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Approximate analytical solutions and mean energies of stationary Schrödinger equation for general molecular potential

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The Schrödinger equation is solved with general molecular potential via the improved quantization rule. Expression for bound state energy eigenvalues, radial eigenfunctions, mean kinetic energy, and potential energy are obtained in compact form. In modeling the centrifugal term of the effective potential, a Pekeris-like approximation scheme is applied. Also, we use the Hellmann–Feynman theorem to derive the relation for expectation values. Bound state energy eigenvalues, wave functions and meanenergies of Woods–Saxon potential, Morse potential, Möbius squared and Tietz–Hua oscillators are deduced from the general molecular potential. In addition, we use our equations to compute the bound state energy eigenvalues and expectation values for four diatomic molecules *viz.* H_2, CO, HF, and O_2. Results obtained are in perfect agreement with the data available from the literature for the potentials and molecules. Studies also show that as the vibrational quantum number increases, the mean kinetic energy for the system in a Tietz–Hua potential increases slowly to a threshold value and then decreases. But in a Morse potential, the mean kinetic energy increases linearly with vibrational quantum number increasing.

Keywords: general molecular potential, Schrödinger equation, improved quantization rule

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1. Introduction

The wave equations are of tremendous importance in the field of quantum mechanics due to the fact that they can provide the information about the quantum mechanical system.[1,2] However, the wave functions are obtained by solving Schrödinger equation with potential energy function describing the system. For a given quantum state defined by the vibrational and rotational quantum numbers v and J respectively, the exact solution of the Schrödinger equation is limited to the harmonic oscillator and Coulombic potential.[3,4] For many other potential energy functions, the exact solution can be obtained only for the state $J = 0$ (also known as the pure vibrational state).[5] For majority of the known potential energy functions, exact solutions of the Schrödinger equation are not feasible as a result of the spin-orbit or centrifugal term coupled to the effective potential.[1,5] For such potentials, approximate numerical or analytical solutions are necessary.[6,7]

Analytical solutions have the advantage of being obtained in close form, a form that makes them useful in exploring the physical properties of the system which they represent.[8–10] It must be mentioned here that not all analytical solutions are reliable, the most accurate analytical solution is one that approximates more closely to its corresponding numerical solution.[11,12] Approximate analytical solution of the Schrödinger equation involves the application of a suitable approximation model to the spin–orbit term[13–15] and an appropriate solution method. Researchers have proposed an almost endless solution methods to solve the Schrödinger equation. Some of the solution methods include ansatz method,[16] asymptotic iteration method,[17] exact quantization rule,[18] Nikiforov–Uvarov method,[19] improved or proper quantization rule,[20] and so,on.

Various models of potential energy functions have been used by researchers to solve the Schrödinger equation.[21–23] In their quest for constructing a potential energy function suitable for explaining molecular interactions, Yanar *et al*. have suggested the general molecular potential (GMP).[24] It is given by the following expression:

$$V(r) = \frac{A - B\,\mathrm{e}^{-\alpha(r-r_\mathrm{e})} + \tilde{q}\left\{C - D\,\mathrm{e}^{-\alpha(r-r_\mathrm{e})}\right\}^2}{\left\{1 - q\,\mathrm{e}^{-\alpha(r-r_\mathrm{e})}\right\}^2}, \quad (1)$$

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where A, B, C, D, $\tilde{q}$, and q are adjustable real potential parameters: $\tilde{q}$ and q are dimensionless parameters, r_e is the equilibrium bond length, and $r \in (0, \infty)$ is the internuclear separation of the interacting atoms.

The Schrödinger equation has been solved in the presence of GMP, and the expression for the ro-vibrational energy was used to model the interaction among six diatomic molecules.[24] Ikot *et al*. have employed the asymptotic iteration method to solve the radial Schrödinger equation with GMP and used the obtained energy spectra to study the thermodynamic properties of potassium dimer.[17] Finally, to the best of our knowledge, these are the only researches reported in the literature about the (GMP).

The researches about the GMP, which were earlier carried out are as follows. (i) In Ref. [24], the ansatz solution approach was used to solve the Schrödinger equation. However, explicit expression for energy eigenvalues was not given, which now entails obtaining separate explicit expression for energy eigenvalues for each of the potentials considered as special case. (ii) In Ref. [17], the expression for eigen energies of the GMP was obtained via asymptotic iteration method. Nonetheless, the result was neither subjected to a numerical test nor reduced into energy eigenvalues of other potential energy functions derivable from the GMP. (iii) The energy eigenvalues obtained for the GMP in previous researches are not valid for $q = 0$. (iv) Even though the GMP remains finite as $q \to 0$, the form of the Pekeris approximation model used in Refs. [17,24] is infinite as $q \to 0$.

The present work aims at obtaining approximate analytical solutions and mean energies of stationary Schrödinger equation with the general molecular potential. The objectives to be studied include: i) deriving the eigen energies of the GMP via the improved quantization rule and eigenfunctions by ansatz solution, with consideration for the cases of $q \neq 0$ and $q = 0$; ii) using a Pekeris-like approximation recipe to model the pseudo-spin orbit term of the effective potential; iii) deriving the formulas of expectation values of kinetic energy, potential energy, and total energy of the GMP, iv) computing the mean energies of the GMP for four diatomic molecules: H_2, CO, HF, and O_2; v) comparing the obtained results with those available from the literature.

The rest of this paper is organized as follows. In Section 2, a brief review of the improved quantization rule is presented. In Section 3, we use ideas of improved quantization rule to derive the expression for bound state energy eigenvalues of the GMP, and obtain the corresponding eigenfunctions via ansatz solution. Mean kinetic energy and potential energy for the system are discussed in Section 4. Section 5 is devoted to the special cases of the GMP and numerical computations. Finally, some conclusions are drawn from the present work in Section 6.

2. Review of improved quantization rule

In this section, a brief outline of the rudiments of improved quantization rule applicable to the present work is given. A detailed narration of this concept is presented elsewhere.[25] The improved quantization rule comes into being due to the need to overcome some of the complicated integrals encountered in exact quantization rule. At the beginning, the exact quantization rule was used to solve the one-dimensional Schrödinger equation given by[25]

$$\psi''(x) + k^2(x)\psi(x) = 0, \tag{2}$$

where double prime denotes the second derivative of $\psi(x)$ with respect to argument x, $\psi(x)$, $x \in (-\infty, \infty)$ is the one-dimensional wave function, and $k(x)$ is the momentum of the system, and given in terms of the energy E and effective potential $V_{\text{eff}}(x)$ by[18,25,26]

$$k(x) = \frac{1}{\hbar}\sqrt{2\mu\{E - V_{\text{eff}}(x)\}}. \tag{3}$$

In the usual notation, equation (2) expressed as a nonlinear Riccati equation is given as[18,25,26]

$$\phi'(x) + \phi^2(x) + k^2(x) = 0. \tag{4}$$

The logarithmic derivative $\phi(x) = \psi'(x)/\psi(x)$ of the wave function $\psi(x)$ is the phase angle.[18,26] For the Sturm–Liouville problem, the phase angle must be monotonic with respect to the energy.[18,26] Therefore, from Eq. (2), $\psi(x)$ must decreases monotonically with respect to x between two turning points where $E \geq V_{\text{eff}}(x)$. Specifically, as x increases across a node of the wave function $\psi(x)$, $\phi(x)$ decreases to $-\infty$, jumps to $+\infty$, and then decreases again.[26] Having carefully studied the one-dimensional Schrödinger equation, the exact quantization rule is given as[18,25,26]

$$\int_{x_A}^{x_B} k(x)\,\mathrm{d}x = N\pi + \int_{x_A}^{x_B} k'(x)\frac{\phi(x)}{\phi'(x)}\mathrm{d}x, \tag{5}$$

where the turning points x_A and x_B are the roots of the equation $V_{\text{eff}}(x) = E$. The number of nodes N of $\phi(x)$ in the region $E \geq V_{\text{eff}}(x)$ is by 1 greater than the number of nodes ν of the wave function $\psi(x)$. That is,

$N = \nu + 1$.[18,26] In Eq. (5), $N\pi$ is the contribution from the nodes of the phase angle while the second term on the right-hand side is the quantum correction. The quantum correction is independent of ν for all exactly solvable quantum systems. Accordingly, it is evaluated for the ground state ($\nu = 0$). For a spherically symmetric potential, equations (2)–(4) are expressed as[18,20,25,26]

$$H\,\psi_{\nu J}(r) = E_{\nu J}\,\psi_{\nu J}(r), \tag{6}$$

$$k_{\nu J}(r) = \frac{1}{\hbar}\sqrt{2\mu\{E_{\nu J} - V_{\rm eff}(r)\}}, \tag{7}$$

$$\phi'_{\nu J}(r) + \phi^2_{\nu J}(r) + k^2_{\nu J}(r) = 0, \tag{8}$$

where

$$H = -\frac{\hbar^2}{2\mu}\frac{{\rm d}^2}{{\rm d}r^2} + V_{\rm eff}(r) \tag{9}$$

is the Hamiltonian operator of the system and the effective potential is defined by

$$V_{\rm eff}(r) = V(r) + \frac{L\hbar^2}{2\mu r^2}, \tag{10}$$

with $L = J(J+1)$ being the angular momentum of the system. In a spherical coordinate system, equation (5) takes the form[18]

$$I_{\nu J} = N\pi + Q_{\rm c}, \tag{11}$$

where

$$I_{\nu J} = \int_{r_{\nu A}}^{r_{\nu B}} k_{\nu J}(r)\,{\rm d}r, \tag{12}$$

$$Q_{\rm c} = \int_{x_{\nu A}}^{x_{\nu B}} \frac{\phi_{0J}(r)}{\phi'_{0J}(r)} k'_{0J}(r)\,{\rm d}r. \tag{13}$$

Setting $\nu = 0$ in Eq. (11) and eliminating $Q_{\rm c}$, the improved quantization rule is written in compact form as follows:[18]

$$I_{\nu J} = I_{0J} + \nu\pi. \tag{14}$$

3. Solution of stationary Schrödinger equation with GMP

3.1. Solution of stationary Schrödinger equation with GMP corresponding to $q \neq 0$

Substituting Eq. (1) into Eq. (10), we have

$$V_{\rm eff}(r) = \frac{A - B\,{\rm e}^{-\alpha(r-r_{\rm e})} + \tilde{q}\left\{C - D\,{\rm e}^{-\alpha(r-r_{\rm e})}\right\}^2}{\left\{1 - q\,{\rm e}^{-\alpha(r-r_{\rm e})}\right\}^2} + \frac{L\hbar^2}{2\mu r^2}. \tag{15}$$

Equation (6) has an exact solution in the presence of Eq. (15) only for the pure vibrational state ($J = 0$). However, approximate analytical solutions are achievable if a suitable approximation scheme is employed to model the centrifugal term of the effective potential. In the earlier studies, the Pekeris-like approximation scheme used is given as[17,24]

$$\frac{1}{r^2} \simeq c_0 + \frac{c_1}{1 - q\,{\rm e}^{-\alpha(r-r_{\rm e})}} + \frac{c_2}{\left\{1 - q\,{\rm e}^{-\alpha(r-r_{\rm e})}\right\}^2}, \tag{16}$$

where the constant coefficients c_{-1+j} $(j = 1, 2, 3)$ are given by[17,24]

$$c_0 = \frac{(3 - \alpha r_{\rm e}) - 2(3 + \alpha r_{\rm e})q + \left(3 + 3\alpha r_{\rm e} + \alpha^2 r_{\rm e}^2\right)q^2}{\alpha^2 q^2 r_{\rm e}^4}, \tag{17a}$$

$$c_1 = \frac{2(q-1)^2(-3 + \alpha r_{\rm e} + 3q + 2\alpha q r_{\rm e})}{\alpha^2 q^2 r_{\rm e}^4}, \tag{17b}$$

$$c_2 = \frac{(q-1)^3[3(q-1) + (q+1)\alpha r_{\rm e}]}{\alpha^2 q^2 r_{\rm e}^4}. \tag{17c}$$

Clearly, as $q \to 0$, GMP remains finite but $\lim\limits_{q\to 0} c_{-1+j}$ $(j = 1, 2, 3) \to \infty$. Thus equation (16) is not suitable for the case in which $q = 0$. In this work, the centrifugal term is modeled by a Pekeris-like approximation recipe given as[2]

$$\frac{L\hbar^2}{2\mu r^2} \simeq \frac{L\hbar^2}{2\mu}\left\{d_0 + \frac{d_1\,{\rm e}^{-\alpha(r-r_{\rm e})}}{1 - q\,{\rm e}^{-\alpha(r-r_{\rm e})}} + \frac{d_2\,{\rm e}^{-2\alpha(r-r_{\rm e})}}{\left[1 - q\,{\rm e}^{-\alpha(r-r_{\rm e})}\right]^2}\right\}, \tag{18}$$

where the constant coefficients d_{-1+j} $(j = 1, 2, 3)$ are given in a compact form as

$$d_{-1+j} = \frac{(2-j)(3-j)}{2r_{\rm e}^2} + \frac{(-1)^j 2}{(-1+j)!(3-j)!\alpha r_{\rm e}^3}(4 - j + q)(1-q)^j + \frac{(-1)^{-1+j}6}{(-1+j)!(3-j)!\alpha^2 r_{\rm e}^4}(1-q)^{1+j}. \tag{19}$$

Evidently, as $q \to 0$, equation (1) is finite. Also, from Eq. (19) we have

$$\lim_{q\to 0} d_{-1+j} \to d^{(\mathrm{M})}_{-1+j} = \frac{(2-j)(3-j)}{2r_{\mathrm{e}}^2} + \frac{(-1)^j(8-2j)}{(-1+j)!(3-j)!\alpha_{\mathrm{M}} r_{\mathrm{e}}^3} + \frac{(-1)^{-1+j}6}{(-1+j)!(3-j)!\alpha_{\mathrm{M}}^2 r_{\mathrm{e}}^4}, \tag{20}$$

which is also finite. Therefore, equation (18) holds for both $q \neq 0$ and $q = 0$. The "M" appearing in Eq. (20) is designated as "expression corresponding to $q = 0$". In the remainder part of this work, This notation will be used unless otherwise stated. Substituting Eq. (18) into Eq. (15) we have

$$V_{\mathrm{eff}}(r) = \frac{A - B\,\mathrm{e}^{-\alpha(r-r_{\mathrm{e}})} + \tilde{q}\left\{C - D\,\mathrm{e}^{-\alpha(r-r_{\mathrm{e}})}\right\}^2}{\left\{1 - q\,\mathrm{e}^{-\alpha(r-r_{\mathrm{e}})}\right\}^2} + \frac{L\hbar^2}{2\mu}\left\{d_0 + \frac{d_1\,\mathrm{e}^{-\alpha(r-r_{\mathrm{e}})}}{1 - q\,\mathrm{e}^{-\alpha(r-r_{\mathrm{e}})}} + \frac{d_2\,\mathrm{e}^{-2\alpha(r-r_{\mathrm{e}})}}{\left[1 - q\,\mathrm{e}^{-\alpha(r-r_{\mathrm{e}})}\right]^2}\right\}. \tag{21}$$

Letting

$$\mathrm{e}^{-\alpha(r-r_{\mathrm{e}})} = \frac{1}{\tau} + q, \tag{22}$$

where $\tau \in \left\{(\mathrm{e}^{-\alpha r_{\mathrm{e}}} - q)^{-1}, 0\right\}$. Equation (21) is expressed with the variable τ as

$$\begin{aligned} V_{\mathrm{eff}}(\tau) = &\left\{q^2 A - qB + \tilde{q}(qC - D)^2 + \frac{L\hbar^2 d_2}{2\mu}\right\}\tau^2 \\ &+ \left\{2qA - B + 2\tilde{q}C(qC - D) + \frac{L\hbar^2 d_1}{2\mu}\right\}\tau \\ &+ A + \tilde{q}C^2 + \frac{L\hbar^2 d_0}{2\mu}, \end{aligned} \tag{23}$$

which is written in close form as

$$V_{\mathrm{eff}}(\tau) = \frac{\hbar^2}{2\mu}\sum_{j=1}^{3}\eta^2_{-1+j}\,\tau^{3-j}, \tag{24}$$

where for $j = 1, 2, 3$,

$$\eta^2_{-1+j} = L d_{3-j} + \frac{2\mu}{\hbar^2}\delta^{(-1+j)}, \tag{25}$$

such that

$$\begin{aligned} \delta^{(-1+j)} \equiv &\frac{1}{(-1+j)!} \\ &\cdot\frac{\partial^{-1+j}}{\partial q^{-1+j}}\left\{q^2 A - qB + \tilde{q}(qC - D)^2\right\}. \end{aligned} \tag{26}$$

With the notation given by Eqs. (25) and (26), the coefficients of τ^2, τ, and τ^0 in Eq. (23) are $\delta^{(0)} + L\hbar^2 d_2/2\mu$, $\delta^{(1)} + L\hbar^2 d_1/2\mu$, and $\delta^{(2)} + L\hbar^2 d_0/2\mu$, respectively. The turning points $\tau_{\nu A} = \left\{\mathrm{e}^{\alpha(r_{\nu A}-r_{\mathrm{e}})} - q\right\}^{-1}$ and $\tau_{\nu B} = \left\{\mathrm{e}^{\alpha(r_{\nu B}-r_{\mathrm{e}})} - q\right\}^{-1}$ required in the solution are determined by solving the equation $V_{\mathrm{eff}}(\tau) = \mathrm{e}_{\nu J}$. Substituting Eq. (24) into this relation, we have

$$\sum_{j=1}^{3}\eta^2_{-1+j}\,\tau^{3-j} = \frac{2\mu\,\mathrm{e}_{\nu J}}{\hbar^2} \equiv \eta^2_{\nu J}. \tag{27}$$

The sum and product of the turning points (which are also roots of Eq. (27)) are obtained as

$$\tau_{\nu A} + \tau_{\nu B} = -\frac{\eta_1^2}{\eta_0^2}, \tag{28}$$

$$\tau_{\nu A}\,\tau_{\nu B} = \frac{\eta_2^2 - \eta_{\nu J}^2}{\eta_0^2}. \tag{29}$$

Equation (7) expressed in terms of parameter τ gives the momentum as

$$\begin{aligned} k_{\nu J}(\tau) &= \left\{\eta^2_{\nu J} - \sum_{j=1}^{3}\eta^2_{-1+j}\,\tau^{3-j}\right\}^{1/2} \\ &\equiv \sqrt{(\tau - \tau_{\nu A})(\tau_{\nu B} - \tau)}. \end{aligned} \tag{30}$$

Using Eq. (22) to transform Eq. (8) into one involving variable τ, the Riccati equation leads to

$$-\alpha\,\tau(1 + q\,\tau)\,\phi'_{\nu J}(\tau) + \phi^2_{\nu J}(\tau) - \sum_{j=1}^{3}\eta^2_{-1+j}\,\tau^{3-j} + \eta^2_{\nu J} = 0. \tag{31}$$

In order to satisfy the Sturm–Liouville requirement, we choose a first-degree polynomial as a trial wave function for the ground state *viz*

$$\phi_{0J}(\tau) = -\omega\,\tau + \gamma, \tag{32}$$

where ω and γ are constant coefficients. Substituting Eq. (32) into Eq. (31) for $\nu = 0$, we have

$$\left(\alpha\,\omega q + \omega^2 - \eta_0^2\right)\tau^2 + \left(\alpha\,\omega - 2\omega\,\gamma - \eta_1^2\right)\tau + \gamma^2 - \eta_2^2 + \eta_{\nu 0}^2 = 0. \tag{33}$$

Equation (33) is true if and only if the separate coefficients of τ^2, τ, and τ^0 each are equal to zero. This yields the following expressions

$$\alpha\,\omega\,q+\omega^2=\eta_0^2, \tag{34a}$$
$$\alpha\,\omega-2\omega\,\gamma=\eta_1^2, \tag{34b}$$
$$\gamma^2=\eta_2^2-\eta_{\nu 0}^2. \tag{34c}$$

The parameter ω is obtained from Eq. (34a) as

$$\omega=-\alpha\,q\,\lambda, \tag{35}$$

where

$$\lambda=\frac{1}{2}\pm\left(\frac{1}{4}+\frac{\eta_0^2}{\alpha^2\,q^2}\right)^{1/2}$$
$$\equiv\frac{1}{2}\pm\frac{1}{2}\sqrt{1+\frac{4\,L\,d_2}{\alpha^2\,q^2}+\frac{8\,\mu\,\delta^{(0)}}{\alpha^2\,q^2\,\hbar^2}}. \tag{36}$$

With ω and γ given by Eqs. (35) and (34b) respectively, our trial solution defined by Eq. (32) is completely known. Our next task is to evaluate the momentum integral. Substituting Eq. (22) into Eq. (12) and inserting Eq. (30) into the resulting relation, we have

$$I_{\nu J}=-\frac{\eta_0}{\alpha}\int_{\tau_{\nu A}}^{\tau_{\nu B}}\frac{\sqrt{(\tau-\tau_{\nu A})\,(\tau_{\nu B}-\tau)}}{\tau\,(1+q\,\tau)}\,\mathrm{d}\,\tau. \tag{37}$$

With the help of standard integral (A1) in Appendix A, equation (37) gives

$$I_{\nu J}=\frac{\pi}{\alpha}\left\{\frac{\eta_0}{q}+\sqrt{\eta_2^2-\eta_{\nu J}^2}-\sqrt{\frac{\eta_0^2-q\,\eta_1^2}{q^2}+\eta_2^2-\eta_{\nu J}^2}\right\}. \tag{38}$$

Corresponding to $\nu=0$, equation (38) yields

$$I_{0J}=\frac{\pi}{\alpha}\left\{\frac{\eta_0}{q}+\sqrt{\eta_2^2-\eta_{0J}^2}-\sqrt{\frac{\eta_0^2}{q^2}-\frac{\eta_1^2}{q}+\eta_2^2-\eta_{0J}^2}\right\}. \tag{39}$$

Inserting Eqs. (34a)–(34c) into Eq. (39) and conducting simplification, the resulting equation is obtained as follows:

$$I_{0J}=\frac{\pi}{\alpha}\left(\frac{\eta_0}{q}+\alpha\,\lambda\right). \tag{40}$$

Substitution of Eqs. (38) and (40) into Eq. (14) leads to

$$\eta_{\nu J}^2=\eta_2^2-\alpha^2\left\{\frac{\eta_0^2-q\,\eta_1^2}{2\,\alpha^2\,q^2\,(\nu+\lambda)}-\frac{\nu+\lambda}{2}\right\}^2. \tag{41}$$

Using Eqs. (25) and (27) to eliminate $\eta_{-1+j}^2\ (j=1,2,3)$ and $\eta_{\nu J}^2$ respectively from Eq. (41), we obtain

$$E_{\nu J}=\delta^{(2)}+\frac{L\hbar^2\,d_0}{2\,\mu}-\frac{\alpha^2\hbar^2}{2\,\mu}\left(\frac{\kappa_3}{\kappa_2}-\frac{\kappa_2}{4}\right)^2, \tag{42}$$

where

$$\kappa_3=\frac{L}{\alpha^2\,q^2}\,(d_2-q\,d_1)+\frac{2\,\mu}{\alpha^2\,\hbar^2}\left(\delta^{(0)}-q\,\delta^{(1)}\right), \tag{43a}$$
$$\kappa_2=2\,\nu+1+\kappa_1, \tag{43b}$$
$$\kappa_1=2\,\lambda-1. \tag{43c}$$

To obtain the corresponding eigenfunctions of the GMP, the Riccati equation given by Eq. (31) is solved. Letting $z=1+q\,\tau$ where $z=\in\left((1-q\,\mathrm{e}^{\alpha\,r_\mathrm{e}})^{-1},0\right)$ and employing the phase angle-wave function relationship to recover the wave function, we have

$$z\,(1-z)\,\psi_{\nu J}''(z)+(1-2\,z)\,\psi_{\nu J}'(z)+\left\{\frac{\eta_0^2}{\alpha^2\,q^2}-\frac{1}{\alpha^2}\left(\frac{\eta_0^2}{q^2}-\frac{\eta_1^2}{q}+\eta_2^2-\eta_{\nu J}^2\right)\frac{1}{z}-\frac{\eta_2^2-\eta_{\nu J}^2}{\alpha^2}\frac{1}{1-z}\right\}\psi_{\nu J}(z)=0. \tag{44}$$

The substitution of the following expression into Eq. (44) is conducted:

$$\psi_{\nu J}(z)=N_{\nu J}\,z^s\,(1-z)^t\,\varphi_{\nu J}(z), \tag{45}$$

where s and t are constants, $N_{\nu J}$ is the normalization constant and $\varphi_{\nu J}(z)$ is an unknown function, then equation (44) is transformed into Gauss hypergeometric differential equation given by

$$z\,(1-z)\,\varphi_{\nu J}''(z)+\{2\,s+1-(2\,s+2\,t+2)\,z\}\,\varphi_{\nu J}'(z)+\left\{(s+t)^2+s+t-\frac{\eta_0^2}{\alpha^2\,q^2}\right\}\varphi_{\nu J}(z)=0, \tag{46}$$

subject to the following constraints:

$$s=\frac{1}{\alpha}\left(\frac{\eta_0^2}{q^2}-\frac{\eta_1^2}{q}+\eta_2^2-\eta_{\nu J}^2\right)^{1/2}, \tag{47}$$

$$t=\frac{1}{\alpha}\left(\eta_2^2-\eta_{\nu J}^2\right)^{1/2}. \tag{48}$$

For a polynomial solution,[24] equation (46) has a solution given by

$$\varphi_{\nu J}={}_2\mathrm{F}_1\left(-\nu,\,\nu+2s+2t+1;\,2s+1;\,z\right), \tag{49}$$

where ${}_2\mathrm{F}_1\left(-\nu,\,\nu+2s+2t+1;\,2s+1;\,z\right)$ is the hypergeometric function. Equations (42) and (45) give the complete solution of the Schrödinger equation with the GMP, and these equations remain valid for none zero values of q.

3.2. Solution of stationary Schrödinger equation with GMP corresponding to $q=0$

To obtain the solution of the Schrödinger equation with the GMP for $q=0$, first, it must be observed that by taking limits, equation (21) remains valid since

$$\lim_{q\to 0}V_{\mathrm{eff}}(r)\equiv V_{\mathrm{eff\,M}}(r)=A_{\mathrm{M}}-B_{\mathrm{M}}\,\mathrm{e}^{-\alpha_{\mathrm{M}}(r-r_{\mathrm{e}})}+\tilde{q}_{\mathrm{M}}\left\{C_{\mathrm{M}}-D_{\mathrm{M}}\,\mathrm{e}^{-\alpha_{\mathrm{M}}(r-r_{\mathrm{e}})}\right\}^2$$
$$+\frac{L\hbar^2}{2\mu}\left\{d_{0\mathrm{M}}+d_{1\mathrm{M}}\,\mathrm{e}^{-\alpha_{\mathrm{M}}(r-r_{\mathrm{e}})}+d_{2\mathrm{M}}\,\mathrm{e}^{-2\alpha_{\mathrm{M}}(r-r_{\mathrm{e}})}\right\}. \tag{50}$$

Letting $q=0$ in Eqs. (42) and (45), $\lim\limits_{q\to 0}\mathrm{e}_{\nu J}\equiv\mathrm{e}_{\nu JM}\to\infty$ and $\lim\limits_{q\to 0}\psi_{\nu J}\equiv\psi_{\nu JM}\to\infty$ are obtained, respectively. These results are contrary to expectations because the potential represented by Eq. (50) is real and finite. To arrive at a physically realistic solution of the Schrödinger equation with the GMP corresponding to $q=0$, one needs to re-evaluate Eqs. (34a)–(34c), thus yielding

$$\omega_{\mathrm{M}}=-\eta_{0\mathrm{M}}, \tag{51a}$$

$$\alpha_{\mathrm{M}}\,\omega_{\mathrm{M}}-2\omega_{\mathrm{M}}\,\gamma_{\mathrm{M}}=\eta_{1\mathrm{M}}^2, \tag{51b}$$

$$\gamma_{\mathrm{M}}^2=\eta_{2\mathrm{M}}^2-\eta_{\nu JM}^2. \tag{51c}$$

Note that in arriving at Eq. (51a) from Eq. (34a), the negative square root is considered to meet the Sturm–Liouville requirements of a trial wave function of one node and zero-pole. For $q=0$, equation (37) gives

$$I_{\nu JM}=-\frac{\eta_{0\mathrm{M}}}{\alpha_{\mathrm{M}}}\int_{\tau_{\nu A}}^{\tau_{\nu B}}\frac{\sqrt{(\tau-\tau_{\nu A})(\tau_{\nu B}-\tau)}}{\tau}\,\mathrm{d}\,\tau. \tag{52}$$

Using the standard integral (A2) in Appendix A and the mapping $\eta_{0\mathrm{M}}\to-\eta_{0\mathrm{M}}$, equation (52) gives

$$I_{\nu JM}=\frac{\pi}{\alpha_{\mathrm{M}}}\left(-\frac{\eta_{1\mathrm{M}}^2}{2\,\eta_{0\mathrm{M}}}+\sqrt{\eta_{2\mathrm{M}}^2-\eta_{\nu JM}^2}\right). \tag{53}$$

Taking $\nu=0$ in Eq. (53) and substituting Eqs. (51a)–(51c) into the resulting expression, we obtain

$$I_{0JM}=\pi/2. \tag{54}$$

Inserting Eqs. (53) and (54) into Eq. (14), and eliminating $\eta_{0\mathrm{M}}$, $\eta_{1\mathrm{M}}$, $\eta_{2\mathrm{M}}$, and $\eta_{\nu JM}$, we obtain

$$E_{\nu JM}=\delta_{\mathrm{M}}^{(2)}+\frac{L\hbar^2\,d_{0\mathrm{M}}}{2\,\mu}-\frac{\alpha_{\mathrm{M}}^2\hbar^2}{2\,\mu}\left\{\nu+\frac{1}{2}+\frac{\mu\,\delta_{\mathrm{M}}^{(1)}/\alpha_{\mathrm{M}}\hbar^2+Ld_{1\mathrm{M}}/2\,\alpha_{\mathrm{M}}}{\sqrt{2\,\mu\,\delta_{\mathrm{M}}^{(0)}/\hbar^2+Ld_{2\mathrm{M}}}}\right\}^2. \tag{55}$$

The radial eigenfunctions are obtained by setting $q=0$ in Eq. (31), resulting in

$$\tau^2\,\psi''_{\nu JM}(\tau)+\tau\,\psi'_{\nu JM}(\tau)-\frac{1}{\alpha_{\mathrm{M}}^2}\left(\eta_{0\mathrm{M}}^2\,\tau^2+\eta_{1\mathrm{M}}^2\,\tau+\eta_{2\mathrm{M}}^2-\eta_{\nu JM}^2\right)\psi_{\nu JM}(\tau)=0. \tag{56}$$

In order to solve Eq. (56), we assume a trial solution in the form of (Ref. [1])

$$\psi_{\nu JM}(\tau)=N_{\nu JM}\,\mathrm{e}^{-(1/2)\tau\rho}\,\tau^{(1/2)\upsilon}\,\varphi_{\nu JM}(\tau), \tag{57}$$

where ρ and υ are the parameters, $N_{\nu JM}$ is the normalization constant, and $\varphi_{\nu JM}(\tau)$ is an unknown function of τ. Substitution of Eq. (57) into Eq. (56) gives the Laguerre hypergeometric differential equation

$$\tau\,\varphi''_{\nu JM}(\tau)+(\upsilon+1-\rho\,\tau)\,\varphi'_{\nu JM}(\tau)-\left(\frac{1}{2}\rho\,\upsilon+\frac{1}{2}\rho+\frac{\eta_{1\mathrm{M}}^2}{\alpha_{\mathrm{M}}^2}\right)\varphi_{\nu JM}(\tau)=0, \tag{58}$$

on condition that

$$\rho = \frac{2\,\eta_{0\mathrm{M}}}{\alpha_{\mathrm{M}}}, \tag{59}$$

$$\upsilon = \frac{2\left(\eta_{2\mathrm{M}}^2 - \eta_{\upsilon J\mathrm{M}}^2\right)^{1/2}}{\alpha_{\mathrm{M}}}. \tag{60}$$

For bound state solution, equation (58) gives

$$\varphi_{\upsilon J\mathrm{M}}(\tau) = {}_1\mathrm{F}_1\left(-n,\, \upsilon+1;\, \rho\,\tau\right), \tag{61}$$

where ${}_1\mathrm{F}_1\left(-n,\, \upsilon+1;\, \rho\,\tau\right)$ is the Laguerre hypergeometric function.

4. Mean values of kinetic energy and potential energy in GMP

Now that we have obtained explicit analytical relations for bound state energy eigenvalues of the GMP for cases where $q=0$ and $q\neq 0$, we are in the position to apply these expressions to driving the important formulas for mean values of kinetic energy and potential energy. The Hellmann–Feynman theorem (HFT)[1,9,10] is used, and it states that if the Hamiltonian H of a quantum mechanical system is a function of some parameter ζ, then $H(\zeta)$, $\psi_{\upsilon J}(\zeta)$, and $E_{\upsilon J}(\zeta)$ are related by[1,9,10]

$$E_\zeta(\zeta) = \langle \psi_{\upsilon J}(\zeta) \left| H_\zeta(\zeta) \right| \psi_{\upsilon J}(\zeta)\rangle, \tag{62}$$

where $E_\zeta(\zeta) = \partial E_{\upsilon J}(\zeta)/\partial\zeta$, $H_\zeta(\zeta) = \partial H_{\upsilon J}(\zeta)/\partial\zeta$, and in general, the notation f_λ will be assumed to mean $\partial f/\partial\lambda$. We begin by substituting Eq. (15) in Eq. (9), and obtain

$$H = -\frac{\hbar^2}{2\mu}\frac{\mathrm{d}^2}{\mathrm{d}\,r^2} + \frac{A - B\,\mathrm{e}^{-\alpha(r-r_\mathrm{e})} + \tilde{q}\left\{C - D\,\mathrm{e}^{-\alpha(r-r_\mathrm{e})}\right\}^2}{\left\{1 - q\,\mathrm{e}^{-\alpha(r-r_\mathrm{e})}\right\}^2} + \frac{L\hbar^2}{2\mu\,r^2}. \tag{63}$$

4.1. Mean values of kinetic energy and potential energy of system in GMP for $q\neq 0$

Choosing $\zeta = L$, equations (62) and (63) give

$$E_L(L) = \langle \psi_{\upsilon J}(L) \left| H_L(L) \right| \psi_{\upsilon J}(L)\rangle, \tag{64}$$

$$H_L = \frac{\hbar^2}{2\mu\,r^2}, \tag{65}$$

respectively. Substituting Eq. (65) into Eq. (64), we obtain

$$\langle r^{-2}\rangle = \frac{2\mu E_L}{\hbar^2}. \tag{66}$$

E_L is obtained by differentiating Eq. (42) with respect to L, and expressed as

$$E_L = \frac{\hbar^2 d_0}{2\mu} + \frac{\hbar^2\,\Xi^{1/2}}{\mu\,q^2}\left(\frac{2\,d_2}{\kappa_1\,\kappa_4} - \frac{d_2 - q\,d_1}{\kappa_2}\right), \tag{67}$$

where

$$\Xi = \left(\frac{\kappa_3}{\kappa_2} - \frac{\kappa_2}{4}\right)^2, \tag{68}$$

$$\frac{1}{\kappa_4} = \frac{\kappa_3}{\kappa_2^2} + \frac{1}{4}. \tag{69}$$

The expectation value of the centrifugal term is given by

$$\langle V_L\rangle = \left\langle \frac{L\hbar^2}{2\mu\,r^2}\right\rangle \equiv L E_L. \tag{70}$$

The mean value of the kinetic energy is found by setting $\zeta = \mu$, separately, in Eqs. (62), (63), and (42). Thus, we have

$$E_\mu = \langle \psi_{\upsilon J}(\mu) \left| H_\mu(\mu) \right| \psi_{\upsilon J}(\mu)\rangle, \tag{71}$$

$$H_\mu = \frac{\hbar^2}{2\mu^2}\frac{\mathrm{d}^2}{\mathrm{d}\,r^2} - \frac{L\hbar^2}{2\mu^2 r^2}, \tag{72}$$

$$E_\mu = -\frac{L\hbar^2 d_0}{2\mu^2} + \frac{\alpha^2\hbar^2\,\Xi}{2\mu^2} + \frac{2\,\Xi^{1/2}}{\mu}\left(\frac{2\,\delta^{(0)}}{\kappa_1\,\kappa_4\,q^2} + \frac{q\,\delta^{(1)} - \delta^{(0)}}{\kappa_2\,q^2}\right). \tag{73}$$

From Eqs. (80) and (81), we find the expectation value of the kinetic energy to be

$$\langle T\rangle \equiv \langle \psi_{\upsilon J}(\mu) \left| -\frac{\hbar^2}{2\mu}\frac{\mathrm{d}^2}{\mathrm{d}\,r^2} \right| \psi_{\upsilon J}(\mu)\rangle = -\mu E_\mu - L E_L. \tag{74}$$

Another important relation which is deduced by the HFT is the expectation value of the GMP. Taking ζ separately as potential parameters A, B, and $\tilde{q}$, we have the mean value of the GMP $\langle V\rangle$ as given below:

$$\langle V\rangle = A E_A + B E_B + \tilde{q} E_{\tilde{q}}, \tag{75}$$

where E_A, E_B, and $E_{\tilde{q}}$ are obtained from Eq. (42) to be

$$E_A = 1 + 2\,\Xi^{1/2}\left(\frac{2}{\kappa_1\,\kappa_4} + \frac{1}{\kappa_2}\right), \tag{76}$$

$$E_B = \frac{-4\,\Xi^{1/2}}{\kappa_1\,\kappa_4\,q}, \tag{77}$$

$$E_{\tilde{q}} = C^2 + 2\,\Xi^{1/2}$$

$$\times\left\{\frac{2}{\kappa_1\,\kappa_4}\left(C-\frac{D}{q}\right)^2+\frac{1}{\kappa_2}\left(C^2-\frac{D^2}{q^2}\right)\right\}. \quad (78)$$

Let Ω_{vJ} be the sum of kinetic energy and potentials, then we have

$$\Omega_{vJ}=-\mu\,E_\mu+A\,E_A+B\,E_B+\tilde{q}\,E_{\tilde{q}}\equiv E_{vJ}. \quad (79)$$

4.2. Mean values of kinetic energy and potential energy of system in GMP for $q=0$

In the previous section, the equations derived for expectation values of kinetic energy and potential energy are valid only for nonzero values of q. Corresponding to $q=0$, equations (70) and (74) transform into

$$\langle V_{L\mathrm{M}}\rangle=\langle\left(\frac{L\hbar^2}{2\,\mu\,r^2}\right)_{\mathrm{M}}\rangle\equiv L E_{L\mathrm{M}}, \quad (80)$$

$$\langle T_{\mathrm{M}}\rangle=-\mu\,E_{\mu\,\mathrm{M}}-L E_{L\mathrm{M}}, \quad (81)$$

where

$$E_{L\mathrm{M}}=\frac{\hbar^2\,d_{0\mathrm{M}}}{2\,\mu}-\frac{\alpha_{\mathrm{M}}^2\hbar^2\,\Pi^{1/2}}{2\,\mu}\left(\frac{d_{1\mathrm{M}}}{\alpha_{\mathrm{M}}\,\kappa_5}-\frac{d_{2\mathrm{M}}}{2\,\kappa_5\,\kappa_7}\right), \quad (82)$$

$$E_{\mu\,\mathrm{M}}=-\frac{L\hbar^2\,d_{0\mathrm{M}}}{2\,\mu^2}+\frac{\alpha_{\mathrm{M}}^2\hbar^2\,\Pi}{2\,\mu^2}-\frac{\alpha_{\mathrm{M}}^2\,\Pi^{1/2}}{\mu}\left(\frac{\delta_{\mathrm{M}}^{(1)}}{\alpha_{\mathrm{M}}\,\kappa_5}-\frac{\delta_{\mathrm{M}}^{(0)}}{\kappa_5\,\kappa_7}\right) \quad (83)$$

are obtained from Eq. (64) by taking ζ separately as L and as μ, with the following expressions:

$$\Pi=\left(\nu+\frac{1}{2}+\frac{\kappa_6}{\kappa_5}\right)^2, \quad (84)$$

$$\kappa_7=\frac{\kappa_5^2}{\kappa_6}, \quad (85a)$$

$$\kappa_6=\frac{L d_{1\mathrm{M}}}{2\,\alpha_{\mathrm{M}}}+\frac{\mu\,\delta_{\mathrm{M}}^{(1)}}{\alpha_{\mathrm{M}}\hbar^2}, \quad (85b)$$

$$\kappa_5=\sqrt{L d_{2\mathrm{M}}+\frac{2\,\mu\,\delta_{\mathrm{M}}^{(0)}}{\hbar^2}}. \quad (85c)$$

Similarly, the mean value of the GMP $\langle V\rangle_{\mathrm{M}}$, for $q=0$ is deduced from Eq. (75) and expressed as

$$\langle V_{\mathrm{M}}\rangle=A_{\mathrm{M}}\,E_{A_{\mathrm{M}}}+B_{\mathrm{M}}\,E_{B_{\mathrm{M}}}+\tilde{q}_{\mathrm{M}}\,E_{\tilde{q}_{\mathrm{M}}}, \quad (86)$$

where $E_{A_{\mathrm{M}}}$, $E_{B_{\mathrm{M}}}$, and $E_{\tilde{q}_{\mathrm{M}}}$ are obtained by differentiating Eq. (55) with respect to A_{M}, B_{M}, and $\tilde{q}_{\mathrm{M}}$, their expressions are given below:

$$E_{A_{\mathrm{M}}}=1, \quad (87)$$

$$E_{B_{\mathrm{M}}}=\frac{\alpha_{\mathrm{M}}\,\Pi^{1/2}}{\kappa_5}, \quad (88)$$

$$E_{\tilde{q}_{\mathrm{M}}}=C_{\mathrm{M}}^2+\alpha_{\mathrm{M}}^2\,\Pi^{1/2}\left(\frac{2C_{\mathrm{M}}D_{\mathrm{M}}}{\alpha_{\mathrm{M}}\,\kappa_5}+\frac{D_{\mathrm{M}}^2}{\kappa_5\,\kappa_7}\right). \quad (89)$$

The sum of energy and potentials for $q=0$ is then

$$\Omega_{vJ\mathrm{M}}=-\mu\,E_{\mu\,\mathrm{M}}+A_{\mathrm{M}}\,E_{A_{\mathrm{M}}}+B_{\mathrm{M}}\,E_{B_{\mathrm{M}}}+\tilde{q}_{\mathrm{M}}\,E_{\tilde{q}_{\mathrm{M}}}\equiv E_{vJ\mathrm{M}}. \quad (90)$$

5. Results and discussion

Having obtain the explicit expressions for energy eigenvalues, eigenfunctions and expectation values of the GMP, at this point we will test the accuracy of our results. Through the suitable choice of parameters A, B, C, D, q, and $\tilde{q}$, we deduce the bound state energy eigenvalues, radial wave functions and expectation values of some potential models that are special cases of the GMP.

5.1. Woods–Saxon potential

The Woods–Saxon potential is a useful potential energy function and used as a major part of nuclear shell model to obtain nuclear energy level spacing and properties of electron distribution in atoms, nuclei and atomic clusters.[20] By choosing $\delta^{(0)}=\delta^{(2)}=0$, $\delta^{(1)}=-V_0$, and the mappings

$$q\to -q,\quad \alpha\to\alpha/R_0,\quad r_{\mathrm{e}}\to R_0,$$
$$L\to 2\,\mu\,\delta^2\,Q^2/\hbar^2,\quad d_{-1+j}\to d_{-1+j}/R_0^2$$

in Eqs. (23) and (42), we obtain Eqs. (B1) and (B2) in Appendi B. These equations are identical to Eqs. (9) and (29) of Ref. [20], the effective potential and bound state energy eigenvalue of the Woods–Saxon potential in D dimensions. Here, since $q\neq 0$, it follows that equations (70) and (75) are applicable for the computation of expectation values of spin–orbit term and potential energy function. On the other hand, equation (74) is suitable for the mean kinetic energy of the potential.

5.2. Morse potential

The Morse potential has been described as an important empirical potential model suitable for representing vibration–rotation states of diatomic molecules.[2,24,28] Equations (B3) and (B4) shown in Appendix B are obtained for the following choice of potential parameters applied to Eqs. (23) and (42) respectively:

$$\delta_{\mathrm{M}}^{(0)}=-(1/2)\delta_{\mathrm{M}}^{(1)}=\delta_{\mathrm{M}}^{(2)}=d_{\mathrm{e}}.$$

By comparison, equarions (B3) and (B4) are identical to Eqs. (48) and (56) for the Morse potential in Ref. [1]. In this case, since $q = 0$, equations (81), (80), and (86) are employed to compute mean values of kinetic energy, centrifugal term, and Morse potential function respectively.

5.3. Tietz–Hua oscillator

Equations (B5) and (B6) shown in Appendix B are obtained from Eqs. (23) and (42) respectively, subject to the following choice of potential parameters: $\delta^{(2)} = d_e$, $\tilde{q}D^2 = D_e$, and $B + 2\tilde{q}CD = 2D_e$. As it is evident that, equation (B5) corresponds to the expression for effective potential of the Tietz–Hua oscillator.[2,28,31] On the other hand, with $q = c_h$ and $b_h = \alpha_M(1 - c_h)$, equation (B6) is just the Eq. (13) of Ref. [31] for the ro-vibrational energy. The Tietz–Hua oscillator is known to be more realistic than the Morse potential in the description of molecular dynamics at moderate and high rotational and vibrational quantum number, and it reduces to Morse potential when $c_h = 0$.[28] For $c_h \neq 0$, equations (70), (75), and (74) are appropriate for the computation of the mean value of centrifugal term, the mean value of the Tietz–Hua potential energy function, and the mean value of kinetic energy.

5.4. Möbius squared oscillator

The Möbius squared oscillator is a very important potential energy model that has wide applications in chemical physics, nuclear physics, molecular physics, and solid-state physics.[1,29] Bound state energy eigenvalues and some expectation values of this oscillator have been studied in the literature.[1,29] It is noted that with the following expressions

$$q = -D' \, e^{-\alpha r_e}/C', \quad \delta^{(2)} = V_0 \left(A'^2/C'^2 + \eta\right),$$
$$B + 2\tilde{q}C'D' = -2V_0 \left(A'B'/C'^{,2} + \eta D'/C'\right) e^{-\alpha r_e},$$
$$\tilde{q}D^2 = V_0 \left(B'^2/C'^2 + \eta D'^2/C'^2\right) e^{-2\alpha r_e},$$

equations (23) and (46) are transformed into the forms given by Eqs. (B7) and (B8) in the Appendix B. Except for the coefficients d_1, d_2, and d_3, equations (B7) and (B8) are respectively equivalent to Eqs. (16) and (37) in Ref. [1] for the effective potential energy and ro-vibrational energy of shifted-rotating Möbius squared oscillator. If in addition, η is reduced to zero and the coefficients d_{-1+j} $(j = 1, 2, 3)$ are chosen as α^2, $2\alpha^2 e^{-\alpha r_e}$, and $\alpha^2 e^{-2\alpha r_e}$ in Eqs. (B7) and (B8), the first term and second term of Eq. (B7) are correspondingly equivalent to Eqs. (5) and (6) of Ref. [29] for the Mobius squared potential and the approximation to the centrifugal term respectively, where for validity, $D' = -C'$. Furthermore, if L is replaced with $(D + 2\ell - 3)(D + 2\ell - 1)/4$, equation (B8) is identical to the energy eigenvalues of Möbius squared oscillator in D dimensions given by Eq. (17b) in Ref. [29], the parameter λ is related to γ of Eq. (17c) by $\lambda = \gamma + 1/2$.

The data in Table 1 show spectroscopic constants of four diatomic molecules *viz.* H_2, CO, HF, and O_2 studied in the present work.

Table 1. Spectroscopic parameters of selected diatomic molecules used in the present study.

Molecule	Molecular state	Molecular parameters					
		c_h	μ (10^{-23} g)	r_e (Å)	α_M (Å^{-1})	b_h (Å^{-1})	D_e (cm^{-1})
H_2 (Refs. [2,28])	$X^1\Sigma_g^+$	0.170066	0.084	0.741	1.9506	1.61890	38318
HF (Ref. [28])	$X^1\Sigma^+$	0.127772	0.160	0.917	2.2266	1.94207	49382
O_2 (Ref. [28])	$X^3\Sigma_g^-$	0.027262	1.337	1.207	2.6636	2.59103	42041
CO (Refs. [2,28])	$X^1\Sigma^+$	0.149936	1.146	1.128	2.5937	2.20481	90531

We compute the bound state energy eigenvalues, expectation values of centrifugal term, potential energy function, kinetic energy, and total energy. The calculations are carried out for arbitrary rotational and vibrational quantum numbers. The results obtained using Eqs. (42), (70), (75), (74), and (79) for the parameters defined in Subsection 5.3 of the Tietz–Hua oscillator are shown in Tables 2–5. Also reported in the tables are the corresponding results for the parameters of Morse potential given in Subsection 5.2, which are calculated through Eqs. (55), (80), (86), (81), and (90). To enable our results to be compared with the existing data in the literature, we compute the binding energy $d_e - E_{vJ}$ and $d_e - E_{vJM}$ for the Tietz–Hua and Morse potentials respectively. The computed results and those extracted from the literature are shown in the tables. For the four diatomic

molecules considered in the present work, our computed bound state energy values are in nearly perfect agreement with the results obtained by generalized pseudospectral method[30] and by Nikiforov–Uvarov method.[2]

Variations of expectation values of the kinetic energy, the potential energy, and the total energy with the vibrational quantum number are shown graphically in the following Figs. 1–4.

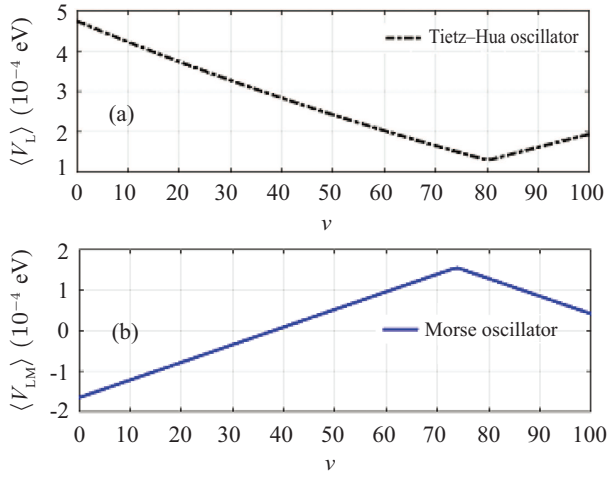


Fig. 1. The variation of the mean centrifugal term with the vibrational quantum number for (a) the Tietz–Hua oscillator, and (b) the Morse oscillator.

Figure 1 shows the plot of expectation values of the centrifugal term *versus* ν. As indicated by the plot in Fig. 1(a), when ν is increased from zero, $\langle V_L \rangle$ decreases linearly to some threshold value and afterwards increases. However, the opposite is true for the variation of $\langle V_{LM} \rangle$ with ν as represented in Fig. 1(b).

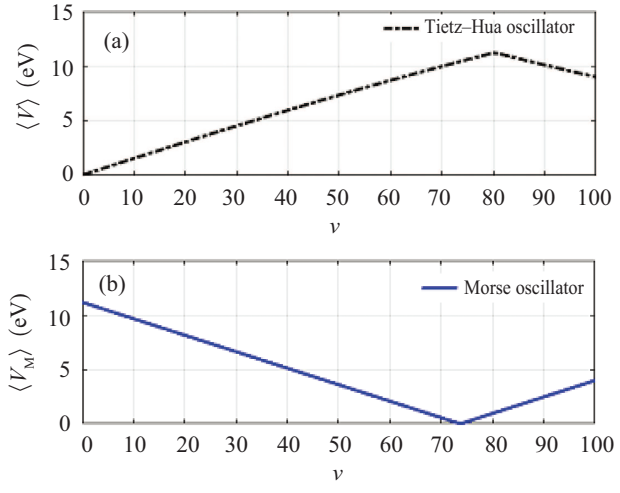


Fig. 2. The variation of the mean GMP with the vibrational quantum number for (a) the Tietz–Hua oscillator and (b) the Morse oscillator.

The variation of the expectation value of GMP with ν is shown in Fig. 2. In this case, as ν is gradually raised from zero, $\langle V \rangle$ increases to a peak value, then decreases as ν is further increased (Fig. 2(a)). Like the previous case, the variation of $\langle V_M \rangle$ with ν is opposite to the variation of $\langle V \rangle$ with ν.

In Fig. 3, we plot the expectation values of the kinetic energy *versus* ν. Figure 3(a) shows that as ν is varied positively, $\langle T \rangle$ increases to a maximum value and afterwards decreases with the ν further increasing. In Fig. 3(b), $\langle T_M \rangle$ increases approximately linearly with the ν increasing.

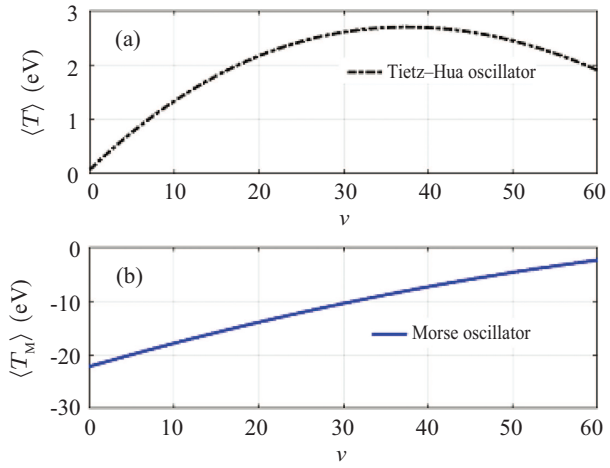


Fig. 3. The variation of the mean kinetic energy with the vibrational quantum number for (a) the Tietz–Hua oscillator, and (b) the Morse oscillator.

The variations of total energy of the GMP with ν are shown in Figs. 4(a) and 4(b) for the Tietz–Hua potential and Morse potential. The plots reveal that as ν increases from zero, the total energy for each of the two oscillators increases slowly, then attains a maximum value, and finally decreases.

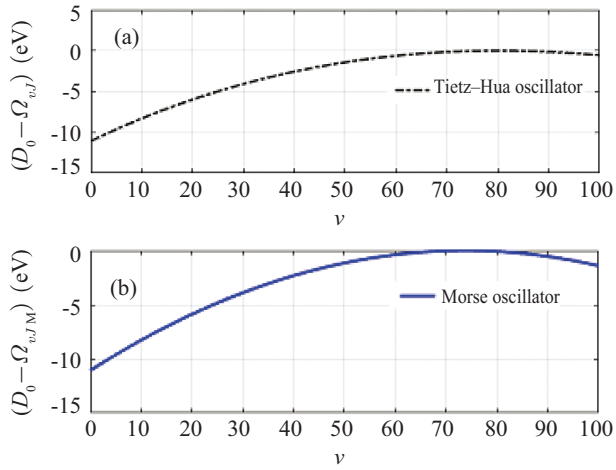


Fig. 4. The variation of the total energy with the vibrational quantum number for (a) the Tietz–Hua oscillator and (b) the Morse oscillator.

Table 2. Expectation values, bound state eidenenergy values: $-(E_{vJ}-D_{\rm e})$ for $q=c_{\rm h}$ and $-(E_{vJM}-D_{\rm e})$ for $q=0$ computed for the H_2 molecule, all in units of eV.

State		$q=c_{\rm h}$							$q=0$					
v	J	$\langle V_L\rangle$	$\langle V\rangle$	$\langle T\rangle$	$D_{\rm e}-\Omega_{vJ}$	$D_{\rm e}-E_{vJ}$	$De-E_{vJ}$[30]	$De-E_{vJ}$[2]	$\langle V_{LM}\rangle$	$\langle V_{M}\rangle$	$\langle T_{M}\rangle$	$De-\Omega_{vJM}$	$De-E_{vJM}$	$De-E_{vJM}$[2]
0	0	0.000000	0.136645	0.132607	4.481576496	4.481576496	4.4815797825	4.4815718267	0.000000	4.614185	−9.095656	4.481471132	4.481471132	4.481466458
	1	0.014579	0.136878	0.132396	4.466975068	4.466975068	4.4669801579	–	−0.003880	4.614024	−9.076865	4.466720568	4.466720568	–
	2	0.043477	0.137471	0.131976	4.437903424	4.437903424	4.4379154622	–	−0.011376	4.613574	−9.039550	4.437352006	4.437352006	–
	5	0.209858	0.144409	0.129520	4.267041353	4.267041353	–	4.2658220403	−0.049339	4.607484	−8.822871	4.264725242	4.264725242	4.264716547
	10	0.689967	0.201427	0.122027	3.737406384	3.737406384	–	3.733630436	−0.103317	4.554452	−8.179801	3.728665450	3.728665450	3.728647519
1	0	0.000000	0.409629	0.369136	3.972063521	3.972063521	–	–	0.000000	4.340897	-8.307235	3.966337746	3.966337746	–
	1	0.013763	0.410250	0.368535	3.958280201	3.958280201	–	–	−0.003328	4.340462	−8.289273	3.952139847	3.952139847	–
	2	0.041045	0.411608	0.367339	3.930835985	3.930835985	–	–	−0.009733	4.339470	−8.253607	3.923870469	3.923870469	–
	5	0.198200	0.422788	0.360341	3.769499403	3.769499403	–	–	−0.041478	4.330376	−8.046570	3.757671727	3.757671727	–
	10	0.652555	0.490364	0.338968	3.268940858	3.268940858	–	–	−0.078221	4.269888	−7.432835	3.241168821	3.241168821	–
2	0	0.000000	0.681736	0.570667	3.498425401	3.498425401	–	–	0.000000	4.067610	−7.550256	3.482645595	3.482645595	–
	1	0.012983	0.682711	0.569711	3.485423206	3.485423206	–	–	−0.002777	4.066899	−7.533123	3.469000360	3.469000360	–
	2	0.038722	0.684764	0.567810	3.459532948	3.459532948	–	–	−0.008090	4.065366	−7.499105	3.441830166	3.441830166	–
	5	0.187063	0.699796	0.556675	3.307294681	3.307294681	–	–	−0.033617	4.053268	−7.301710	3.282059447	3.282059447	–
	10	0.616751	0.776908	0.522630	2.834539243	2.834539243	–	–	−0.053126	3.985324	−6.717311	2.785113428	2.785113428	–
3	0	0.000000	0.952446	0.738868	3.059515091	3.059515091	3.0595425362	–	0.000000	3.794323	−6.824717	3.030394679	3.030394679	–
	1	0.012238	0.953743	0.737588	3.047259519	3.047259519	3.0474413866	–	−0.002225	3.793336	−6.808414	3.017302108	3.017302108	–
	2	0.036502	0.956429	0.735043	3.022854685	3.022854685	3.0233638406	–	−0.006448	3.791262	−6.776045	2.991231099	2.991231099	–
	5	0.176410	0.974967	0.720135	2.879316180	2.879316180	–	–	−0.025756	3.776160	−6.588292	2.837888402	2.837888402	–
	10	0.582449	1.060699	0.674505	2.433175185	2.433175185	–	–	−0.028031	3.700760	−6.033228	2.360499270	2.360499270	–
5	0	0.000000	1.487845	0.981430	2.281554187	2.281554187	2.2815913849	2.66965093	0.000000	3.247748	−5.467965	2.220216551	2.220216551	2.220195358
	1	0.010841	1.489704	0.979586	2.270697478	2.270697478	2.2710928924	–	−0.001122	3.246211	−5.453319	2.208229309	2.208229309	–
	2	0.032341	1.493495	0.975916	2.249075999	2.249075999	2.2502130058	–	−0.003162	3.243053	−5.424248	2.184356668	2.184356668	–
	5	0.156432	1.518141	0.954409	2.121846456	2.121846456	–	2.107007299	−0.010035	3.221943	−5.255779	2.043870016	2.043870016	2.043845951
	10	0.517959	1.618755	0.888435	1.725679685	1.725679685	–	–	0.022159	3.131631	−4.759385	1.605594657	1.605594657	1.605563961
7	0	0.000000	2.012597	1.108209	1.630022143	1.630022143	–	1.613091100	0.000000	2.701173	−4.236977	1.535803363	1.535803363	1.535779780
	1	0.009557	2.014928	1.105891	1.620452179	1.620452179	–	–	−0.000018	2.699086	−4.223989	1.524921450	1.524921450	–
	2	0.028513	2.019646	1.101278	1.601391314	1.601391314	–	–	0.000123	2.694845	−4.198215	1.503247176	1.503247176	–
	5	0.138031	2.049401	1.074221	1.489174886	1.489174886	–	1.472279959	0.005687	2.667727	−4.049031	1.375616570	1.375616570	1.375590575
	10	0.458363	2.162311	0.991042	1.139112307	1.139112307	–	1.122535653	0.072350	2.562503	−3.611308	0.976454984	0.976454984	0.976423401

Table 3. Expectation values, bound state eigenenergy values: $-(E_{vJ}-D\mathrm{e})$ for $q=c_\mathrm{h}$ and $-(E_{vJ\mathrm{M}}-D\mathrm{e})$ for $q=0$ computed for CO molecule, all in units of eV.

State		$q=c_\mathrm{h}$						$q=0$					
v	J	$\langle V_L\rangle$	$\langle V\rangle$	$\langle T\rangle$	$D\mathrm{e}-\Omega_{vJ}$	$D\mathrm{e}-E_{vJ}$	$D\mathrm{e}-E_{vJ}$[2]	$\langle V_{L\mathrm{M}}\rangle$	$\langle V_\mathrm{M}\rangle$	$\langle T_\mathrm{M}\rangle$	$D\mathrm{e}-\Omega_{vJ\mathrm{M}}$	$D\mathrm{e}-E_{vJ\mathrm{M}}$	$D\mathrm{e}-E_{vJ\mathrm{M}}$[2]
0	0	0.000000	0.075611	0.075090	11.073716231	11.073716231	11.07370964	0.000000	11.148807	−22.222511	11.073704790	11.073704790	11.07369820
	1	0.000473	0.075612	0.075089	11.073242852	11.073242852	–	−0.000164	11.148805	−22.221872	11.073230921	11.073230921	–
	2	0.001420	0.075615	0.075086	11.072296109	11.072296109	–	−0.000493	11.148803	−22.220593	11.072283197	11.072283197	–
	5	0.007100	0.075631	0.075071	11.066616045	11.066616045	11.06659606	−0.002464	11.148790	−22.212923	11.066597248	11.066597248	11.06659052
	10	0.026022	0.075691	0.075017	11.047687401	11.047687401	11.04763173	−0.009026	11.148740	−22.187363	11.047648989	11.047648989	11.04764190
1	0	0.000000	0.226825	0.221560	10.776032799	10.776032799	–	0.000000	10.997584	−21.772919	10.775335097	10.775335097	–
	1	0.000468	0.226829	0.221556	10.775564704	10.775564704	–	−0.000160	10.997581	-21.772287	10.774865556	10.774865556	–
	2	0.001404	0.226837	0.221548	10.774628529	10.774628529	–	−0.000480	10.997575	−21.771021	10.773926489	10.773926489	–
	5	0.007020	0.226885	0.221501	10.769011874	10.769011874	–	−0.002400	10.997535	−21.763428	10.768292482	10.768292482	–
	10	0.025731	0.227050	0.221342	10.750294581	10.750294581	–	−0.008788	10.997399	−21.738128	10.749517363	10.749517363	–
2	0	0.000000	0.378015	0.363325	10.483078036	10.483078036	–	0.000000	10.846362	−21.327402	10.481040119	10.481040119	–
	1	0.000463	0.378021	0.363318	10.482615195	10.482615195	–	−0.000156	10.846357	−21.326776	10.480574907	10.480574907	–
	2	0.001388	0.378035	0.363305	10.481689528	10.481689528	–	−0.000467	10.846346	−21.325523	10.479644497	10.479644497	–
	5	0.006942	0.378114	0.363227	10.476135918	10.476135918	–	−0.002335	10.846280	−21.318008	10.474062432	10.474062432	–
	10	0.025442	0.378382	0.362965	10.457628768	10.457628768	–	−0.008550	10.846057	−21.292968	10.455460453	10.455460453	–
3	0	0.000000	0.529165	0.500433	10.194819940	10.194819940	–	0.000000	10.695140	−20.885960	10.190819857	10.190819857	–
	1	0.000458	0.529174	0.500424	10.194362323	10.194362323	–	−0.000151	10.695132	−20.885340	10.190358973	10.190358973	–
	2	0.001373	0.529192	0.500405	10.193447104	10.193447104	–	−0.000454	10.695117	−20.884100	10.189437220	10.189437220	–
	5	0.006863	0.529302	0.500296	10.187956180	10.187956180	–	−0.002270	10.695026	−20.876663	10.183907098	10.183907098	–
	10	0.025155	0.529673	0.499931	10.169657972	10.169657972	–	−0.008312	10.694716	−20.851883	10.165478259	10.165478259	–
5	0	0.000000	0.831285	0.760866	9.632267339	9.632267339	9.629868985	0.000000	10.392696	−20.015299	9.622603479	9.622603479	9.622583913
	1	0.000447	0.831299	0.760852	9.631820081	9.631820081	–	−0.000143	10.392684	−20.014692	9.622151253	9.622151253	–
	2	0.001342	0.831327	0.760823	9.630925578	9.630925578	–	−0.000428	10.392660	−20.013478	9.621246814	9.621246814	–
	5	0.006708	0.831498	0.760653	9.625558955	9.625558955	9.623148913	−0.002140	10.392516	−20.006197	9.615820577	9.615820577	9.615800888
	10	0.024585	0.832071	0.760087	9.607675063	9.607675063	9.605233875	−0.007836	10.392034	−19.981936	9.597738017	9.597738017	9.597717999
7	0	0.000000	1.133065	1.003228	9.088125314	9.088125314	9.084920084	0.000000	10.090251	−19.160937	9.070685965	9.070685965	9.070661765
	1	0.000437	1.133084	1.003209	9.087688297	9.087688297	–	−0.000134	10.090235	−19.160343	9.070242395	9.070242395	–
	2	0.001311	1.133122	1.003170	9.086814276	9.086814276	–	−0.000402	10.090202	−19.159156	9.069355271	9.069355271	–
	5	0.006554	1.133352	1.002941	9.081570544	9.081570544	9.078354525	−0.002010	10.090007	−19.152030	9.064032918	9.064032918	9.064008590
	10	0.024022	1.134122	1.002178	9.064096266	9.064096266	9.060851540	−0.007360	10.089351	−19.128288	9.046296637	9.046296637	9.046271986

Table 4. Expectation values, bound state energy eigenvalues: $-(E_{vJ}-D\mathrm{e})$ for $q=c_{\mathrm{h}}$ and $-(E_{vJ\mathrm{M}}-D\mathrm{e})$ for $q=0$ computed for HF molecule, all in units of eV.

State		$q=c_{\mathrm{h}}$			$q=0$							
v	J	$\langle V_L\rangle$	$\langle V\rangle$	$\langle T\rangle$	$D\mathrm{e}-\Omega_{vJ}$	$D\mathrm{e}-E_{vJ}$	$D\mathrm{e}-E_{vJ}$ [2]	$\langle V_{LM}\rangle$	$\langle V_{\mathrm{M}}\rangle$	$\langle T_{\mathrm{M}}\rangle$	$D\mathrm{e}-\Omega_{vJ\mathrm{M}}$	$D\mathrm{e}-E_{vJ\mathrm{M}}$
0	0	0.000000	0.128297	0.125567	5.868726107	5.868726107	5.8687195228	0.000000	5.994290	−11.862969	5.868678884	5.868678884
	1	0.005056	0.128349	0.125516	5.863668945	5.863668945	5.8636625262	−0.002493	5.994249	−11.855357	5.863601751	5.863601751
	2	0.015156	0.128457	0.125416	5.853560796	5.853560796	5.8535547327	−0.007467	5.994159	−11.840146	5.853453683	5.853453683
	5	0.075411	0.129282	0.124813	5.793084404	5.793084404	–	−0.036967	5.993452	−11.749224	5.792738306	5.792738306
	10	0.272043	0.134113	0.122817	5.593616062	5.593616062	–	−0.131087	5.989013	−11.450400	5.592473838	5.592473838
1	0	0.000000	0.384784	0.357883	5.379922916	5.379922916	–	0.000000	5.737691	−11.114678	5.376987965	5.376987965
	1	0.004857	0.384933	0.357735	5.375064639	5.375064639	–	−0.002331	5.737568	−11.107310	5.372072914	5.372072914
	2	0.014560	0.385237	0.357440	5.365354102	5.365354102	–	−0.006981	5.737317	−11.092584	5.362248902	5.362248902
	5	0.072439	0.387224	0.355668	5.307259026	5.307259026	–	−0.034543	5.735643	−11.004574	5.303474828	5.303474828
	10	0.261259	0.395852	0.349804	5.115674870	5.115674870	–	−0.122279	5.728037	−10.715402	5.109644125	5.109644125
2	0	0.000000	0.640954	0.566555	4.915081044	4.915081044	–	0.000000	5.481091	−10.387896	4.906805385	4.906805385
	1	0.004662	0.641197	0.566313	4.910417980	4.910417980	–	−0.002169	5.480887	−10.380771	4.902052416	4.902052416
	2	0.013975	0.641689	0.565829	4.901097717	4.901097717	–	−0.006495	5.480474	−10.366531	4.892552459	4.892552459
	5	0.069522	0.644796	0.562932	4.845340041	4.845340041	–	−0.032120	5.477833	−10.281433	4.835719688	4.835719688
	10	0.250672	0.657082	0.553341	4.661495092	4.661495092	–	−0.113472	5.467061	−10.001911	4.648322751	4.648322751
3	0	0.000000	0.896612	0.752195	4.473783802	4.473783802	4.4737571516	0.000000	5.224491	−9.682622	4.458131143	4.458131143
	1	0.004470	0.896945	0.751862	4.469312385	4.469312385	4.4692935886	−0.002007	5.224207	−9.675740	4.453540257	4.453540257
	2	0.013400	0.897617	0.751197	4.460375269	4.460375269	4.4603723647	−0.006009	5.223632	−9.661987	4.444364356	4.444364356
	5	0.066658	0.901803	0.747216	4.406912342	4.406912342	–	−0.029696	5.220024	−9.579801	4.389472887	4.389472887
	10	0.240278	0.917612	0.734034	4.230665787	4.230665787	–	−0.104665	5.206084	−9.309929	4.208509715	4.208509715
5	0	0.000000	1.405648	1.056731	3.660210444	3.660210444	3.6601740988	0.000000	4.711292	−8.336600	3.625307676	3.625307676
	1	0.004098	1.406153	1.056227	3.656112031	3.656112031	3.6560952745	−0.001683	4.710845	−8.330203	3.621040954	3.621040954
	2	0.012282	1.407168	1.055220	3.647920639	3.647920639	3.6479433575	−0.005037	4.709947	−8.317422	3.612513165	3.612513165
	5	0.061083	1.413396	1.049187	3.598924103	3.598924103	–	−0.024850	4.704406	−8.241060	3.561504302	3.561504302
	10	0.220043	1.435872	1.029206	3.437467887	3.437467887	–	−0.087050	4.684132	−7.990490	3.393408660	3.393408660
7	0	0.000000	1.910515	1.275994	2.936080646	2.936080646	–	0.000000	4.198093	−7.076610	2.878517564	2.878517564
	1	0.003738	1.911179	1.275331	2.932342159	2.932342159	–	−0.001359	4.197484	−7.070700	2.874575007	2.874575007
	2	0.011203	1.912512	1.274005	2.924870348	2.924870348	–	−0.004066	4.196262	−7.058891	2.866695330	2.866695330
	5	0.055704	1.920639	1.266063	2.880183750	2.880183750	–	−0.020003	4.188787	−6.988353	2.819569072	2.819569072
	10	0.200514	1.949314	1.239761	2.733001286	2.733001286	–	−0.069435	4.162179	−6.757084	2.664340961	2.664340961

Table 5. Expectation values, bound state energy eigenvalues: $-(E_{vJ}-De)$ for $q=c_{\rm h}$ and $-(E_{vJ{\rm M}}-De)$ for $q=0$ computed for O_2 molecule, all in units of eV.

State		$q=c_{\rm h}$			$q=0$							
v	J	$\langle V_L\rangle$	$\langle V\rangle$	$\langle T\rangle$	$De-\Omega_{vJ}$	$De-E_{vJ}$	$De-E_{vJ}$[2]	$\langle V_{L{\rm M}}\rangle$	$\langle V_{\rm M}\rangle$	$\langle T_{\rm M}\rangle$	$De-\Omega_{vJ{\rm M}}$	$De-E_{vJ{\rm M}}$
0	0	0.000000	0.048273	0.047826	5.116322738	5.116322738	5.1163223113	0.000000	5.164155	−10.280490	5.116334845	5.116334845
	1	0.000344	0.048274	0.047825	5.115978867	5.115978867	5.1159784440	−0.000097	5.164154	−10.280048	5.115990893	5.115990893
	2	0.001032	0.048276	0.047823	5.115291138	5.115291138	5.1152907228	−0.000291	5.164152	−10.279164	5.115303002	5.115303002
	5	0.005157	0.048290	0.047810	5.111165141	5.111165141	–	−0.001452	5.164139	−10.273863	5.111176032	5.111176032
	10	0.018900	0.048339	0.047767	5.097416442	5.097416442	–	−0.005313	5.164091	−10.256202	5.097424091	5.097424091
1	0	0.000000	0.144818	0.140700	4.926903989	4.926903989	–	0.000000	5.067621	−9.994464	4.926842973	4.926842973
	1	0.000340	0.144821	0.140696	4.926564395	4.926564395	–	−0.000093	5.067618	−9.994028	4.926503141	4.926503141
	2	0.001019	0.144828	0.140690	4.925885220	4.925885220	–	−0.000278	5.067612	−9.993157	4.925823490	4.925823490
	5	0.005093	0.144867	0.140652	4.921810548	4.921810548	–	−0.001390	5.067574	−9.987930	4.921745960	4.921745960
	10	0.018664	0.145001	0.140523	4.908232937	4.908232937	–	−0.005087	5.067444	-9.970516	4.908158826	4.908158826
2	0	0.000000	0.241359	0.229910	4.741153370	4.741153370	–	0.000000	4.971087	−9.712014	4.740926698	4.740926698
	1	0.000335	0.241364	0.229904	4.740818047	4.740818047	–	−0.000089	4.971082	−9.711585	4.740590986	4.740590986
	2	0.001006	0.241375	0.229894	4.740147414	4.740147414	–	−0.000266	4.971072	−9.710726	4.739919575	4.739919575
	5	0.005029	0.241439	0.229830	4.736123993	4.736123993	–	−0.001328	4.971010	−9.705573	4.735891486	4.735891486
	10	0.018429	0.241659	0.229616	4.722717222	4.722717222	–	−0.004860	4.970797	−9.688406	4.722469159	4.722469159
3	0	0.000000	0.337892	0.315464	4.559065193	4.559065193	4.5590745476	0.000000	4.874554	−9.433140	4.558586021	4.558586021
	1	0.000331	0.337900	0.315457	4.558734134	4.558734134	4.5587436240	−0.000084	4.874546	−9.432716	4.558254429	4.558254429
	2	0.000993	0.337914	0.315442	4.558072031	4.558072031	4.5580817907	−0.000253	4.874532	−9.431870	4.557591259	4.557591259
	5	0.004965	0.338004	0.315352	4.554099787	4.554099787	–	−0.001266	4.874445	−9.426791	4.553612610	4.553612610
	10	0.018195	0.338309	0.315054	4.540863608	4.540863608	–	−0.004633	4.874150	−9.409872	4.540355090	4.540355090
5	0	0.000000	0.530926	0.475642	4.205853481	4.205853481	4.2058686976	0.000000	4.681486	−8.886118	4.204631462	4.204631462
	1	0.000323	0.530938	0.475630	4.205530933	4.205530933	4.2055464879	−0.000076	4.681475	−8.885707	4.204308110	4.204308110
	2	0.000968	0.530962	0.475607	4.204885852	4.204885852	4.2049020823	−0.000229	4.681452	−8.884885	4.203661419	4.203661419
	5	0.004837	0.531102	0.475466	4.201015738	4.201015738	–	−0.001143	4.681316	−8.879955	4.199781651	4.199781651
	10	0.017727	0.531576	0.474999	4.188120002	4.188120002	–	−0.004180	4.680856	−8.863530	4.186853747	4.186853747
7	0	0.000000	0.723899	0.621299	3.867223629	3.867223629	–	0.000000	4.488419	−8.353398	3.864979295	3.864979295
	1	0.000314	0.723915	0.621283	3.866909568	3.866909568	–	−0.000068	4.488403	−8.352999	3.864664182	3.864664182
	2	0.000942	0.723947	0.621251	3.866281459	3.866281459	–	−0.000204	4.488372	−8.352202	3.864033972	3.864033972
	5	0.004710	0.724138	0.621061	3.862513180	3.862513180	–	−0.001019	4.488186	−8.347420	3.860253085	3.860253085
	10	0.017260	0.724780	0.620425	3.849956901	3.849956901	–	−0.003727	4.487562	−8.331490	3.847654795	3.847654795

6. Conclusions

In the present work, bound state energy eigenvalues and radial eigenfunctions of the general molecular potential are obtained within the frameworks of improved quantization rule and ansatz solution method respectively. A Pekeris-like approximation model is used to model the pseudo-spin orbit term of the Schrödinger equation. With the help of Hellmann–Feynman theorem, closed form expressions for mean kinetic energy and mean potential energy are derived for the system. Equations for ro-vibrational energy, wave functions and mean energy of Woods–Saxon potential, Morse potential, Möbius squared, and Tietz–Hua oscillators are deduced from the general molecular potential energy. Furthermore, we numerically compute the values for bound state energy eigenvalues and mean energy values for four diatomic molecules *viz.* H_2, CO, HF, and O_2. The results obtained are in perfect agreement with existing data in the literature for the potentials and molecules. Our studies also reveal that as the vibrational quantum number increases, the mean kinetic energy of the system in Tietz–Hua potential increases slowly to a threshold value then decreases. On the other hand, in a Morse potential, the mean kinetic energy increases approximately linearly with the vibrational quantum number increasing.

Appendix A: List of standard definite integral used in this work

$$\int_a^b \frac{\sqrt{(x-a)\,(b-x)}}{x\,(1+qx)}\,z\,dx = \pi\left\{\frac{\sqrt{(1+qa)\,(1+qb)}}{q} - \frac{1}{q} - \sqrt{ab}\right\},\ \text{(Ref. [27])}, \tag{A1}$$

$$\int_a^b \frac{\sqrt{(x-a)\,(b-x)}}{x}\,\mathrm{d}\,x = \pi\left\{\frac{1}{2}\,(a+b) - \sqrt{ab}\right\},\ \text{(Ref. [18])}. \tag{A2}$$

Appendix B: List of derived expressions of effective potential and bound state ro-vibrational energy for the special cases of general molecular potentials considered in this work

B1. Woods–Saxon potential

$$V_{\text{eff}}^{(\text{WS})}(r) = -\frac{V_0}{\mathrm{e}^{\alpha(r-R_0)/R_0}+q} + \frac{L\hbar^2}{2\mu}\left\{d_0 + \frac{d_1}{\mathrm{e}^{\alpha(r-R_0)/R_0}+q} + \frac{d_2}{\left[\mathrm{e}^{\alpha(r-R_0)/R_0}+q\right]^2}\right\}, \tag{B1}$$

$$E_{\nu J}^{(\text{WS})} = \frac{L\hbar^2 d_0}{2\mu R_0^2} - \frac{\alpha^2\hbar^2}{2\mu R_0^2}\left\{\frac{(L/\alpha^2)\,(q\,d_1+d_2) - (2\mu V_0 R_0^2/\alpha^2\hbar^2 q)}{2\nu+1-\sqrt{1+(4Ld_2/\alpha^2 q^2)}} - \frac{2\nu+1-\sqrt{1+(4Ld_2/\alpha^2 q^2)}}{4}\right\}^2. \tag{B2}$$

B2. Morse potential

$$V_{\text{eff M}}^{(\text{Morse})}(r) = D\mathrm{e}\left\{1-e^{-\alpha_{\text{M}}(r-r\mathrm{e})}\right\}^2 + \frac{L\hbar^2}{2\mu}\left\{d_{0\text{M}} + d_{1\text{M}}\,\mathrm{e}^{-\alpha_{\text{M}}(r-r\mathrm{e})} + d_{2\text{M}}\,\mathrm{e}^{-2\,\alpha_{\text{M}}(r-r\mathrm{e})}\right\}, \tag{B3}$$

$$E_{\nu J\text{M}}^{(\text{Morse})} = D_{\text{e}} + \frac{L\hbar^2 d_{0\text{M}}}{2\mu} - \frac{\alpha_{\text{M}}^2\hbar^2}{2\mu}\left(\nu+\frac{1}{2}+\frac{(Ld_{1\text{M}}/2\,\alpha_{\text{M}}) - (2\mu D\mathrm{e}/\alpha_{\text{M}}\hbar^2)}{\sqrt{Ld_{2\text{M}}+2\mu D\mathrm{e}/\hbar^2}}\right)^2. \tag{B4}$$

B3. Tietz–Hua potential

$$V_{\text{eff}}^{(\text{TH})}(r) = D_{\text{e}}\left\{\frac{1-\mathrm{e}^{-b_{\text{h}}(r-r_{\text{e}})}}{1-c_{\text{h}}\,\mathrm{e}^{-b_{\text{h}}(r-r_{\text{e}})}}\right\}^2 + \frac{L\hbar^2}{2\mu}\left\{d_0 + \frac{d_1\,\mathrm{e}^{-b_{\text{h}}(r-r_{\text{e}})}}{1-c_{\text{h}}\,\mathrm{e}^{-b_{\text{h}}(r-r_{\text{e}})}} + \frac{d_2\,\mathrm{e}^{-b_{\text{h}}(r-r_{\text{e}})}}{\left[1-c_{\text{h}}\,\mathrm{e}^{-b_{\text{h}}(r-r_{\text{e}})}\right]^2}\right\}, \tag{B5}$$

$$E_{\nu J}^{(\text{TH})} = D_{\text{e}} + \frac{L\hbar^2 d_0}{2\mu} - \frac{b_{\text{h}}^2\hbar^2}{2\mu}\left\{\frac{(L/b_{\text{h}}^2 c_{\text{h}}^2)\,(d_2 - c_{\text{h}}\,d_1) - (2\mu D_{\text{e}}/b_{\text{h}}^2\hbar^2)\,(1-1/c_{\text{h}}^2)}{2\nu+1+\sqrt{1+(4Ld_2/b_{\text{h}}^2 c_{\text{h}}^2)+(8\mu D_{\text{e}}/b_{\text{h}}^2\hbar^2)\,(1-(1/c_{\text{h}}))^2}}\right.$$
$$\left. - \frac{2\nu+1+\sqrt{1+(4Ld_2/b_{\text{h}}^2 c_{\text{h}}^2)+(8\mu D_{\text{e}}/b_{\text{h}}^2\hbar^2)\,(1-1/c_{\text{h}})^2}}{4}\right\}^2. \tag{B6}$$

B4. Möbius squared oscillator

$$V_{\rm eff}(r) = V_0\left(\frac{A'+B'\,{\rm e}^{-\alpha r}}{C'+D'\,{\rm e}^{-\alpha r}}\right)^2 + \frac{L\hbar^2}{2\mu}\left\{d_0 + \frac{C'\,d_1\,{\rm e}^{-\alpha r_{\rm e}}\,{\rm e}^{-\alpha r}}{C'+D'\,{\rm e}^{-\alpha r}} + \frac{C'^2\,d_2\,{\rm e}^{-2\alpha r_{\rm e}}\,{\rm e}^{-2\alpha r}}{(C'+D'\,{\rm e}^{-\alpha r})^2}\right\} + \eta\,V_0, \tag{B7}$$

$$E_{\nu J}^{(\rm MS)} = V_0\left(\frac{A'^2}{C'^2}+\eta\right) + \frac{\alpha^2\hbar^2 L}{2\mu} - \frac{\alpha^2\hbar^2}{8\mu(\nu+\lambda)^2}\left\{-\frac{L}{\alpha^2}\left(\frac{C'^2}{D'^2}\frac{d_2}{{\rm e}^{-2\alpha re}} + \frac{C'}{D'}\frac{d_1}{\rm e}^{-\alpha r_{\rm e}}\right)\right.$$
$$\left. + \frac{2\mu V_0}{\alpha^2\hbar^2}\left(\frac{A'^2}{C'^2}+\frac{B'^2}{D'^2}+2\eta\right) + \frac{1}{4}(\nu+\lambda)\right\}^2. \tag{B8}$$

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