Energy Eigenvalues and Eigen functions of a Diatomic Molecule in Quadratic Exponential-type Potential

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Abstract

We employed the exact quantization rule to obtain closed form expression for the bound state energy eigenvalues of a molecule in quadratic exponential-type potential. To deal with the spin-orbit centrifugal term of the effective potential energy function, we have used a Pekeris-type approximation scheme, we have also obtained closed form expression for the normalized radial wave functions by solving the Riccati equation with quadratic exponential-type potential. Using our derived energy eigenvalue formula, we have deduced expressions for the bound state energy eigenvalues of the Hulthén, Eckart and Deng-Fan potentials, considered as special cases of the quadratic exponential-type potential. Our deduced energy eigenvalues are in excellent agreement with those in the literature. We have computed bound states energy eigenvalues for six diatomic molecules *viz*: HCl, LiH, H_2, SeH, VH and TiH. Our results are in total agreement with existing results in the literature for the s-wave and in good agreement for higher quantum states. By solving the Riccati equation, we have obtained normalized radial wave functions of the quadratic exponential-type potential, our results show higher probabilities of finding the molecule in the region $0.1 \leq y \leq 0.2$

Key words: eigenvalues, eigen functions, quadratic exponential-type potential, exact quantization rule, Riccati equation

Introduction

In the subject of wave mechanics, much emphasis is placed on the wave functions of a system owing to the fact that all the required information about the system are derivable from the wave functions (Eyube, Jabil and Umar, 2019a; Qiang and Dong, 2009; Jia, Liu and Wang, 2008). However, obtaining the wave function of a system requires solving the Schrödinger equation, a second order differential equation for a given potential energy function. The solution of the Schrödinger equation is either exact (Eyube, Sanda and Jabil, 2019b; Ikot, Awoga, Hassanabadi and Maghoodi, 2014; Hamzavi, Rajabi and Hassanabadi, 2012) or inexact (Khordad and Mirhosseini, 2015; Ikhdair and Sever, 2009) for the quantum state nℓ, where n is the principal quantum number and ℓ is the principal angular momentum quantum number. The Coulomb and harmonic oscillator potentials are two well-known potential energy functions which have exact solutions (Hitler *et al*., 2017) for all values of ℓ ($\ell = 0$ as well as $\ell \neq 0$), on the other hand fewer other potential energy functions have exact solutions only for state $\ell = 0$, such solutions are often referred to as s-wave solutions (Tsaur and Wang, 2014; Serano, Gu and Dong, 2010). Most of the known potential energy functions have no exact solutions with the Schrödinger equation, therefore, for these class of potentials, approximate numerical (Nasser, Abdelmonem and Abdel-Hady, 2012; Lucha and Schöberl, 1999) or analytical (Yanar, Tas, Salti and Aydogdu, 2020; Okorie, Ikot, Chukwuocha and Rampho, 2020; Gu and Dong. 2011) solutions are acceptable. There are two steps involved in arriving at an analytical solution, first, an approximation scheme (Falaye, Ikhdair and Hamzavi, 2015; Greene and Aldrich, 1976; Pekeris, 1934) must be applied on the centrifugal term of the Schrödinger equation, secondly the solution method to be used to solve the resulting equation. It must be emphasized that no two different approximation schemes and/or two different solution methods give the same analytical solutions, thus, the better analytical solution is the one which approximates more closely to a corresponding numerical solution (Khodja *et al*., 2019; Eyube *et al*., 2019c; Tang, Liang, Zhang, Zhao and Jia., 2013). Various solution methods have been proposed and used to solve the Schrödinger equation, some of these methods include: parametric Nikiforov-Uvarov method (Khordad and Mirhosseini, 2015; Ikot, Awoga, Hassanabadi and Maghoodi, 2014), exact and proper quantization rules (Qiang, Gao and Zhou, 2008; Dong, Morales and Garcia-Ravelo, 2007; Ma and Xu, 2005), factorization method (Pahlavani, Rahbar and Ghezelbash, 2013), path integral method (Khodja, *et a*l., 2019) and ansatz solution method (Taskin and Kocal, 2010; Qiang and Dong, 2009). The quadratic exponential-type potential (QEP) is a useful analytical model in the description of molecular and vibrational dynamics of diatomic molecules (Okorie, Ikot, Onyeaju and Chukwuocha, 2018; Ikot *et al*., 2014), it has wide applications in chemical physics, molecular, atomic and solid state physics. In a previous study, the arbitrary ℓ-state solution in D-dimensions of the Schrödinger equation with QEP was obtained by Ikot *et al*. (2014) within the frameworks of Nikiforov-Uvarov method, the Greene and Aldrich approximation scheme was used to deal with the centrifugal term of the effective potential, in their result, special cases of Woods-Saxon, Hulthén and generalized Morse potentials were considered. In a related work, Okorie *et al*. (2018) solved the Schrödinger equation in D-dimension via ansatz solution method, the Greene and Aldrich approximation scheme was also applied on the centrifugal term of the effective potential, they used their result to explore the thermodynamic properties of this potential. Ezzatpour and Akbarieh (2016) obtained the analytical solution of Klein-Gordon equation with the QEP. Motivated by the successes in the application of exact quantization rule as a solution method of the Schrödinger equation (Falaye *et al*., 2015; Ikhdair and Sever, 2009), we are encouraged to solve the radial Schrödinger equation with QEP to obtain closed form expressions for bound state energy eigenvalues and radial wave functions within the frameworks of exact quantization rule, to deal with the centrifugal term, instead of the previously used Greene and Aldrich approximation scheme by other authors, we will employ the Pekeris-type approximation scheme which has proved to be better approximation model over the Greene and Aldrich approximation scheme (Yanar *et al*., 2020), which to the best of our knowledge has not been considered by other researchers, we will use our results to deduce closed form expressions for the bound state energy eigenvalues and radial wave functions of Eckart, Hulthén and Deng-Fan potentials, we will compare our results with those in the literature where they exist.

Theoretical Formulation

Review of the concepts of exact quantization rule

Here we give a summary of the necessary concepts of exact quantization rule, the full details are given by Ma and Xu (2005). The exact quantization rule was proposed to solve the one-dimensional Schrödinger equation *viz*.

$$\psi''_{n\ell}(z)+k^2_{n\ell}(z)\psi_{n\ell}(z)=0 \qquad 1$$

where prime denotes derivative with respect to the argument, z and $k_{n\ell}$ (z) is the linear momentum of the system, it is given by:

$$k_{n\ell}(z)=\sqrt{\frac{2\mu}{\hbar^2}\left\{E_{n\ell}-V_{eff}(z)\right\}} \qquad 2$$

with μ as the mass of the system, $E_{\ell n}$ is the energy eigenvalue, V_{eff} (z) is the effective potential energy function which is a piecewise continuous real function of z. Eq. (1) can be reduced to the well-known Riccati nonlinear differential equation given by:

$$\varphi'_{n\ell}(z)+\frac{2\mu}{\hbar^2}\left\{E_{n\ell}-V_{eff}(z)\right\}+\varphi^2_{n\ell}(z)=0 \qquad (3)$$

where the phase angle, $\varphi_{n\ell}(z)=\psi'_{n\ell}(z)/\psi_{n\ell}(z)$ is the logarithmic derivative of the wave function $\psi_{n\ell}(z)$. Due to Sturm-Liouville theorem, $\varphi_{n\ell}(z)$ decreases monotonically with respect to z between two turning points determined by the equation $E_{ne} \geq V_{eff}(z)$. Particularly, increases across a node of the wave function, $\psi_{n\ell}(z)$ where, $E_{ne} \geq V_{eff}(z)$, $\varphi_{n\ell}(z)$ decreases to ∞– and jumps to ∞+ and then decreases again. By carefully studying the one-dimensional Schrödinger equation, the exact quantization rule was proposed (Ma and Xu, 2005) as:

$$\int_{z_{nA}}^{z_{nB}} k_{n\ell}(z)dx = N\pi + \int_{z_{nA}}^{z_{nB}} \varphi_{n\ell}(z)\left[\frac{dk_{n\ell}(z)}{dz}\right]\left[\frac{d\varphi_{n\ell}(z)}{dz}\right]^{-1} dz \qquad 4$$

where z_{nA} and z_{nB} are two turning points determined by solving the equation $E_{n\ell}=V_{eff}(z)$ and $z_{nA}<z_{nB}$. N is the number of nodes of $\varphi_{n\ell}(z)$ in the neighborhood of $E_{n\ell} \geq V_{eff}(z)$ and it is larger by one than the number of nodes n of the wave function $\psi_{n\ell}(z)$, clearly, $N=n+1$. The first term, $N\pi$ relates to the contribution from the nodes of the wave function, and the second term is referred to as the quantum correction. The quantum correction is independent of the number of nodes for the exactly solvable systems (Falaye *et al.*, 2015; Dong *et al* ., 2007), therefore, it can be evaluated for the ground state ($n=0$), this can conveniently be represented by:

$$Q_c=\int_{z_{nA}}^{z_{nB}} \varphi_{n\ell}(z)\left[\frac{dk_{n\ell}(z)}{dz}\right]\left[\frac{d\varphi_{n\ell}(z)}{dz}\right]^{-1} dz \equiv \int_{z_{0A}}^{z_{0B}} \varphi_{0\ell}(z)\left[\frac{dk_{0\ell}(z)}{dz}\right]\left[\frac{d\varphi_{0\ell}(z)}{dz}\right]^{-1} dx \qquad 5$$

In three dimensional spherical coordinates, the exact quantization rule assumes the following form:

$$\int_{r_{nA}}^{r_{nB}} k_{n\ell}(r)dr = N\pi + \int_{r_{nA}}^{r_{nB}} \varphi_{0\ell}(r)\left[\frac{dk_{0\ell}(r)}{dr}\right]\left[\frac{d\varphi_{0\ell}(r)}{dr}\right]^{-1} dr \qquad 6$$

In compact form, Eq. (6) can be written as:

$$I=N\pi+Q_c \qquad 7$$

where the momentum integral is given by:

$$I=\int_{r_{nA}}^{r_{nB}} k_{n\ell}(r)dr \qquad 8$$

and the quantum correction is:

$$Q_c=\int_{r_{nA}}^{r_{nB}} \varphi_{0\ell}(r)\left[\frac{dk_{0\ell}(r)}{dr}\right]\left[\frac{d\varphi_{0\ell}(r)}{dr}\right]^{-1} dr \qquad 9$$

The Schrödinger equation (Okorie *et al.*, 2020) in three dimensions for a spherically symmetric potential is given as:

$$\left\{-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}+V_{eff}(r)\right\}u_{n\ell}(r)=E_{n\ell}u_{n\ell}(r) \qquad 10$$

$u_{n\ell}(r)$ is the radial wave function, $E_{n\ell}$ is the energy eigenvalue and r is the separation

The effective quadratic exponential -type potential

The effective quadratic exponential - type potential (Okorie *et al* ., 2018; Ikot *et al* ., 2014) including the spin - orbit centrifugal term is given by:

$$V_{eff}(r)=\frac{V_0\left(p\,e^{2\delta r}+q\,e^{\delta r}+s\right)}{\left(e^{\delta r}-1\right)^2}+\frac{L\hbar^2}{2\mu r^2} \qquad 11$$

where p, q and s are adjustable constants, V_0 and δ are the potential depth and screening parameters respectively and $L=\ell(\ell+1)$. Exact solution of Eq. (10) with effective QEP of Eq. (11) is limited only to s-wave solutions. However, by employing suitable approximation scheme to deal with the spin - orbit term of the effective potential, approximate analytical solution can be obtained. In this article we will employ the Pekeris-type approximation scheme (Tang *et al*., 2014, Hamzavi *et al*., 2012), which has proved to be better than the Greene and Aldrich approximation scheme in solving the Schrödinger equation with various exponential-type potentials, the approximation model is given as:

$$\frac{1}{r^2}\cong\eta+\frac{\kappa}{e^{\delta r}-1}+\frac{\lambda}{\left(e^{\delta r}-1\right)^2} \qquad 12$$

where η, κ and λ are adjustable parameters, thus, inserting Eq. (12) in Eq. (11), this gives:

$$V_{eff}(r)=\frac{V_0\left(p\,e^{2\delta r}+q\,e^{\delta r}+s\right)}{\left(e^{\delta r}-1\right)^2}+\frac{L\hbar^2}{2\mu}\left\{\eta+\frac{\kappa}{e^{\delta r}-1}+\frac{\lambda}{\left(e^{\delta r}-1\right)^2}\right\} \qquad 13$$

using the transformation equation,

$$e^{\delta r}=1/z+1 \qquad 14$$

Eq. (14) transforms to:

$$V_{eff}(z)=\frac{\hbar^2}{2\mu}\left\{L\lambda+\frac{2\mu V_0}{\hbar^2}(p+q+s)\right\}z^2+\frac{\hbar^2}{2\mu}\left\{L\kappa+\frac{2\mu V_0}{\hbar^2}(2p+q)\right\}z+\frac{\hbar^2}{2\mu}\left(L\eta+\frac{2\mu pV_0}{\hbar^2}\right) \qquad 15$$

Introduction of the following constants:

$$\varepsilon_1^2=L\lambda+\frac{2\mu V_0}{\hbar^2}(p+q+s) \qquad 16$$

$$\varepsilon_2^2=L\kappa+\frac{2\mu V_0}{\hbar^2}(2p+q) \qquad 17$$

$$\varepsilon_3^2=L\eta+\frac{2\mu pV_0}{\hbar^2} \qquad 18$$

allows Eq. (15) to be written in the more simplified form as:

$$V_{eff}(z)=Az^2+Bz+C \qquad 19$$

where

$$A=\frac{\hbar^2\varepsilon_1^2}{2\mu} \qquad 20$$

$$B=\frac{\hbar^2\varepsilon_2^2}{2\mu} \qquad 21$$

$$C=\frac{\hbar^2\varepsilon_3^2}{2\mu} \qquad 22$$

To establish the Riccati equation (Gu and Dong, 2011; Dong *et al*., 2007), first we need to determine the turning points by imposing the requirement:

$$V_{eff}(z)=E_{n\ell} \qquad 23$$

Substituting Eq. (19) in Eq. (23) leads to:

$$Az^2+Bz+C-E_{n\ell}=0 \qquad 24$$

The turning points Z_{nA} and Z_{nB} (with $z_{nB}>z_{nA}$ which are roots Eq. (24) are given by:

$$z_{nA}=-\frac{B+\sqrt{B^2-4A\left(C-E_{n\ell}\right)}}{2A} \qquad 25$$

and

$$z_{nB}=-\frac{B-\sqrt{B^2-4A\left(C-E_{n\ell}\right)}}{2A} \qquad 26$$

From Eqs. (25) and (26), the sum and products of these roots are:

$$z_{nA}+z_{nB}=-\frac{B}{A} \qquad 27$$

$$z_{nA}\,z_{nB}=\frac{C-E_{n\ell}}{A} \qquad 28$$

For the ground (0=*n*) state, Eqs. (27) and (28) give respectively:

$$z_{0A}+z_{0B}=-\frac{B}{A} \qquad 29$$

$$z_{0A}\,z_{0B}=\frac{C-E_{0\ell}}{A} \qquad 30$$

Using Eq, (2), the momentum of the system is given by:

$$k_{n\ell}(z)=\sqrt{\frac{2\mu}{\hbar^2}\left(E_{n\ell}-Az^2-Bz-C\right)} \qquad 31$$

In what will be required later, Eq. (31) can be expressed in terms of the turning points as follows,

$$k_{n\ell}(z)=\sqrt{\frac{2\mu A}{\hbar^2}\left(\frac{C-E_{n\ell}}{A}-z^2-\frac{B}{A}z\right)} \qquad 32$$

Using Eqs. (27), (28) and (20) in (32), we find:

$$k_{n\ell}(z) = \varepsilon_1 \sqrt{(z - z_{nA})(z_{nB} - z)} \tag*{33}$$

The derivative of Eq. (33) with respect to z is given by:

$$k'_{n\ell}(z) = -\varepsilon_1 \frac{z - \frac{1}{2}(z_{nA} + z_{nB})}{\sqrt{(z - z_{nA})(z_{nB} - z)}} \tag*{34}$$

Since the ground state derivative of the momentum will be needed for evaluating the quantum correction, Eq. (34) gives for the ground state (0=n), and using Eq. (29):

$$k'_{0\ell}(z) = -\varepsilon_1 \frac{z + B/2A}{\sqrt{(z - z_{0A})(z_{0B} - z)}} \tag*{35}$$

Using Eq. (3), the Riccati equation in three dimensional spherical coordinates (Falaye *et al.*, 2015) is:

$$\varphi'_{n\ell}(r) + \frac{2\mu}{\hbar^2}\{E_{n\ell} - V_{eff}(r)\} + \varphi^2_{n\ell}(r) = 0 \tag*{36}$$

To obtain the corresponding Riccati equation in terms of variable z, we substitute Eq. (14) in (36), this results in the following first order nonlinear differential equation given by:

$$-\delta\, z(1+z)\varphi'_{n\ell}(z) + \frac{2\mu}{\hbar^2}\left(E_{n\ell} - Az^2 - Bz - C\right) + \varphi^2_{n\ell}(z) = 0 \tag*{37}$$

where we have used Eq. (19) to eliminate $V_{n\ell}(z)$. Eq. (37) gives for the ground state;

$$-\delta\, z(1+z)\varphi'_{0\ell}(z) + \frac{2\mu}{\hbar^2}\left(E_{0\ell} - Az^2 - Bz - C\right) + \varphi^2_{0\ell}(z) = 0 \tag*{38}$$

Since $\varphi_{\ell 0}$ (z) has one zero and no pole, it has to assume a linear form in z, for a trial solution, we assume:

$$\varphi_{0\ell}(y) = -c_1\, y + c_2 \tag*{39}$$

c_1 and c_2 being constants, substituting Eq. (39) in (38), get:

$$\delta\, c_1 (z + z^2) + \frac{2\mu}{\hbar^2}\left(E_{0\ell} - C - Az^2 - Bz\right) + c_1^2 z^2 - 2c_1 c_2 z + c_2^2 = 0 \tag*{40}$$

$$\left(\delta\, c_1 - \frac{2\mu A}{\hbar^2} + c_1^2\right) z^2 + \left(\delta\, c_1 - \frac{2\mu B}{\hbar^2} - 2c_1 c_2\right) y + \frac{2\mu}{\hbar^2}\left(E_{0\ell} - C\right) + c_2^2 = 0 \tag*{41}$$

By equating corresponding coefficients of z^2, z and z^0 respectively on both sides of Eq. (41), this results in the following relations:

$$c_1^2 + \delta\, c_1 = \frac{2\mu A}{\hbar^2} \equiv \varepsilon_1^2 \tag*{42}$$

$$\delta\, c_1 - 2c_1 c_2 = \frac{2\mu B}{\hbar^2} = \varepsilon_2^2 \tag*{43}$$

$$c_2^2 = \frac{2\mu}{\hbar^2}\left(C - E_{0\ell}\right) \tag*{44}$$

Therefore, solving for c^1 in Eq. (42), we obtained:

$$c_1 = -\delta\,\omega \tag*{45}$$

where

$$\omega = \tfrac{1}{2}\left\{1 + \left(1 + \frac{4\varepsilon_1^2}{\delta^2}\right)^{\frac{1}{2}}\right\} \tag*{46}$$

Clearly, Eq. (46) leads to;

$$\varepsilon_1 = \delta\left(\omega^2 - \omega\right)^{\frac{1}{2}} \tag*{47}$$

From Eq. (43), we find:

$$c_2 = \frac{\delta}{2} + \frac{\varepsilon_2^2}{2\delta\,\omega} \tag*{48}$$

Now that both c^1 and c^2 have been obtained we are in position to compute the various integrals appearing in Eq. (7), starting with the quantum correction, in terms of the variable z, Eq. (9) and (14) give:

$$Q_c = -\frac{1}{\delta}\int_{z_{0A}}^{z_{nB}} \frac{\varphi_{0\ell}(z)}{\varphi'_{0\ell}(z)} k'_{0\ell}(z) \frac{dz}{z(1+z)} \tag*{49}$$

Using Eq. (35) and (39) in (49), we have that:

$$Q_c = \frac{\varepsilon_1}{\delta}\int_{z_{0A}}^{z_{nB}} \frac{(z - c_2/c_1)(z + B/2A)}{z(1+z)} \frac{dz}{\sqrt{(z - z_{0A})(z_{0B} - z)}} \tag*{50}$$

Eq. (50) can be expressed as:

$$Q_c = \frac{\varepsilon_1}{\delta}\int_{z_{0A}}^{z_{nB}} \left\{1 - \frac{c_2 B}{2c_1 Az} - \frac{(c_1 + c_2)(2A - B)}{2c_1 A(1+z)}\right\} \frac{dz}{\sqrt{(z - z_{0A})(z_{0B} - z)}} \tag*{51}$$

The integral given by Eq. (51) can be evaluated by means of the following standard integral (Falaye *et al.*, 2015):

$$\int_{z_{nA}}^{z_{nB}} \frac{dz}{(P + Qz)\sqrt{(z - z_{nA})(z_{nB} - z)}} = \frac{\pi}{\sqrt{(P + Qz_{nB})(P + Qz_{nA})}} \tag*{52}$$

application of Eq. (52) in (51) leads to the following:

$$Q_c = \frac{\pi\,\varepsilon_1}{\delta}\left\{1 - \frac{c_2 B}{2c_1 A} I_1 - \frac{(c_1 + c_2)(2A - B)}{2c_1 A} I_2\right\} \tag*{53}$$

where

$$I_1^{-2} = z_{0A}\, z_{0B} = \frac{C - E_{0\ell}}{A} \equiv \frac{c_2^2}{\varepsilon_1^2} \tag*{54}$$

Thus, we find:

$$I_1 = \frac{\varepsilon_1}{c_2} \tag*{55}$$

similarly; we find:

$$I_2^{-2} = 1 + z_{0A} + z_{0B} + z_{0A}\, z_{0B} \tag*{56}$$

upon substituting Eq. (29) and (30) in Eq. (56), this gives:

$$I_2^{-2} = 1 - \frac{B}{A} + \frac{C - E_{0\ell}}{A} \qquad 57$$

By putting Eq. (42) – (44) in Eq. (57) we have:

$$I_2^{-2} = 1 - \frac{\delta\, c_1 - 2 c_1 c_2}{c_1^2 + \delta\, c_1} + \frac{c_2^2}{c_1^2 + \delta\, c_1} \equiv \frac{(c_1 + c_2)^2}{c_1^2 + \delta\, c_1} \qquad 58$$

so that:

$$I_2 = \frac{\left(c_1^2 + \delta\, c_1\right)^{\frac{1}{2}}}{c_1 + c_2} \equiv \frac{\varepsilon_1}{c_1 + c_2} \qquad 59$$

Substituting Eq. (55) and (59) in Eq. (53) and eliminate${}_1c$from Eq. (45), we have for the quantum correction:

$$Q_c = \frac{\pi\, \varepsilon_1}{\delta}\left(1 + \frac{\varepsilon_1}{\delta\, \omega}\right) \qquad 60$$

The other integral on the right hand side of Eq. (7) is given in terms of variable z as:

$$I = -\frac{1}{\delta}\int_{z_{nA}}^{z_{nB}} k_{n\ell}(z)\frac{dz}{z(1+z)} \qquad 61$$

Putting Eq. (45) in Eq. (61), this gives:

$$I = -\frac{\varepsilon_1}{\delta}\int_{z_{nA}}^{z_{nB}} \frac{\sqrt{(z - z_{nA})(z_{nB} - z)}}{z(1+z)}dy \qquad 62$$

In order to evaluate the integral in Eq. (62) we use the following standard integral (Falaye *et al.*, 2015)

$$\int_{z_{nA}}^{z_{nB}} \frac{\sqrt{(z - z_{nA})(z_{nB} - z)}}{z(1+Qz)}dz = \pi\left\{-\frac{1}{Q} - \sqrt{z_{nA} z_{nB}} + \frac{\sqrt{(Q z_{nA} + 1)(Q z_{nB} + 1)}}{Q}\right\} \qquad 63$$

Therefore, by using the definite integral of Eq. (63) and subsequently, Eq. (27) and (28) we obtained,

$$I = -\frac{\pi\, \varepsilon_1}{\delta}\left\{-1 - \sqrt{\frac{C - E_{n\ell}}{A}} + \sqrt{1 - \frac{B}{A} + \frac{C - E_{n\ell}}{A}}\right\} \qquad 64$$

It follows that, by substituting Eq. (60) and (64) in the exact quantization rule expressed by Eq. (7) and replacing N by $n+1$, get:

$$E_{n\ell} = \frac{\hbar^2 \varepsilon_3^2}{2\mu} - \frac{\hbar^2 \delta^2}{2\mu}\left\{\frac{\varepsilon_1^2 - \varepsilon_2^2}{2\delta^2 (n+\omega)} - \frac{n+\omega}{2}\right\}^2 \qquad 65$$

Thus, by using Eq. (16), (17), (18) and (46) to eliminate ε_1^2, , ε_2^2, ε_3^2 and ω respectively from Eq. (65), we obtained the energy eigenvalues of the QEP as:

$$E_{n\ell} = pV_0 + \frac{\ell(\ell+1)\eta\hbar^2}{2\mu} - \frac{\hbar^2\delta^2}{2\mu}\left\{\frac{\frac{2\mu V_0}{\hbar^2\delta^2}(s-p) + \frac{\ell(\ell+1)}{\delta^2}(\lambda - \kappa)}{2n+1+\sqrt{1+\frac{4\ell(\ell+1)\lambda}{\delta^2}+\frac{8\mu V_0}{\hbar^2\delta^2}(p+q+s)}} - \frac{2n+1+\sqrt{1+\frac{4\ell(\ell+1)\lambda}{\delta^2}+\frac{8\mu V_0}{\hbar^2\delta^2}(p+q+s)}}{4}\right\}^2 \qquad 66$$

Radial wave function of the quadratic exponential-type potential

By solving the R iccati equation given by Eq. (37), one obtains the function $\varphi_{n\ell}(z)$, we also need to recover the radial wave function $u_{n\ell}(z)$. Consider the following transformation relation on Eq. (37):

$$y = \frac{z}{1+z} \qquad 67$$

and using the logarithmic definition of the phase angle $\varphi_{n\ell}(z)$, we obtained:

$$y^2 u''_{n\ell}(y) + y\,u'_{n\ell}(y) + \left\{-\varepsilon_4 \frac{y^2}{(1-y)^2} + \varepsilon_5 \frac{y}{1-y} - \varepsilon_6\right\}u_{n\ell}(y) = 0 \qquad 68$$

where

$$\varepsilon_4 = \frac{2\mu A}{\delta^2\hbar^2} \qquad 69$$

$$\varepsilon_5 = -\frac{2\mu B}{\delta^2\hbar^2} \qquad 70$$

$$\varepsilon_6 = \frac{2\mu}{\delta^2\hbar^2}\left(C - E_{n\ell}\right) \qquad 71$$

Eq. (68) has solution (Eyube *et al.*, 2019b) given by:

$$u_{n\ell}(y) = N_{n\ell}\, y^{\tau}(1-y)^{\upsilon} f_{n\ell}(y) \qquad 72$$

where the constants τ, υ and the function $f_{n\ell}(y)$ are chosen such that:

$$\tau = \varepsilon_6^{\frac{1}{2}} \qquad 73$$

$$\upsilon^2 - \upsilon = \varepsilon_4 \qquad 74$$

and $f_{n\ell}(y)$ is the Gaussian hypergeometric function given by:

$$f_{n\ell}(y) = {}_2F_1(-n, n+2\tau+2\upsilon; 2\tau+1; y) \qquad 75$$

The normalization constant, $N_{n\ell}$ is evaluated from normalization condition, following Qiang and Dong (2009), we find:

$$N_{n\ell} = \left(\frac{\delta}{M}\right)^{\frac{1}{2}} \qquad 76$$

with M given by

$$M = \frac{n!(n+\upsilon)\Gamma(n+2\upsilon)\Gamma(2\tau)\Gamma(2\tau+1)}{(n+\tau+\upsilon)\Gamma(n+2\tau+1)\Gamma(n+2\tau+2\upsilon)} \qquad 77$$

Results and Discussion

By choosing appropriate values for the parameters p, q, s, η, κ and λ, we can use our results for effective potential and energy eigenvalues of QEP given by Eqs. (13) and (66) to deduce effective potential and energy eigenvalues of other potential models.

The Hulthén potential

If we choose $p = 0$, $q = -s = -Ze^2\delta$ and $V_0 = 1$, Eqs. (13) yield:

$$V_{eff}(r) = -\frac{Ze^2\delta}{e^{\delta r}-1} + \frac{L\hbar^2}{2\mu}\left\{\eta + \frac{\kappa}{e^{\delta r}-1} + \frac{\lambda}{(e^{\delta r}-1)^2}\right\} \qquad 78$$

$$E_{n\ell} = \frac{\ell(\ell+1)\eta\hbar^2}{2\mu} - \frac{\hbar^2\delta^2}{2\mu}\left\{\frac{\frac{2\mu Ze^2}{\delta\hbar^2} + \frac{\ell(\ell+1)}{\delta^2}(\lambda-\kappa)}{2n+1+\sqrt{1+\frac{4\ell(\ell+1)\lambda}{\delta^2}}} - \frac{2n+1+\sqrt{1+\frac{4\ell(\ell+1)\lambda}{\delta^2}}}{4}\right\}^2 \qquad 79$$

Letting $\eta = 0$, $\kappa = \omega\delta^2$ and $\lambda = \delta^2$, Eq. (78) and (79) reduces to the effective Hulthén potential and the corresponding energy eigenvalue derived by Jia *et al*. (2008). In the same manner, if we let $\eta = \delta^2 d_0$, $\kappa = \lambda = \delta^2$ in Eqs. (78) and (79) respectively we get the effective Hulthén potential and the energy eigenvalues derived by Ikhdair (2009).

The Eckart potential

By suitable choice of parameters, the Eckart potential is considered here as a special case of the QEP , choosing $p = 0$, $q = \beta - \alpha$, $s = \alpha$ and $V_0 = 1$, Eqs. (13) and (66) give the effective Eckart potential as

$$V_{eff}(r) = -\frac{\alpha}{(e^{\delta r}-1)^2} + \frac{\beta e^{\delta r}}{(e^{\delta r}-1)^2} + \frac{L\hbar^2}{2\mu}\left\{\eta + \frac{\kappa}{e^{\delta r}-1} + \frac{\lambda}{(e^{\delta r}-1)^2}\right\} \qquad 80$$

and the energy eigenvalues of the Eckart potential as:

$$E_{n\ell} = \frac{\ell(\ell+1)\eta\hbar^2}{2\mu} - \frac{\hbar^2\delta^2}{2\mu}\left\{\frac{\frac{2\mu\alpha}{\hbar^2\delta^2} + \frac{\ell(\ell+1)}{\delta^2}(\lambda-\kappa)}{2n+1+\sqrt{1+\frac{4\ell(\ell+1)\lambda}{\delta^2}+\frac{8\mu\beta}{\hbar^2\delta^2}}} - \frac{2n+1+\sqrt{1+\frac{4\ell(\ell+1)\lambda}{\delta^2}+\frac{8\mu\beta}{\hbar^2\delta^2}}}{4}\right\}^2 \qquad 81$$

Taking $\eta = 0$, $\delta = 1/a$, $\kappa = \xi/a^2$ and replacing λ by λ/a in Eqs. (80) and (81) reproduces the effective Eckart potential and energy eigenvalues respectively as obtained by Taskin and Kocal (2010)

The Deng-Fan potential

The Deng-Fan potential has been reported to be very important in the description of diatomic molecular energy spectra and electromagnetic transitions (Diaf, 2014). If we choose $p = 1$, $q = -2e^{\delta r_e}$, $s = e^{2\delta r_e}$ and $V_0 = D_e$, effective QEP given by Eq. (13) transforms to the effective Deng-Fan potential *viz*:

$$V_{eff}(r) = D_e\left(1 - \frac{e^{\delta r_e} - 1}{e^{\delta r} - 1}\right)^2 + \frac{L\hbar^2}{2\mu}\left\{\eta + \frac{\kappa}{e^{\delta r} - 1} + \frac{\lambda}{\left(e^{\delta r} - 1\right)^2}\right\} \qquad 82$$

where D_e is the dissociation energy and r_e is the equilibrium bond length, it follows that by substituting the values of these parameters in Eq. (66), the energy eigenvalues of the Deng-Fan molecular potential can be deduced as:

$$E_{n\ell} = D_e + \frac{\ell(\ell+1)\eta\hbar^2}{2\mu} - \frac{\hbar^2\delta^2}{2\mu}\left\{\frac{\frac{2\mu D_e}{\hbar^2\delta^2}\left(e^{2\delta r_e} - 1\right) + \frac{\ell(\ell+1)}{\delta^2}(\lambda - \kappa)}{2n+1+\sqrt{1+\frac{4\ell(\ell+1)\lambda}{\delta^2}+\frac{8\mu D_e}{\hbar^2\delta^2}\left(e^{\delta r_e}-1\right)^2}} - \frac{2n+1+\sqrt{1+\frac{4\ell(\ell+1)\lambda}{\delta^2}+\frac{8\mu D_e}{\hbar^2\delta^2}\left(e^{\delta r_e}-1\right)^2}}{4}\right\}^2 \qquad 83$$

To test the accuracy of our results, we have used Eq. (83) to compute bound state energy eigenvalues of six diatomic molecules: HCl, LiH, H_2, SeH, VH and TiH. Following Tang *et al*. (2014), we have chosen the parameters η, κ and λ such that:

$$\eta = 1 + \frac{1}{\delta r_e^2}\left(1 - e^{-\delta r_e}\right)\left(3 + e^{-\delta r_e}\right) - \frac{3}{\delta^2 r_e^3}\left(1 - e^{-\delta r_e}\right)^2 \qquad 84$$

$$\kappa = \frac{2e^{\delta r_e}}{\delta r_e^2}\left(1 - e^{-\delta r_e}\right)^2\left(2 + e^{-\delta r_e}\right) - \frac{6e^{\delta r_e}}{\delta^2 r_e^3}\left(1 - e^{-\delta r_e}\right)^3 \qquad 85$$

$$\lambda = -\frac{e^{2\delta r_e}}{\delta r_e^2}\left(1 - e^{-\delta r_e}\right)^3\left(1 + e^{-\delta r_e}\right) + \frac{3e^{2\delta r_e}}{\delta^2 r_e^3}\left(1 - e^{-\delta r_e}\right)^4 \qquad 86$$

The data in Table 1 (Oyewumi, Oluwadare, Sen and Babalola, 2012) shows model parameters of the diatomic molecules used in our computation of bound state energy eigenvalues.

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

molecule	D_e (eV)	r_e (Å)	δ ($Å^{-1}$)	μ (amu)
HCl	4.619061175	1.2746	1.8677	0.9801045
LiH	2.515283695	1.5956	1.1280	0.8801221
H_2	4.7446	0.7416	1.9426	0.50391
SeH	2.25	1.776	1.41113	0.986040
VH	2.33	1.719	1.44370	0.988005
TiH	2.05	1.781	1.32408	0.987371

The results shown in Table 2 are computed bound state energy eigenvalues for HCl, LiH, H_2, SeH, VH and TiH. To enable us compare results with existing data in the literature, we have included bound state energy eigenvalues of the Deng-Fan potential obtained within the frameworks of Nikiforov-Uvarov (NU) via the improved Greene and Aldrich approximation scheme. Comparison of the present result (PR) and that obtained by NU method shows excellent agreement for the case of $\ell = 0$, both EQR and NU methods give exact analytical solutions for the s-wave. However, for the other states with $\ell \neq 0$, approximation schemes used contributes to the analytical solutions, the results tends to be in good agreement for higher quantum states. Figures 1 and 2 shows plots in atomic units ($\mu = \hbar = 1$) and $\delta = 0.025$, $V_0 = 1$ of normalized radial wave functions (Fig 1a and 2a) given by Eq. (77) and corresponding probability amplitude (b) given by $\left|u_{n\ell}(y)\right|^2$ in atomic units (Fig 1b and 2b) for state 4d. The probability density measures the likelihood of were the system can be located, in Figures 1b and 2b, the plots show that the probability is greatest in the region $0.1 \le y \le 0.2$

Table 2: bound state energies (in eV) for HCl, LiH, H_2, SeH, VH and TiH

state		HCl		LiH		H_2	
		PR	NU	PR	NU	PR	NU
0	0	0.201982172	0.201984174	0.103333625	0.103334650	0.349976783	0.349980221
	1	0.208460872	0.204854248	0.108230843	0.105236729	0.390745131	0.364688765
1	0	0.590742124	0.590747827	0.302003040	0.302005955	0.996767785	0.996777053
	1	0.597127567	0.593537612	0.306826349	0.303838653	1.036337565	1.010323238
2	0	0.960002027	0.960011044	0.490681252	0.490685861	1.580234480	1.580248366
	1	0.966295369	0.962721591	0.495432293	0.492450759	1.618675505	1.592700793
	2	0.978880787	0.968141645	0.504932694	0.495978997	1.695489068	1.617539648
3	0	1.310015915	1.310027865	0.669594907	0.669601019	2.104068759	2.104086156
	1	1.316218292	1.312660203	0.674275270	0.671299648	2.141445176	2.115507769
	2	1.328621793	1.317923855	0.683634354	0.674695388	2.216133717	2.138289195
	3	1.347223909	1.325816775	0.697668878	0.679785205	2.328006349	2.172307398
4	0	1.641032731	1.641047243	0.838963132	0.838970564	2.571660549	2.571680443
	1	1.647145259	1.643602379	0.843574355	0.840604402	2.608031385	2.582129083
	2	1.659369075	1.648711644	0.852795199	0.843870601	2.680712650	2.602968445
	3	1.677701697	1.656373023	0.866622457	0.848766203	2.789584050	2.634083222
	4	1.702139403	1.666583499	0.885051328	0.855286782	2.934466410	2.675301759

state		SeH		VH		TiH	
		PR	NU	PR	NU	PR	NU
0	0	0.104849655	0.104850694	0.109282618	0.109283701	0.095194192	0.095195135
	1	0.108121346	0.106349671	0.112776716	0.110873673	0.098494294	0.096647888
1	0	0.306243588	0.306246538	0.319112328	0.319115401	0.277946427	0.277949104
	1	0.309466023	0.307704129	0.322553285	0.320660504	0.281195886	0.279358078
2	0	0.496946039	0.496950687	0.517706915	0.517711754	0.450920200	0.450924416
	1	0.500119783	0.498367397	0.521095362	0.519212554	0.454119699	0.452290234
	2	0.506466640	0.501200316	0.527871554	0.522213593	0.460517950	0.455021255
3	0	0.677087059	0.677093198	0.705207485	0.705213873	0.614253922	0.614259487
	1	0.680212672	0.678469522	0.708544045	0.706670923	0.617404131	0.615582758
	2	0.686463269	0.681221677	0.715216467	0.709584473	0.623703811	0.618228694
	3	0.695837596	0.685348677	0.725223358	0.713953418	0.633151486	0.622196086
4	0	0.846794248	0.846801673	0.881752400	0.881760121	0.768082994	0.768089723
	1	0.849872278	0.848138097	0.885037683	0.883173966	0.771184571	0.769371041
	2	0.856027714	0.850810460	0.891607559	0.886001113	0.777386995	0.771933083
	3	0.865259311	0.854817791	0.901460646	0.890240476	0.786688808	0.775774658
	4	0.877565203	0.860158632	0.914594870	0.895890425	0.799087823	0.780893985

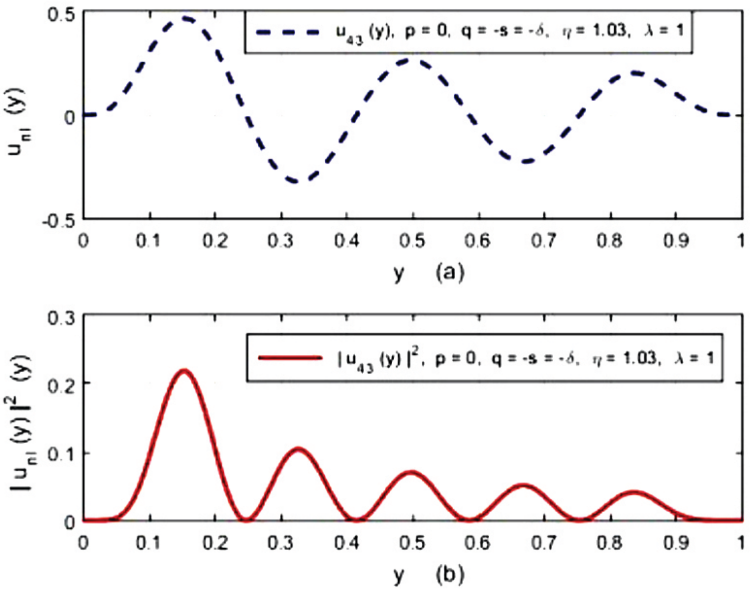

Figure 1 Normalized radial wave function (a) and probability density function (b) of QEP for 4d state

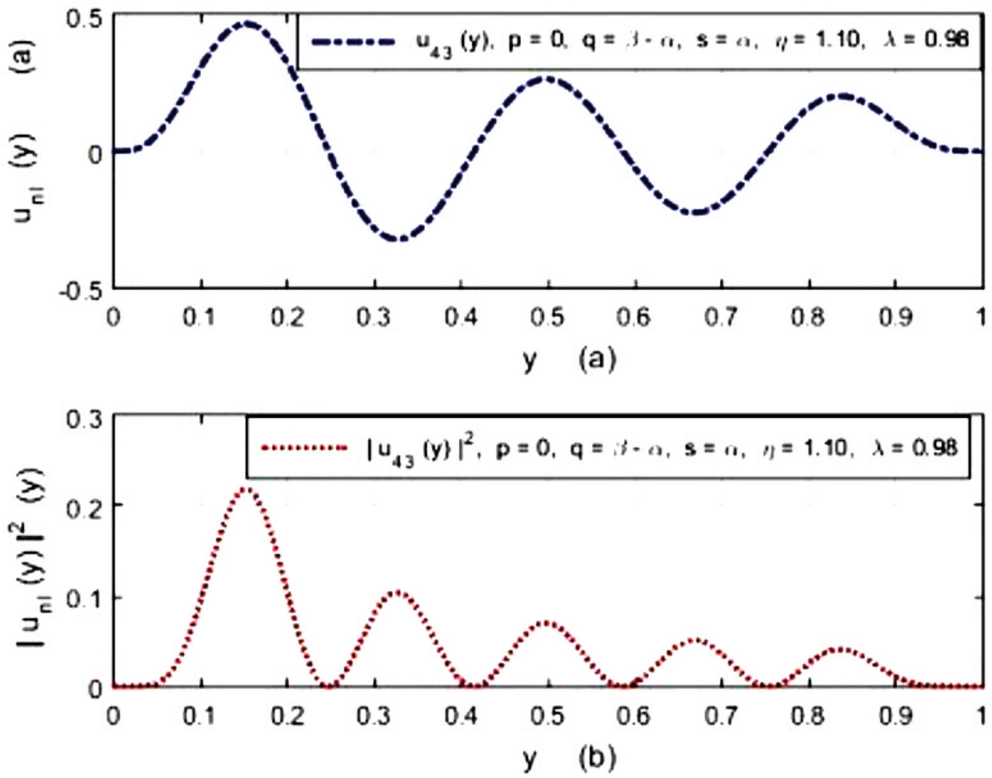

Figure 2 Normalized radial wave function (a) and probability density function (b) of QEP, $\alpha = 40$, $\beta = 0.00005$ for 4d state

Conclusion

In this article we have employed the ideas of exact quantization rule and ansatz solution method to obtain closed form expressions for the bound state energy eigenvalues and normalized radial wave functions of a molecule in a quadratic exponential-type potential, expressions for the bound state energy eigenvalues of the Hulthén, Eckart and Deng-Fan potentials were obtained when considered as special cases of the quadratic exponential-type potential. The results in this article may be useful in areas of solid state physics, atomic, molecular and chemical physics.

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