\alpha u} - q} + \frac{c_2}{(e^{\alpha u} - q)^2} \right\} \tag{16}$$

where c_0, c_1 and c_2 are constants given by:

$$c_0 = 1 - \frac{1}{\alpha}(1-q)(3+q) + \frac{3}{\alpha^2}(1-q)^2 \tag{17}$$

$$c_1 = \frac{2}{\alpha}(1-q)^2(2+q) - \frac{6}{\alpha^2}(1-q)^3 \tag{18}$$

$$c_2 = -\frac{1}{\alpha}(1-q)^3(1+q) + \frac{3}{\alpha^2}(1-q)^4 \tag{19}$$

However, by taking $c_0, c_1,$ and c_2 as $4d_0 r_e^2 \delta^2, r_e^2 \delta^2$ and $r_e^2 \delta^2$ respectively where d_0 has the value $1/3$, the Pekeris-type approximation reduces to the improved Green and Aldrich approximation model [28], we shall use these approximation schemes to test the accuracy of our results where appropriate. By substituting Eq. (16) in (15), the effective potential is then:

$$V_{eff}(u) = De \left\{ \frac{E + F e^{-\alpha u} + G e^{-2\alpha u}}{(1 - q e^{-\alpha u})^2} \right\} + \frac{L\hbar^2}{2\mu r_e^2} \left\{ c_0 + \frac{c_1 e^{-\alpha u}}{1 - q e^{-\alpha u}} + \frac{c_2 e^{-2\alpha u}}{(1 - q e^{-\alpha u})^2} \right\} \tag{20}$$

using the following transformation on Eq. (20)

$$x = \frac{e^{-\alpha u}}{1 - q e^{-\alpha u}} \quad (21)$$

gives

$$V_{\text{eff}}(x) = \left\{ \frac{L \hbar^2 c_2}{2 \mu r_e^2} + D_e (q^2 E + q F + G) \right\} x^2 + \left\{ \frac{L \hbar^2 c_1}{2 \mu r_e^2} + D_e (2q E + F) \right\} x + \frac{L \hbar^2 c_0}{2 \mu r_e^2} + D_e E \quad (22)$$

For brevity, Eq. (22) can be written in the more compact form as:

$$V_{\text{eff}}(x) = Ax^2 + Bx + C \quad (23)$$

with the constants A, B and C given by:

$$A = \frac{\hbar^2 \varepsilon_1^2}{2 \mu r_e^2} \quad (24)$$

$$B = \frac{\hbar^2 \varepsilon_2^2}{2 \mu r_e^2} \quad (25)$$

$$C = \frac{\hbar^2 \varepsilon_3^2}{2 \mu r_e^2} \quad (26)$$

where

$$\varepsilon_1^2 = L c_2 + \frac{2 \mu r_e^2 D_e}{\hbar^2} (q^2 E + q F + G) \quad (27)$$

$$\varepsilon_2^2 = L c_1 + \frac{2 \mu r_e^2 D_e}{\hbar^2} (2q E + F) \quad (28)$$

$$\varepsilon_3^2 = L c_0 + \frac{2 \mu r_e^2 D_e E}{\hbar^2} \quad (29)$$

Following Ma and Xu (2005), we can determine the turning points x_{nA} and x_{nB} ($> x_{nA}$) by imposing the condition:

$$V_{\text{eff}}(x) = E_{n\ell} \quad (30)$$

Substituting Eq. (23) in (30), we find the sum $x_{nA} + x_{nB}$ and the product $x_{nA} x_{nB}$ as given by:

$$x_{nA} + x_{nB} = -\frac{B}{A} \equiv -\frac{\varepsilon_2^2}{\varepsilon_1^2} \quad (31)$$

$$x_{nA} x_{nB} = \frac{C - E_{n\ell}}{A} \quad (32)$$

In what will be required in the evaluation of quantum correction, the ground state equivalents of Eqs. (31) and (32) are required, therefore putting $n = 0$ in Eqs. (31) and (32), we have:

$$x_{0A} + x_{0B} = -\frac{\varepsilon_2^2}{\varepsilon_1^2} \quad (33)$$

$$x_{0A} x_{0B} = \frac{C - E_{0\ell}}{A} \quad (34)$$

Clearly, the sum $x_{nA} + x_{nB}$ is independent of the vibrational and rotational quantum numbers.

The expression for the momentum of the system is given by:

$$k_{n\ell}^2 = \frac{2 \mu}{\hbar^2} (E_{n\ell} - Ax^2 - Bx - C) \quad (35)$$

Expressing Eq. (35) in terms of the turning points, this results to:

$$k_{n\ell}(x) = \frac{\varepsilon_1}{r_e} \sqrt{(x - x_{nA})(x_{nB} - x)} \quad (36)$$

And the derivative of Eq. (36) is given by:

$$k'_{n\ell}(x) = \frac{\varepsilon_1}{r_e} \frac{x + \varepsilon_2^2/2\varepsilon_1^2}{\sqrt{(x - x_{nA})(x_{nB} - x)}} \tag{37}$$

Evaluating the derivative of the momentum for the ground state, this gives:

$$k'_{0\ell}(x) = \frac{\varepsilon_1}{r_e} \frac{x + \varepsilon_2^2/2\varepsilon_1^2}{\sqrt{(x - x_{0A})(x_{0B} - x)}} \tag{38}$$

Expressing the Riccati equation given by Eq. (4) in terms of variable x, we have that:

$$-\frac{\alpha}{r_e}(x + qx^2)\varphi'_{n\ell}(x) + \varphi_{n\ell}^2(x) + \frac{2\mu}{\hbar^2}(E_{n\ell} - Ax^2 - Bx - C) = 0 \tag{39}$$

which for the ground state gives

$$-\frac{\alpha}{r_e}(x + qx^2)\varphi'_{0\ell}(x) + \varphi_{0\ell}^2(x) + \frac{2\mu}{\hbar^2}(E_{0\ell} - Ax^2 - Bx - C) = 0 \tag{40}$$

For a trial solution of Eq. (40), choose:

$$\varphi_{0\ell}(x) = -a_1x + a_2 \tag{41}$$

where a_1 and a_2 are constants. Substituting Eq. (41) in Eq. (40) gives:

$$\frac{a_1\alpha}{r_e}(x + qx^2) + a_1^2x^2 - 2a_1a_2x + a_2^2 + \frac{2\mu}{\hbar^2}(E_{0\ell} - Ax^2 - Bx - C) = 0 \tag{42}$$

From Eq. (42) we have:

$$\left(a_1^2 + \frac{a_1\alpha q}{r_e} - \frac{2\mu A}{\hbar^2}\right)x^2 + \left(\frac{a_1\alpha}{r_e} - 2a_1a_2 - \frac{2\mu B}{\hbar^2}\right)x + \left(a_2^2 - \frac{2\mu}{\hbar^2}(E_{0\ell} - C)\right) = 0 \tag{43}$$

equate the corresponding coefficients of x^2 , x and x^0 respectively on both sides of the Eq. (43) we have the following equations:

$$\frac{a_1\alpha q}{r_e} + a_1^2 = \frac{2\mu}{\hbar^2}A \equiv \frac{\varepsilon_1^2}{r_e^2} \tag{44}$$

$$\frac{a_1\alpha}{r_e} - 2a_1a_2 = \frac{2\mu}{\hbar^2}B \equiv \frac{\varepsilon_2^2}{r_e^2} \tag{45}$$

$$a_2^2 = \frac{2\mu}{\hbar^2}(C - E_{0\ell}) \tag{46}$$

$$a_1 = -\frac{\alpha q}{r_e} \left\{ \frac{1}{2} + \left(\frac{1}{4} + \frac{\varepsilon_1^2}{\alpha^2 q^2} \right)^{\frac{1}{2}} \right\} \tag{47}$$

we have

$$a_1 = -\frac{\alpha q \sigma}{r_e} \tag{48}$$

where

$$\sigma = \frac{1}{2} + \left(\frac{1}{4} + \frac{\varepsilon_1^2}{\alpha^2 q^2} \right)^{\frac{1}{2}} \tag{49}$$

from Eq. (44) and (45), we can get our constants and thus find our trial solution Eq. (11) gives the quantum correction in terms of the variable x as:

$$Q_c = -\frac{r_e}{\alpha} \int_{x_{0A}}^{x_{nB}} \frac{\varphi_{0\ell}(x)}{\varphi'_{0\ell}(x)} k'_{0\ell}(x) \frac{dx}{x(1+qx)} \tag{50}$$

substituting Eq. (41) and (37) and taking $n = 0$ in Eq. (50), we have

$$Q_c = \frac{\varepsilon_1}{\alpha} \int_{x_{0A}}^{x_{nB}} \frac{(x - a_2/a_1)(x + \varepsilon_2^2/2\varepsilon_1^2)}{x(1+qx)} \frac{dx}{\sqrt{(x - x_{0A})(x_{0B} - x)}} \tag{51}$$

the above integral can be evaluated by standard integral eq. (A1) [28], which gives:

$$Q_c = \frac{\pi \varepsilon_1}{\alpha} \left\{ \frac{1}{q} - \frac{a_2 \varepsilon_2^2}{2 a_1 \varepsilon_1^2} \frac{\varepsilon_1}{a_2 r_e} + \frac{(a_1 + q a_2)(q \varepsilon_2^2 - 2 \varepsilon_1^2)}{2 a_1 q \varepsilon_1^2} \frac{\varepsilon_1}{(a_1 + a_2 q) r_e} \right\} \quad (52)$$

Eq. (52) simplifies to:

$$Q_c = \frac{\pi \varepsilon_1}{\alpha} \left(\frac{1}{q} + \frac{\varepsilon_1}{\alpha \sigma q^2} \right) \quad (53)$$

Next, we evaluate the momentum integral on the left hand side of Eq. (8) and applying the transformation given by Eq. (21), we have:

$$I = -\frac{\varepsilon_1}{\alpha} \int_{x_{nA}}^{x_{nB}} \frac{\sqrt{(x - x_{nA})(x_{nB} - x)} dx}{x(1 + qx)} \quad (54)$$

The momentum integral of Eq. (36) was used in arriving at Eq. (54). In order to evaluate the definite integral in (54), we employ the following standard integral Eq. (A2) [29], therefore, Eq. (54) gives:

$$I = -\frac{\pi \varepsilon_1}{\alpha} \left\{ \frac{\sqrt{(q x_{nA} + 1)(q x_{nB} + 1)}}{q} - \frac{1}{q} - \sqrt{x_{nA} x_{nB}} \right\} \quad (55)$$

It follows that by using Eqs. (32), (24), (26) and (55), the energy eigenvalues of the GMO is given by:

$$E_{n\ell} = \frac{\hbar^2 \varepsilon_3^2}{2 \mu r_e^2} - \frac{\hbar^2 \alpha^2}{2 \mu r_e^2} \left\{ \frac{\varepsilon_1^2 - q \varepsilon_2^2}{2 \alpha^2 q^2 (n + \sigma)} - \frac{n + \sigma}{2} \right\}^2 \quad (56)$$

Using Eqs. (27) (28), (29) and (49) to eliminate $\varepsilon_1, \varepsilon_2, \varepsilon_3, \alpha$ and σ in Eq. (56) we have:

$$E_{n\ell} = D_\ell E + \frac{L \hbar^2 c_0}{2 \mu r_e^2} - \frac{\hbar^2 \delta^2}{2 \mu} \left\{ \frac{\frac{L}{\delta^2 q^2 r_e^2} (c_2 - q c_1) - \frac{2 \mu D_\ell}{\delta^2 \hbar^2 q^2} (q^2 E - G)}{2 n + 1 + \sqrt{1 + \frac{4 L c_2}{\delta^2 q^2 r_e^2} + \frac{8 \mu D_\ell}{\delta^2 \hbar^2 q^2} (q^2 E + q F + G)}} - \frac{2 n + 1 + \sqrt{1 + \frac{4 L c_2}{\delta^2 q^2 r_e^2} + \frac{8 \mu D_\ell}{\delta^2 \hbar^2 q^2} (q^2 E + q F + G)}}{4} \right\}^2 \quad (57)$$

To obtain the energy eigenfunctions of the general molecular oscillator, we need to solve the Riccati equation given by (39), this will give the solution for the phase angle $\varphi_{n\ell}(x)$, therefore, by using the definition of the phase angle, the wave function, $\psi_{n\ell}(x)$ can be recovered. Using the following transformation equation:

$$z = 1 + q x \quad (58)$$

and the definition of the phase angle, Eq. (39) gives, with slight simplification:

$$z(1 - z)\psi_{n\ell}''(z) + (1 - 2z)\psi_{n\ell}'(z) + \left\{ \varepsilon_4 - \frac{\varepsilon_4 - \varepsilon_5 + \varepsilon_6}{z} - \frac{\varepsilon_6}{1 - z} \right\} \psi_{n\ell}(z) = 0 \quad (59)$$

where

$$\varepsilon_4 = \frac{2 \mu r_e^2 A}{\alpha^2 q^2 \hbar^2} \quad (60)$$

$$\varepsilon_5 = \frac{2 \mu r_e^2 B}{\alpha^2 q \hbar^2} \quad (61)$$

$$\varepsilon_6 = \frac{2 \mu r_e^2}{\alpha^2 \hbar^2} (C - E_{n\ell}) \quad (62)$$

Following [2] Eq. (59) has solution of the form:

$$\psi_{n\ell}(z) = N_{n\ell} z^\zeta (1-z)^\xi {}_2F_1(-n, n+2\zeta+2\xi+1; z) \tag{63}$$

where ${}_2F_1$ is the hypergeometric function and the constants ζ and ξ are subjected to the following constraints:

$$\zeta = (\varepsilon_4 - \varepsilon_5 + \varepsilon_6)^{\frac{1}{2}} \tag{64}$$

$$\xi = \varepsilon_6^{\frac{1}{2}} \tag{65}$$

4. Discussion

The Morse oscillator

If we let $q=0, E=1, F=-2$ and $G=1$ in Eq. (14), the effective potential reduces to:

$$V_{eff-M}(r) = D_e \left\{ 1 - e^{-\delta(r-r_e)} \right\}^2 + \frac{L\hbar^2}{2\mu r^2} \tag{66}$$

Eq. (66) can be recognized to be the effective Morse oscillator, in which case the constant δ is the Morse constant [13,30]. Therefore, by inserting the above parameters in Eq. (57), the resulting energy eigenvalues are expected to give the energy eigenvalues ($E_{n\ell-M}$) of Morse oscillator, however substituting these values in Eq. (57) leads to $E_{n\ell-M} \rightarrow \infty$, which is physically not acceptable because $V_{eff-M}(r)$ is a finite potential energy function. Thus, in order to obtain a physically acceptable expression for $E_{n\ell-M}$ we need to re-evaluate the quantum correction Q_{cM} and the momentum integral I_M respectively for the Morse oscillator. Note that Eqs. (44) and (51) gives, for $q=0$:

$$a_{1M} = -\frac{\varepsilon_1}{r_e} \tag{67}$$

$$Q_{cM} = -\frac{\varepsilon_1}{\alpha} \int_{x_{0A}}^{x_{0B}} \left(x + \frac{B}{2A} - \frac{a_{1M}}{a_{2M}} - \frac{a_{1M} B}{2 a_{2M} A x} \right) \frac{dx}{\sqrt{(x-x_{0A})(x_{0B}-x)}} \tag{68}$$

using standard integrals (A3-A6 in the appendix) obtained from ref. [29], Eq. (68) simplifies to:

$$Q_{cM} = -\frac{\pi}{2} \tag{69}$$

similarly, Eq. (54) gives for $q=0$,

$$I_M = \frac{\varepsilon_1}{\alpha} \int_{x_{nA}}^{x_{nB}} \frac{\sqrt{(x-x_{nA})(x_{nB}-x)} dx}{x} \tag{70}$$

application of the standard integral (A6) on Eq. (70) gives:

$$I_M = -\frac{\pi \varepsilon_1}{\alpha} \left(\frac{\varepsilon_2^2}{2 \varepsilon_1^2} + \sqrt{x_{nA} x_{nB}} \right) \tag{71}$$

Substituting Eqs. (72) and (69) in the exact quantization rule given by Eq. (9), we have that:

$$E_{n\ell-M} = D_e E + \frac{L\hbar^2 c_0}{2\mu r_e^2} - \frac{\hbar^2 \delta^2}{2\mu} \left(n + \frac{1}{2} + \frac{\frac{Lc_1}{2\delta r_e} + \frac{\mu r_e D_e F}{\delta \hbar^2}}{\sqrt{Lc_2 + \frac{2\mu r_e^2 D_e G}{\hbar^2}}} \right)^2 \tag{72}$$

Table 1

Spectroscopic data of the molecules used in the present work, [6, 28]

Molecule	D_e (eV)	r_e (Å)	μ (amu)	δ (Å ⁻¹)
H ₂	4.7446	0.7416	0.50391	1.9506
LiH	2.5152672118	1.5956	0.8801221	1.128
HCl	4.619030905	1.2746	0.9801045	1.8677
CO	11.2256	1.1283	6.8606719	2.2994

Using Eq. (72) with $q=0$, $E = 1$, $F = -2$ and $G = 1$, we have computed the bound state energy eigenvalues of the GMO, the computed results for the four diatomic molecules (H_2 , CO , HCl and LiH) are shown in Tables 2 and 3, to enable comparison with existing literature results we have included in the table, the bound state energy eigenvalues for these molecules corresponding to the Morse oscillator obtained by generalized pseudospectral method (GPS) and the Nikiforov-Uvarov (NU) method. Firstly, it will be observed that the expressions for the Morse oscillator used in [32] has to be shifted by $+De$ to agree with the GMO given by Eq. (66), for the purpose of comparing results, our computed bound state energy eigenvalues of Eq. (72) must be stepped down by $-De$, the results are shown in the tables from these results it is evident that the present results obtained by exact quantization rule agrees totally with those obtained by other method in the literature for both the low and the high lying quantum states.

Table 2 Bound state energy eigenvalues (in eV) for H_2 , CO , HCl and LiH along with literature results

states		H_2			CO			HCl			LiH			
N	ℓ	PR	[32]	[33]	PR	[32]	[33]	PR	[32]	[33]	PR	[32]	[33]	
0	0	4.474909	4.476	4.476013	11.091535	11.09	11.09105	4.435525	4.435	4.435563	2.428843	2.428	2.428863	
		47	01	13	13	15	88	55	56	94	75	86	21	
	1	4.460126		4.461228	11.091058		11.09010	4.432939		4.432977	2.427002	...	2.427022	
		83	...	5	56	...	57	05	...	53	59	...	1	
	2	4.430694		4.431799	11.090105		11.09010	4.427767		4.427806	2.423322	...	2.423342	
		67	...	8	45	...	57	61	...	3	80	...	44	
	5	4.257701	4.176		11.084387	11.08		4.396782	4.396	...	2.401314	2.401	...	
		00	44	4.17644	29	44	...	97	82	...	80	33	...	
	1	3.720574	3.721		11.065333	11.06		4.294043	4.294	...	2.328817	2.328	...	
		0	13	94	3.72194	05	53	...	32	08	25	84	...	
	1	0	3.959200		3.962315	10.825821		10.82582	4.079673	...	4.079710	2.260529	...	2.260548
			56	...	34	50	...	21	09	...	06	23	...	05
1		3.944973		3.948116	10.825349		10.82534	4.077163	...	4.077201	2.258735	...	2.258755	
		82	...	47	01	...	96	58	...	44	96	...	59	
2		3.916647		3.919864	10.824404		10.82440	4.072146	...	4.072185	2.255151	...	2.255173	
		28	...	23	04	...	47	12	...	79	90	...	24	
5		3.750119			10.818734			4.042084	2.233716	
		26	77	87	86	
1		3.232664			10.799843			3.942417	2.163112	
		0	12	48	88	...	35	
2		0	3.475054		3.479918	10.563329		10.56333	3.738698	...	3.738733	2.098257	...	2.098276
			52	...	82	35	...	03	30	...	84	93	...	11
	1	3.461383		3.466338	10.562860		10.56286	3.736265	...	3.736303	2.096512	...	2.096533	
		68	...	75	93	...	19	78	...	82	54	...	04	
	2	3.434162		3.439328	10.561924		10.56192	3.731402	...	3.731445	2.093024	...	2.093049	
		75	...	36	12	...	52	29	...	39	21	...	5	
	5	3.274100			10.556303			3.702264	2.072162	
		39	73	44	13	
	1	2.776316			10.537575			3.605670	2.003450	
		0	98	39	11	...	66	
	5	0	2.211993	2.220		9.7951817	9.795		2.805039	2.805	...	1.647703	1.647	...
			64	52	...	8	18	...	94	06	...	35	71	...
1		2.199990			9.7947255			2.802838	1.646101	
		49	8	41	62	
2		2.176086			9.7938132			2.798436	1.642900	
		42	1	83	45	
5		2.035421	2.043		9.7883394	9.788		2.772069	2.772	...	1.623757	1.623	...	
		02	55	...	9	33	...	16	09	...	26	77	...	
1		1.596652	1.603		9.7700999	9.770		2.684692	2.684	...	1.560724	1.560	...	
		0	79	91	...	9	09	...	81	71	...	91	74	...
7		0	1.527767	1.537		9.2991908	9.299		2.256989	2.257	...	1.377549	1.377	...
			41	44	...	0	18	...	39	01	...	72	56	...
	1	1.516876			9.2987427			2.254941	1.376043	
		06	5	84	76	
	2	1.495183			9.2978466			2.250848	1.373034	
		22	8	20	04	
	5	1.367449	1.376		9.2924707	9.292		2.226327	2.226	...	1.355036	1.355	...	
		13	56	...	3	46	...	33	34	...	78	05	...	
	1	0.968024	0.975		9.2745571	9.274		2.145096	2.145	...	1.295790	1.295	...	
		0	36	81	...	3	55	...	30	11	50	8	...	

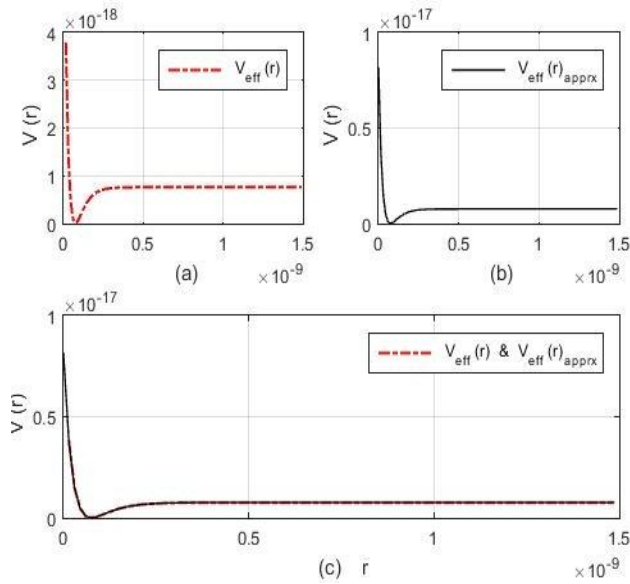


Fig 1. Plot of variation of effective general molecular potential Morse, $V(r)$ in (a), and approximate effective general molecular potential Morse, $V(r)$ in (b) with combined plot of (a) and (b) for H_2 in (c)

The generalized Morse oscillator

For values of the parameters $E = 0$, $F = 2(e^{-\delta r_e} - 1)$, $G = 1 - e^{-2\delta r_e}$ and $q = e^{-\delta r_e}$, the expression for the effective potential in Eq. (14) yields:

$$V_{\text{eff-SGM}}(r) = D_e \left(1 - \frac{e^{\delta r_e} - 1}{e^{\delta r} - 1} \right)^2 - D_e + \frac{L\hbar^2}{2\mu r^2} \tag{73}$$

Eq. (73) is just the effective shifted generalized Morse oscillator, $V_{\text{eff-SGM}}(r)$ [13]. It follows that upon substituting these values of the parameters in the expression for the energy eigenvalues of the general molecular oscillator given by Eq. (57), we have the energy eigenvalues for the shifted generalized Morse oscillator given as:

$$E_{n\ell-SGM} = \frac{L\hbar^2 c_0}{2\mu r_e^2} - \frac{\hbar^2 \delta^2}{2\mu} \left\{ \begin{array}{l} \frac{\frac{L}{\delta^2 r_e^2} (c_2 e^{\delta r_e} - c_1) e^{\delta r_e} + \frac{2\mu D_e}{\delta^2 \hbar^2} (e^{2\delta r_e} - 1)}{2n + 1 + \sqrt{1 + \frac{4Lc_2 e^{2\delta r_e}}{\delta^2 r_e^2} + \frac{8\mu D_e}{\delta^2 \hbar^2} (e^{-\delta r_e} + 1)^2}} \\ - \frac{2n + 1 + \sqrt{1 + \frac{4Lc_2 e^{2\delta r_e}}{\delta^2 r_e^2} + \frac{8\mu D_e}{\delta^2 \hbar^2} (e^{-\delta r_e} + 1)^2}}{4} \end{array} \right\}^2 \tag{74}$$

To further test the accuracy our results we have employed the energy eigenvalues of the GMO of Eq. (74) to compute bound state energy eigenvalues for four diatomic molecules viz: H_2 , CO , HCl and LiH the results of our computation are shown by the entries in Tables 4 and 5 and also the literature results which were obtained by alternative means of proper quantization rule (PQR) and asymptotic iteration method (AIM). The PQR results were available for H_2 and CO and upon comparison our present results is in near perfect agreement with the results for PQR. If we further compare the results EQR, PRQ and AIM, the results we obtained by EQR is almost indistinguishable with the other two methods except for few isolated cases of the H_2 molecule. The results obtained in this study are a clear demonstration of the efficacy of the EQR in obtaining bound state energy for diatomic molecules when considered for low and high quantum states.

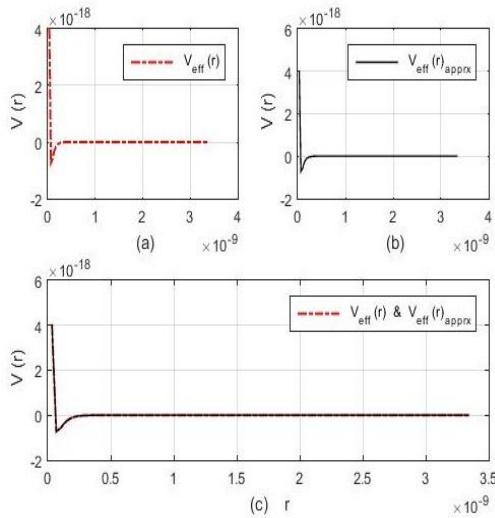


Fig 2. Plot of variation of effective general molecular potential $V(r)$ in (a), and approximate effective general molecular potential $V(r)$ in (b) with combined plot of (a) and (b) for HCl in (c).

Table 3 Bound state energy eigenvalues (in eV) for H_2 , CO, HCl and LiH along with literature results

states	H_2			CO			HCl		LiH		
	N	ℓ	PR	[31]	[29]	PR	[31]	[29]	PR	[31]	
0	0	4.39383750	4.39461978	4.39461978	11.08075134	11.0807518	11.08075178	4.41704940	4.417077	2.41193393	2.41194905
	1	4.37912480	11.08020383	4.41417939	...	2.41003189	...
	2	4.34977450	11.07910881	4.40844043	...	2.40622945	...
	5	4.17575583	4.17661805	4.17661316	11.07253907	11.0725399	11.07253746	4.37403672	4.37406578	2.38346076	2.38347625
	10	3.62064027	3.62183842	3.62182049	11.05064413	11.0506458	11.05064208	4.25972896	4.25976195	2.30813095	2.30814747
1	0	3.74562763	10.79416640	4.02829079	...	2.21326520	...
	1	3.73207676	10.79362281	4.02550106	...	2.21143254	...
	2	3.70504523	10.79253563	4.01992265	...	2.20776881	...
	5	3.54480384	10.78601289	3.98648179	...	2.18583121	...
	10	3.03399921	10.76427465	3.87537764	...	2.11325695	...
2	0	3.16095471	10.51162718	3.65903222	...	2.02458767	...
	1	3.14849738	10.51108749	3.65632173	...	2.02282281	...
	2	3.12364843	10.51000812	3.65090178	...	2.01929464	...
	5	2.97637761	10.50353225	3.61841118	...	1.99816919	...
	10	2.50731885	10.48195021	3.51046879	...	1.92828778	...
5	0	1.75274100	1.75845157	1.75845157	9.68815923	9.68814619	9.688146187	2.66574180	2.66574902	1.51627313	1.51627729
	1	1.74320803	9.68763118	2.66326292	...	1.51470268	...
	2	1.72419619	9.68657510	2.65830616	...	1.51156322	...
	5	1.61162673	1.61741062	1.61740572	9.68023898	9.68022628	9.680226284	2.62859335	2.62860119	1.49276676	1.49277143
	10	1.25440404	1.26045164	1.26043371	9.65912268	9.659164	9.659110919	2.52989351	2.52990569	1.43060825	1.4306143
7	0	1.07146436	1.07763699	1.07763699	9.15918188	9.159164	9.159164003	2.09652455	2.0965248	1.22339249	1.22339354
	1	1.06362899	9.15866154	2.09419521	...	1.22194465	...
	2	1.04800595	9.15762087	2.08953750	...	1.21905034	...
	5	0.95559189s	0.96181478	0.96180989	9.15137718	9.15135966	9.151359661	2.06161809	2.06162002	1.20172274	1.20172434
	10	0.66343343	0.66984407	0.66982613	9.13056901	9.13055243	9.130552425	1.96888561	1.96889204	1.14443549	1.14443859

5. Conclusion

Closed form expressions for bound state energy eigenvalues and radial wavefunctions of the GMO were obtained by solving the Schrodinger equation for this potential energy function, the exact quantization rule and ansatz solution model were used to obtain the solutions, bound state eigen energies and eigenfunctions for the s-wave and for non zero angular momentum of the GMO were deduced, cases of generalized Morse oscillator as well as generalized shifted Morse oscillator were considered. We have computed rotational-vibrational energies for four diatomic molecules viz: H_2 , CO, HCl and LiH and compared our result with existing results in the literature. The results we obtained are quite satisfactory and within the context of non-relativistic Schrodinger equation. This method of EQR presented in this letter is systemic, efficient and gives practical solutions to interacting problems; it can be applied to solve other oscillators of remarkable interest.

Appendix

$$\int_{x_{nA}}^{x_{nB}} \frac{dx}{(P+Qx)\sqrt{(x-x_{nA})(x_{nB}-x)}} = \frac{\pi}{\sqrt{(P+Qx_{nB})(P+Qx_{nA})}} \quad (\text{A1})$$

$$\int_{x_{nA}}^{x_{nB}} \frac{\sqrt{(x-x_{nA})(x_{nB}-x)}}{x(1+Qx)} dx = \pi \left\{ \frac{1}{Q} - \sqrt{x_{nA}x_{nB}} + \frac{\sqrt{(Qx_{nA}+1)(Qx_{nB}+1)}}{Q} \right\} \quad (\text{A2})$$

$$\int_{x_{nA}}^{x_{nB}} \frac{x dx}{\sqrt{(x-x_{nA})(x_{nB}-x)}} = \frac{\pi}{2} (x_{nA} + x_{nB}) \quad (\text{A3})$$

$$\int_{x_{nA}}^{x_{nB}} \frac{dx}{x\sqrt{(x-x_{nA})(x_{nB}-x)}} = \frac{\pi}{\sqrt{x_{nA}x_{nB}}} \quad (\text{A4})$$

$$\int_{x_{nA}}^{x_{nB}} \frac{dx}{\sqrt{(x-x_{nA})(x_{nB}-x)}} = \pi \quad (\text{A5})$$

$$\int_{x_{nA}}^{x_{nB}} \frac{\sqrt{(x-x_{nA})(x_{nB}-x)}}{x} dx = \pi \left\{ \frac{1}{2} (x_{nA} + x_{nB}) - \sqrt{x_{nA}x_{nB}} \right\} \quad (\text{A6})$$

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