Non-relativistic Energy Spectrum of the Deng-Fan Oscillator via the WKB Approximation Method

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Author’s contribution

The sole author designed, analysed, interpreted and prepared the manuscript.

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ABSTRACT

The energy spectrum of the radial Schrodinger equation with the molecular Deng Fan potential has been obtained through the WKB approximation scheme. The radial WKB solution yields a transcendental or an implicit equation. The energy eigenvalues for non-physical and real molecular interacting systems are presented. In comparison with the numerical eigenvalues obtained with MATHEMATICA 3.0 package, the WKB approximation method produces improved results over the results obtained with other analytical methods in the literature.

Keywords: Deng-Fan potential; diatomic molecules; WKB approximation method; Schrodinger equation.

1. INTRODUCTION

The Deng-Fan potential (DFP) has garnered interest recently in chemical and molecular physics for the study of diatomic molecular interacting systems [1]. The potential was proposed by Deng and Fan [2] to account for the irregular behavior of the Morse Oscillator as the...
intermolecular distance \((r)\) approaches zero and infinity \([3]\). Rong et al. \([4]\) states that the DFP has the correct physical boundary conditions at \(r = 0\) and \(r = \infty\). This potential is used in applied physics to study the ro-vibrational states of diatomic molecules. The mathematical representation of the potential as proposed by Deng and Fan \([2]\) is given as

\[
V(r) = D_e \left[ 1 - \frac{b}{e^{\alpha r} - 1} \right]^2, b = e^{\alpha r} - 1, \ r \in (0, \infty) \quad (1)
\]

Where \(D_e\) is the potential depth, \(r_e\) is the internuclear distance, \(\alpha\) is a parameter that determines the range of the potential. The potential is long-range for large \(\alpha\) and short range for small parameter of \(\alpha\). The constant \(b\) is the position of minimum \(r_e\) and \(r\) is the radius of the potential.

The solutions of the bound states of the Schrodinger equation (SE) with the molecular Deng-Fan \(-\) type potential have been reported in the literature \([1,3-12]\). The relativistic bound states solutions of the Deng-Fan potential have also been presented in the literature \([13,14]\).

Several methods have been used to solve wave equations for potential of interest. For the molecular DFP, the quantum system is exactly solvable for the s-wave case using some analytical approaches. However, the solution is not trivial for any arbitrary angular momentum quantum number \(l\) arising from the centrifugal barrier term of the effective potential. In such a case, the wave equation can be approximated by an appropriate analytical technique and numerical method. Oyewume et al. \([3]\) states that the frequently used approximations to deal with the centrifugal term is the Pekeris-type approximation scheme \([15]\) and the one proposed by Greene and Aldrich \([16]\) for short range potential. These approximations enable the solubility of the quantum system of choice for any \(l\) states quantum numbers. Several analytical techniques have been used to solve the SE with the molecular Deng-Fan type potential. Roy \([1]\) obtained the bound states of the SE with the shifted DFP using the generalized pseudospectral (GPS) method. The energy eigenvalues for the diatomic molecules \(\text{H}_2, \text{LiH}, \text{HCl}, \text{CO}\) were obtained for low and high lying vibrational \((n)\) and rotational \((l)\) quantum numbers. Using the Nikiforov- Uvarov (NU) method, Oyewumi et al. \([3]\) obtained bound states of the DFP. They compared their results with the results obtained with other methods in the literature. The potential has been used to calculate the transition frequencies and intensities overtones of \(X-H\) stretching vibrations \([4]\). Diaw \([6]\) obtained the bound state of the SE using the Feynman Integral Method (FIM). Dong and Gu \([5]\) applied an approximation technique to obtain the energy eigenvalues of the DFP. The authors \([5,6]\), compared their results with the energy eigenvalues obtained with the numerical support of MATHEMATICA packet for short range potential \([17]\) as reported in Dong and Gu \([5]\). Oyewumi et al. \([9]\), using the Asymptotic Iterative Method (AIM), studied the thermodynamic properties including the bound state of the SE with the DFP. Hamzavi et al. \([10]\) applied the NU and the Amplitude Phase (AP) methods to estimate the energy spectrum of the SE confined by the shifted DFP. Other methods such as the Exact Quantization Rule (EQR) \([11]\) and the Wentzel-Kramers-Brillouin (WKB) approximation scheme \([12]\) have been applied to find the bound energy eigenvalues of the SE with the shifted DFP. The authors in Oluwadare and Oyewumi \([11]\) obtained the energy spectra and the expectation values of some diatomic molecules generated by the shifted Deng-Fan potential. While Amos et al. \([12]\) obtained the analytical bound state solution of the SE in closed form.

In this present work, we used similar method employed by the authors in Amos et al. \([12]\) to obtain the energy eigenvalues of the molecular DFP. The radial solution of the SE with both the DFP and shifted DFP using the WKB method does not yield a closed form energy expression but rather, it gives a transcendental-type or an implicit equation. In order to test the correctness of the result obtained in this present work, the energy eigenvalues were obtained with the help of MAPLE 18 programme. Furthermore, the energy spectra are obtained for a few selected diatomic molecules such as \(\text{HCl}, \text{LiH}\) and \(\text{SiH}\). Furthermore, by taking the energy difference \((E_n - D_e)\), the energy eigenvalues for the shifted DFP were obtained for \(\text{HCl}\) and \(\text{LiH}\) diatomic molecules. The results show good agreement with the ones obtained by other analytical and numerical methods in the literature and thus indicates that it can be extended to the investigation of other diatomic molecules.

The paper is organized as follows. In section two, we recycle the synopsis of the WKB approximation method in order to make the paper self-contained. Section three contains the analytical bound state solution of the radial SE
generated by the DFP. Numerical results are presented in section four including the possible comparison with other analytical and numerical solutions in the literature. The paper is concluded in section five.

2. THE WKB APPROXIMATION METHOD

In quantum mechanics, the WKB approximation method offers a way of finding approximate solutions of linear differential equations. This semi-classical quantization approximation method has been treated in pedagogical textbooks [18,19]. For the Schrodinger equation, it is used to investigate tunneling rates through a potential barrier and also for the calculation of the energy eigenvalues of potentials of interest. This method is straightforward in that if we know the classical momentum of a quantum particle, then we can obtain the energy eigenvalues with the help of the WKB quantization integral. The method fails at the classical turning points where the energy just equals the potential energy or where the classical momentum vanishes (P(r) = 0). The WKB method yields accurate energy eigenvalues for large values of the radial quantum number and is also accurate for slow varying potentials functions. However, their accuracy varies quite markedly for the ground and other low lying states depending on the potential of interest [20]. Also, the approximation scheme does not yield an exact energy eigenvalues of the radial SE [21]. In order to circumvent this problem, the centrifugal barrier term l(l + 1)ℏ^2/2μr^2 in the effective potential of the radial SE has to be replaced with the term \( l^2 \frac{h^2}{2μr^2} \). This modification is known as the Langer correction [22]. Sergeenko [23], state that the Langer correction regularizes the WKB wave function at the origin and ensures correct asymptotic behaviour at large radial quantum numbers. This implies that the centrifugal barrier term is non-vanishing at \( l = 0 \). This also makes the WKB quantization integral unsolvable for some potential. In such case an approximate approximation scheme is required to deal with the centrifugal barrier term.

The three-dimensional time-independent SE with a reduced mass \( μ \) and wave-function \( ψ(\vec{r}, θ, φ) \) is given as

\[
-\frac{\hbar^2}{2μ} \frac{1}{\sin θ} \frac{\partial}{\partial \theta} (\sin θ \frac{\partial}{\partial \theta}) + \frac{1}{r^2 \sin^2 θ} \frac{\partial^2}{\partial φ^2} ψ + V(\vec{r})ψ(\vec{r}, θ, φ) = Eψ(\vec{r}, θ, φ).
\]

(2)

Using the method of separation of variables in Eq. (2) we can separate the equation into the radial part and the angular part by using the transformation \( ψ(\vec{r}, θ, φ) = \frac{R(r)}{r} Y(θ, φ) \).

With the appropriate separation constant, we will obtain the radial SE as

\[
\frac{d^2 R(r)}{dr^2} + \frac{2μ}{ℏ^2} [E - V_{eff}(r)] R(r) = 0.
\]

(3)

where the effective potential \( V_{eff}(r) \) is given as

\[
V_{eff}(r) = V(r) + \frac{(l^2 + \frac{1}{2}) h^2}{2μr^2}
\]

(4)

We can rewrite Eq. (3) as

\[
\left[ -\frac{\hbar^2}{2μ} \frac{d^2}{dr^2} \right] R(r) = 2μ \left[ E - V(r) - \frac{(l^2 + \frac{1}{2}) h^2}{2μr^2} \right] R(r).
\]

(5)

Equation (5) is a momentum eigenvalue equation with the classical momentum obtained as

\[
P(r) = \left[ 2μ \left[ E - V(r) - \frac{(l^2 + \frac{1}{2}) h^2}{2μr^2} \right] \right]^{\frac{1}{2}}.
\]

(6)

The standard WKB quantization condition [20,23] for a two turning point \( (r_1, r_2) \) problem is given as

\[
∫_{r_1}^{r_2} P(r)dr = \pi \hbar \left( n + \frac{1}{2} \right), \ r_1 < r < r_2 \quad n = 0, 1, 2 \ldots
\]

(7)

The turning points are gotten from Eq. (6) by setting \( P(r) = 0 \).

The semi-classical wave function in the leading \( \hbar \) approximation has the form

\[
ψ^{WKB}(r) = \frac{N}{\sqrt{P(r)}} \exp \left[ ± \frac{i}{\hbar} ∫ P(r)dr \right].
\]

(8)

3. ENERGY EIGENVALUE SOLUTION OF THE RADIAL SCHRODINGER EQUATION

To obtain the energy eigenvalues expression, we will substitute the DFP given in Eq. (1) into the momentum eigenvalues equation given by Eq. (5)
\[
\left[\left(\frac{\hbar a}{dr}\right)^2\right] R(r) = 2\mu \left[E - D_e \left[1 - \frac{b}{e^{ar} - 1}\right]^2 \right] - \frac{(i+\frac{3}{2})^2}{2\mu r^2} R(r) 
\]

From Eq. (9), we obtained the classical momentum as

\[
P(r) = 2\mu \left[E - D_e \left[1 - \frac{b}{e^{ar} - 1}\right]^2 \right] - \frac{(i+\frac{3}{2})^2}{2\mu r^2} 
\]

If we substitute the momentum into the semi-classical quantization condition given in Eq. (7), then we will obtain

\[
\sqrt{2\mu \int_{r_1}^{r_2} \left[E - D_e \left[1 - \frac{b}{e^{ar} - 1}\right]^2 \right] - \frac{(i+\frac{3}{2})^2}{2\mu r^2} dr = \pi \hbar \left(n + \frac{1}{2}\right)} \quad r_1 < r < r_2 
\]

With the WKB approximation method, Eq. (11) is exactly solvable without the centrifugal barrier term but not solvable for any arbitrary \(l\)-states. To find the solution of the SE including the centrifugal term, the Pekeris-type approximation has been used [3,6,9-11] to deal with the centrifugal term of the effective potential, by letting

\[
\frac{1}{r^2} \sim \alpha^2 \left[c_0 + \frac{e^{ar}}{(e^{ar} - 1)^2}\right] 
\]

where \(c_0\) is a dimensionless constant with a value \(9\) \(c_0 = 1.120315\).

If we substitute Eq. (12) into (11) we will obtain

\[
\sqrt{2\mu \int_{r_1}^{r_2} \left[E - D_e \left[1 - \frac{b}{e^{ar} - 1}\right]^2 \right] - \frac{(i+\frac{3}{2})^2}{2\mu r^2} \left[c_0 + \frac{e^{ar}}{(e^{ar} - 1)^2}\right] \left[\frac{r}{2\mu}\right]^\frac{1}{2} dr = \pi \hbar \left(n + \frac{1}{2}\right)} 
\]

Now we let \(y = e^{ar} - 1\), \(y \in [0, \infty]\),

\[
dy = \alpha e^{ar} \alpha(1 + y) dy, 
\]

By changing variable from \(r\) to \(y\) in Eq. (13), we will get

\[
\sqrt{2\mu \int_{y_1}^{y_2} \left[E - D_e \left[1 - \frac{b}{e^{ar} - 1}\right]^2 \right] - \frac{(i+\frac{3}{2})^2}{2\mu r^2} \left[c_0 + \frac{e^{ar}}{(e^{ar} - 1)^2}\right] \left[\frac{r}{2\mu}\right]^\frac{1}{2} dy = \pi \hbar \left(n + \frac{1}{2}\right)} 
\]

If we collect liked terms of the terms inside the squared root of Eq. (15), and simplify, then we will have

\[
\sqrt{\frac{2\mu}{\alpha^2} \int_{y_1}^{y_2} dy \frac{y^{3/2}}{\gamma(1+y)} \left[E y^2 - D_e y^2 + 2D_e by - D_e b^2 - \frac{(i+\frac{3}{2})^2}{2\mu} \hbar^2 y^2 \alpha^2 c_0 - \frac{\hbar^2 a^2 (i+\frac{3}{2})^2}{2\mu} y \gamma^2 a^2 (i+\frac{3}{2})^2 \right]^{\frac{1}{2}}} = \pi \hbar \left(n + \frac{1}{2}\right) 
\]

where

\[
N = D_e - E + \hbar^2 a^2 \left(l + \frac{1}{2}\right)^2 c_0 
\]

\[
W = 2D_e b^2 + \hbar^2 a^2 \left(l + \frac{1}{2}\right)^2 
\]

\[
T = D_e b^2 + \hbar^2 a^2 \left(l + \frac{1}{2}\right)^2 
\]

Equation (16) can further be simplified as

\[
\sqrt{\frac{2\mu}{\alpha^2} \int_{y_1}^{y_2} dy \frac{y^{3/2}}{\gamma(1+y)} \left[-y^2 + By - C\right]^{\frac{1}{2}}} = \pi \hbar \left(n + \frac{1}{2}\right) 
\]

where

\[
B = \frac{W}{N}, 
\]

\[
C = \frac{T}{N} 
\]

To evaluate Eq. (20), we make use of the transformation

\[
z = 1 + 2y \quad z \in (1, \infty) 
\]

By changing variable from \(y\) to \(z\) in Eq. (20), implies that

\[
\sqrt{\frac{2\mu}{\alpha^2} \int_{z_{-1}}^{z_1} \frac{dz}{\gamma^{2} - 1} \sqrt{-z^2 + Fz - G}} = \pi \hbar \left(n + \frac{1}{2}\right), 
\]

where

\[
F = 2 + 2B 
\]

\[
G = 1 + 2B + 4C 
\]
The turning points $z_2$ and $z_1$ are given by
\[ z_1 = \frac{-\sqrt{F^2 - 4G}}{2} \quad (27) \]
\[ z_2 = \frac{F + \sqrt{F^2 - 4G}}{2} \quad (28) \]

We can write Eq. (24) in a regular form as
\[ \int_{z_1}^{z_2} \frac{dz}{z(z - z_1)(z - z_2)} = \frac{\pi}{2} \left( \frac{1}{z_1} + \frac{1}{z_2} \right) \quad (29) \]

With the help of the semi-classical quantization integral standard given in Hruska et al. [20] we have
\[ \int_{z_1}^{z_2} \frac{dz}{z(z - z_1)(z - z_2)} = \frac{\pi}{2} \left( \frac{1}{z_1} + \frac{1}{z_2} \right) - \frac{1}{2} \left( \frac{1}{z_1} - \frac{1}{z_2} \right) \quad (30) \]

By comparing Eq. (29) and (30), implies that
\[ \sqrt{\frac{2\mu N}{\alpha^2}} \left( \frac{1}{z_1} + \frac{1}{z_2} \right) - \frac{1}{2} \left( \frac{1}{z_1} - \frac{1}{z_2} \right) = 2\hbar \left( n + \frac{1}{2} \right) \quad (31) \]

With the help of Eqs. (27) and (28), Eq. (31) becomes
\[ \sqrt{\frac{2\mu N}{\alpha^2}} \left[ \sqrt{1 + F + G} - \sqrt{1 - F + G} \right] = 2\hbar \left( n + \frac{1}{2} \right) \quad (32) \]

Next we substitute $F$ and $G$ given in the respective Eqs. (25) and (26) into Eq. (32) to obtain
\[ \sqrt{\frac{2\mu N}{\alpha^2}} \left[ \sqrt{1 + B + C} - \sqrt{1 - B + C} \right] = \hbar \left( n + \frac{1}{2} \right) \quad (33) \]

Recalling the notations $B$ and $C$ given in Eqs. (21) and (22), Eq. (33) can be written as
\[ \sqrt{\frac{2\mu N}{\alpha^2}} \left[ \sqrt{1 + \frac{W}{N} + \frac{\nu}{N} - \frac{\nu}{N} - 1} \right] = \hbar \left( n + \frac{1}{2} \right) \quad (34) \]

Finally, substituting the notations $N, W$ and $\nu$ in Eqs. (17-19) into Eq. (34) with some algebraic simplifications, we obtained the energy eigenvalues equation of the Deng-Fan Potential as
\[ \sqrt{\frac{2\mu (D_v (b+1)^2 - E_{\text{nu}})}{\hbar^2 \alpha^2}} + c_0 \left( l + \frac{1}{2} \right)^2 - \sqrt{\frac{2\mu D_v \hbar^2}{\hbar^2 \alpha^2}} + \left( l + \frac{1}{2} \right)^2 - \sqrt{\frac{2\mu (D_v - E_{\text{nu}})}{\hbar^2 \alpha^2}} + c_0 \left( l + \frac{1}{2} \right)^2 = \left( n + \frac{1}{2} \right) \quad (35) \]

4. NUMERICAL RESULTS

The energy eigenvalue equation has been found with the use of the WKB approximation method. The result shows that the WKB approximation method does not yield a close form solution for either the DFP or the shifted DFP but rather produces a transcendental-type or an implicit equation. This however is in contrast to the analytical work of Amos and coworkers [12] where they obtained a closed form solution of the shifted DFP with the use of the WKB method. In order to test the accuracy of Eq. (35), the energy spectra for the 2p, 3p, 3d, 4p, 4d, 4f, 5p, 5d, 5f, and 5g quantum states are obtained using MAPLE programme with the arbitrary spectroscopic parameters $D_v$, $r_v$, and $\alpha$ as shown in Tables 2-3. Also, Eq. (35) can be applied to generate the energy eigenvalues of physical systems. To achieve this, the ro-vibrational energy spectrum of some selected diatomic molecules (HCl, LiH and ScH) confined by the DFP are obtained (see Table 4). Furthermore we show that the energy difference $(E_{\text{nu}} - D_v)$ using Eq. (35) is an equivalence of the energy eigenvalues for the shifted DFP (See Tables 5-6). The spectroscopic parameters for the HCl, LiH and ScH molecules were taken from Oyewumi et al. [3] and tabulated in Table 1. We used the conversions $\hbar c = 1973.29$ eVÅ, 1 amu = 931.494028 MeV/c² reported in Falaye et al. [24].

| Molecules | $D_v$(eV) | $r_v$(Å) | $\alpha$(Å⁻¹) | $\mu$(a.m.u.) |
|-----------|-----------|-----------|----------------|---------------|
| HCl       | 4.619061175 | 1.2746    | 1.8677         | 0.981045      |
| LiH       | 2.515283695 | 1.5956    | 1.1280         | 0.8801221     |
| ScH       | 2.25      | 1.776     | 1.41113        | 0.986040      |

Table 1. Spectroscopic parameters for HCl, LiH and ScH diatomic molecules taken from Oyewumi et al. [3]
Table 2. Comparison of ro-vibrational energy eigenvalues $E_{nl}$(eV) for the DFP with spectroscopic parameters $r_e = 0.4$ Å and $D_e = 15$ a.u.
with $\hbar = \mu = 1$

| State | $\alpha$ | This work | NU [3] | AIM [9] | Numerical [5] | Approx. [5] | FIM[6] | GPS [1] |
|-------|----------|-----------|--------|---------|---------------|-------------|--------|--------|
| 2p    | 0.05     | 7.860830507 | 7.860804493 | 7.860804467 | 7.8628 | 7.8606 | 7.86080 | 7.860804466 |
|       | 0.10     | 7.953408639 | 7.953304454 | 7.953304350 | 7.95537 | 7.95247 | 7.95329 |
|       | 0.15     | 8.045338000 | 8.045099870 | 8.045099635 | 8.04724 | 8.04322 | 8.04508 |
|       | 0.20     | 8.136619920 | 8.136203372 | 8.136203356 | 8.13842 | 8.13287 | 8.13613 |
|       | 0.25     | 8.227279483 | 8.226629167 | 8.226628516 | 8.22892 | 8.22142 | 8.22655 |
|       | 0.30     | 8.317325475 | 8.316389030 | 8.316388092 | 8.31874 | 8.30869 | 8.31629 |
| 3p    | 0.05     | 10.99778906 | 10.99776305 | 10.99776302 | 10.9998 | 10.9976 | 10.99776 |
|       | 0.10     | 11.16266460 | 11.16256046 | 11.16256036 | 11.1647 | 11.1617 | 11.16255 |
|       | 0.15     | 11.32448272 | 11.32424872 | 11.32424848 | 11.32647 | 11.3224 | 11.32422 |
|       | 0.20     | 11.48325379 | 11.48283762 | 11.48283721 | 11.48513 | 11.4795 | 11.48280 |
|       | 0.25     | 11.63898698 | 11.63833667 | 11.63833602 | 11.64068 | 11.6331 | 11.63827 |
|       | 0.30     | 11.79169146 | 11.79075502 | 11.79075408 | 9.67565 | 9.7833 | 11.79066 |
| 3d    | 0.05     | 10.21600623 | 10.21598027 | 10.21598019 | 10.21651 | 10.2154 | 10.21597 |
|       | 0.10     | 10.35364341 | 10.35353947 | 10.35353916 | 10.35409 | 10.3510 | 10.35350 |
|       | 0.15     | 10.48958790 | 10.48935439 | 10.48935369 | 10.48992 | 10.4837 | 10.48928 |
|       | 0.20     | 10.62387907 | 10.62346374 | 10.62346249 | 10.62403 | 10.6135 | 10.62334 |
|       | 0.25     | 10.75655542 | 10.75590641 | 10.75590446 | 10.75645 | 10.7403 | 10.75571 |
|       | 0.30     | 10.88765606 | 10.88721251 | 10.8871869 | 10.88719 | 10.8642 | 10.88644 |
| 4p    | 0.05     | 12.49762844 | 12.49760242 | 12.49760240 | 12.4992 | 12.4974 | 12.49760 |
|       | 0.10     | 12.69690015 | 12.69679604 | 12.69679594 | 12.69851 | 12.696 | 12.69678 |
|       | 0.15     | 12.88858217 | 12.88834813 | 12.88834790 | 12.8901 | 12.8865 | 12.88832 |
|       | 0.20     | 13.07266080 | 13.07224462 | 13.07224420 | 13.07400 | 13.0689 | 13.07220 |
|       | 0.25     | 13.24912075 | 13.24847044 | 13.24846979 | 13.2501 | 13.2433 | 13.24840 |
| 4d    | 0.05     | 12.09831623 | 12.09829027 | 12.09829019 | 12.0989 | 12.0977 | 12.09828 |
|       | 0.10     | 12.28511332 | 12.28500942 | 12.28500910 | 12.2857 | 12.2825 | 12.28498 |
|       | 0.15     | 12.46665293 | 12.46641937 | 12.46641867 | 12.46715 | 12.4608 | 12.46635 |
|       | 0.20     | 12.64298290 | 12.64256756 | 12.64256631 | 12.64324 | 12.6326 | 12.64244 |
| 4f    | 0.05     | 11.82081212 | 11.82078623 | 11.82078608 | 11.8209 | 11.8195 | 11.82077 |
|       | 0.10     | 11.99806481 | 11.99796058 | 11.99796058 | 11.9981 | 11.993 | 11.99790 |
|       | 0.15     | 12.17192945 | 12.17169661 | 12.17169520 | 12.1718 | 12.1604 | 12.17156 |
|       | 0.20     | 12.34248626 | 12.34207217 | 12.34206967 | 12.3421 | 12.3221 | 12.34182 |
Table 3. Comparison of ro-vibrational energy eigenvalues $E_{nl}$ (eV) for the DFP with spectroscopic parameters $r_e = 0.8$ a.u and $D_e = 15$ a.u with $\hbar = \mu = 1$

| State | $\alpha$ | This work | NU [3] | AIM [9] | Numerical [5] | Approx. [5] | FIM [6] | GPS [1] |
|-------|----------|-----------|--------|---------|--------------|------------|--------|--------|
| 5p    | 0.10     | 13.5424659 | 13.54214250 | 13.54214240 | 13.5434 | 13.5413 | 13.54213643 |
|       | 0.20     | 13.92940251 | 13.92898633 | 13.92898591 | 13.9301 | 13.9257 | 13.92894 |
| 5d    | 0.10     | 13.30690079 | 13.30679690 | 13.30679659 | 13.3075 | 13.3043 | 13.306777642 |
|       | 0.20     | 13.69307930 | 13.69266395 | 13.69266270 | 13.6931 | 13.6827 | 13.6827 |
| 5f    | 0.10     | 13.14770129 | 13.14759771 | 13.14759709 | 13.1478 | 13.1426 | 13.14756936 |
|       | 0.20     | 13.53385635 | 13.53344225 | 13.53343975 | 13.5333 | 13.5134 | 13.5134 |
| 5g    | 0.10     | 13.03807936 | 13.03797622 | 13.03797516 | 13.0379 | 13.0296 | 13.037943909 |
|       | 0.20     | 13.42752509 | 13.42711266 | 13.42710850 | 13.4267 | 13.3938 | 13.3938 |

Note: The values are rounded for simplicity.
Table 4. Comparison of energy eigenvalues $E_{nl}$ (eV) of the DFP for the diatomic molecules HCl, LiH, and ScH. The spectroscopic parameters are taken from Oywumi et al. [3]

| State | $\alpha$ | This work | NU [3] | AIM [9] | Numerical [5] | Approx. [5] | GPS [1] |
|-------|----------|-----------|--------|---------|---------------|-------------|---------|
| 4d    | 0.25     | 10.66262419 | 10.66197388 | 10.66197323 | 10.665 | 10.6568 | 10.661857334 |
|       | 0.05     | 8.493369573 | 8.493343486 | 8.493343408 | 8.4948 | 8.49272 | 8.493343095 |
|       | 0.10     | 8.707214778 | 8.707110984 | 8.707110672 | 8.7087 | 8.70461 | 8.70710618 |
|       | 0.15     | 8.918041256 | 8.917807599 | 8.917806896 | 8.9194 | 8.91218 | 8.917778045 |
|       | 0.20     | 9.125920478 | 9.125505093 | 9.125503844 | 9.1272 | 9.11551 | 9.125505093 |
| 4f    | 0.05     | 7.434731843 | 7.434705654 | 7.434705654 | 7.4351 | 7.43346 | 7.434705351 |
|       | 0.10     | 7.586522280 | 7.586418806 | 7.586418181 | 7.5868 | 7.58142 | 7.586418181 |
|       | 0.15     | 7.735965234 | 7.735732273 | 7.735730867 | 7.7361 | 7.72448 | 7.735697652 |
|       | 0.20     | 7.883171622 | 7.882755012 | 7.88275512 | 7.8831 | 7.86276 | 7.88275512 |
| 5p    | 0.10     | 11.30217646 | 11.30207244 | 11.30207233 | 11.3047 | 11.3012 | 11.30207244 |
|       | 0.20     | 11.91363994 | 11.91322375 | 11.91322333 | 11.9161 | 11.9099 | 11.91322375 |
| 5d    | 0.10     | 10.52018988 | 10.52008608 | 10.52008576 | 10.5219 | 10.5176 | 10.52008608 |
|       | 0.20     | 11.06978698 | 11.06937161 | 11.06937036 | 11.0713 | 11.0594 | 11.06937161 |
| 5f    | 0.10     | 9.796761519 | 9.79665803 | 9.796657408 | 9.7975 | 9.79166 | 9.796641911 |
|       | 0.20     | 10.27345118 | 10.27303707 | 10.2730347 | 10.2738 | 10.253 | 10.27303707 |
| 5g    | 0.10     | 9.152326416 | 9.152223355 | 9.15222313 | 9.1524 | 9.14389 | 9.152206082 |
|       | 0.20     | 9.553281943 | 9.552869479 | 9.552865312 | 9.5528 | 9.51954 | 9.552869479 |
This work

| State | HCL | LiH | ScH |
|-------|-----|-----|-----|
| 0     | 0.792936901 | 0.792936901 | 0.792936901 |
| 1     | 0.792936901 | 0.792936901 | 0.792936901 |
| 2     | 0.792936901 | 0.792936901 | 0.792936901 |
| 3     | 0.792936901 | 0.792936901 | 0.792936901 |
| 4     | 0.792936901 | 0.792936901 | 0.792936901 |

Table 5. Comparison of the shifted DFP eigenvalues \((E_{nl} - D_C)\) in eV for HCl molecule for various vibrational \(n\) and rotational \(l\) quantum numbers

| \(n\) | \(l\) | This work | AP [10] | NU [10] | AIM [9] | GPS [1] |
|-------|-------|-----------|---------|---------|---------|---------|
| 0     | 0     | 4.16922040 | 4.41705 | 4.41705 | 4.417077001 | 4.4170494559 |
| 5     | 1     | 4.3790853 | 4.37843 | 4.37403 | 4.374065784 |
| 10    | 1     | 4.25960994 | 4.25791 | 4.25973 | 4.259761948 |
| 5     | 0     | 2.66593059 | 2.66574 | 2.66574 | 2.665748019 | 2.6657422481 |
| 5     | 1     | 2.62844225 | 2.63411 | 2.62859 | 2.628601192 | 2.6341202067 |
| 10    | 1     | 2.52975073 | 2.55027 | 2.52989 | 2.529905688 | 2.5502777586 |
| 7     | 0     | 2.09636984 | 2.09652 | 2.09652 | 2.096524802 | 2.0965250897 |
| 5     | 1     | 2.06146505 | 2.06768 | 2.06161 | 2.061620202 | 2.067682795 |
| 10    | 1     | 1.96873708 | 1.99127 | 1.96888 | 1.968892038 | 1.9912752181 |
Table 6. Comparison of the shifted DFP eigenvalues \((E_n - D_0)\) in eV for LiH molecule for various vibrational \(n\) and rotational \(l\) quantum numbers

| \(n\) | \(l\) | This work | AP [10] | NU [10] | AIM [9] | GPS [1] |
|------|------|----------|--------|--------|--------|--------|
| 0    | 0    | 2.411860999 | 2.41195 | 2.41195 | 2.411949045 | 2.41193395635 |
| 5    | 0    | 2.383413301 | 2.38458 | 2.38348 | 2.383476249 |        |
| 10   |      | 2.308084518 | 2.31229 | 2.30815 | 2.308147473 |        |
| 5    | 0    | 1.516214349 | 1.51628 | 1.51628 | 1.516277294 | 1.5162733601 |
| 5    | 1    | 1.492708486 | 1.49429 | 1.49278 | 1.492771433 | 1.4942942044 |
| 10   |      | 1.430551348 | 1.43627 | 1.43062 | 1.430614300 | 1.4362755837 |
| 7    | 0    | 1.223330593 | 1.22340 | 1.22340 | 1.223393538 | 1.2233927653 |
| 5    |      | 1.201661396 | 1.20344 | 1.20173 | 1.201724433 | 1.2034455538 |
| 10   |      | 1.144375642 | 1.15083 | 1.14444 | 1.144438594 | 1.1508305492 |

5. CONCLUSION

In this paper, the energy spectrum of the radial SE generated by the DFP has been obtained by using the WKB approximation method. The Pekeris type approximation scheme was used to deal with the centrifugal barrier term of the effective potential. The WKB method yields an implicit energy equation. This equation is applied in generating energy spectrum for the non-physical and also for real molecular systems such as HCl LiH and ScH diatomic molecules. In comparison with the numerical eigenvalues obtained with MATHEMATICA package, the WKB approximation method produces improved results over the results obtained by other analytical methods in the literature.

COMPETING INTERESTS

Author has declared that no competing interests exist.

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