



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

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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

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

Where D_e is the potential depth, r_e is the internuclear distance, α is a parameter that determines the range of the potential. The potential is long-range for large α and short range for small parameter of α . 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 H_2 , LiH, HCl, 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]. Diaf [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 package 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 HCl, LiH and ScH. Furthermore, by taking the energy difference $(E_{nl} - D_e)$, the energy eigenvalues for the shifted DFP were obtained for HCl and 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 straight forward 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 function or where the classical momentum vanishes ($P(r) = 0$). The WKB method yield 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 $l(l + 1)\hbar^2/2\mu r^2$ in the effective potential of the radial SE has to be replaced with the term $(l + \frac{1}{2})^2 \hbar^2/2\mu r^2$. 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 term is non-vanishing at $l = 0$. This also makes the WKB quantization integral unsolvable for some potential. In such case an appropriate 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 $\psi(r, \theta, \phi)$ is given as

$$-\frac{\hbar^2}{2\mu} \left[\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right] \psi(r, \theta, \phi) + V(r) \psi(r, \theta, \phi) = E \psi(r, \theta, \phi). \quad (2)$$

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 $\psi(r, \theta, \phi) = \frac{R(r)Y(\theta, \phi)}{r}$.

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

$$\frac{d^2 R(r)}{dr^2} + \frac{2\mu}{\hbar^2} [E - V_{eff}(r)] R(r) = 0. \quad (3)$$

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

$$V_{eff}(r) = V(r) + \frac{(l + \frac{1}{2})^2 \hbar^2}{2\mu r^2} \quad (4)$$

We can rewrite Eq. (3) as

$$\left[\left(-\frac{i\hbar d}{dr} \right)^2 \right] R(r) = 2\mu \left[E - V(r) - \frac{(l + \frac{1}{2})^2 \hbar^2}{2\mu r^2} \right] R(r). \quad (5)$$

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

$$P(r) = \left\{ 2\mu \left[E - V(r) - \frac{(l + \frac{1}{2})^2 \hbar^2}{2\mu r^2} \right] \right\}^{\frac{1}{2}}. \quad (6)$$

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

$$\int_{r_1}^{r_2} P(r) dr = \pi \hbar \left(n + \frac{1}{2} \right). \quad r_1 < r < r_2 \quad n = 0, 1, 2 \dots \quad (7)$$

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

$$\psi^{WKB}(r) = \frac{N}{\sqrt{P(r)}} \exp \left[\pm \frac{i}{\hbar} \int P(r) dr \right]. \quad (8)$$

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)

$$\left[\left(-\frac{i\hbar d}{dr} \right)^2 \right] R(r) = 2\mu \left[E - D_e \left[1 - \frac{b}{e^{\alpha r - 1}} \right]^2 - \frac{\left(l + \frac{1}{2} \right)^2 \hbar^2}{2\mu r^2} \right] R(r) \quad (9)$$

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

$$P(r) = 2\mu \left[E - D_e \left[1 - \frac{b}{e^{\alpha r - 1}} \right]^2 - \frac{\left(l + \frac{1}{2} \right)^2 \hbar^2}{2\mu r^2} \right] \quad (10)$$

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

$$\sqrt{2\mu} \int_{r_1}^{r_2} \left[E - D_e \left[1 - \frac{b}{e^{\alpha r - 1}} \right]^2 - \frac{\left(l + \frac{1}{2} \right)^2 \hbar^2}{2\mu r^2} \right]^{\frac{1}{2}} dr = \pi \hbar \left(n + \frac{1}{2} \right). \quad r_1 < r < r_2 \quad n = 0, 1, 2 \dots \quad (11)$$

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

$$\frac{1}{r^2} \sim \alpha^2 \left[c_0 + \frac{e^{\alpha r}}{(e^{\alpha r - 1})^2} \right] \quad (12)$$

Where c_0 is a dimensionless constant with a value [9] $c_0 = \frac{1}{12.0015}$.

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

$$\sqrt{2\mu} \int_{r_1}^{r_2} \left[E - D_e \left[1 - \frac{b}{e^{\alpha r - 1}} \right]^2 - \frac{\left(l + \frac{1}{2} \right)^2 \hbar^2 \alpha^2 \left[c_0 + \frac{e^{\alpha r}}{(e^{\alpha r - 1})^2} \right]^{\frac{1}{2}}}{2\mu} \right] dr = \pi \hbar \left(n + \frac{1}{2} \right) \quad (13)$$

Now we let $y = e^{\alpha r} - 1, \quad y \in [0, \infty]$,

$$dy = \alpha e^{\alpha r} = \alpha(1 + y)dr,$$

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

$$\sqrt{2\mu} \int_{y_1}^{y_2} \frac{dy}{1+y} \left[E - D_e \left[\frac{y-b}{y} \right]^2 - \frac{\left(l + \frac{1}{2} \right)^2 \hbar^2 \alpha^2 \left[c_0 + \frac{1+y}{y^2} \right]^{\frac{1}{2}}}{2\mu} \right] = \pi \hbar \left(n + \frac{1}{2} \right) \quad (14)$$

$$\Rightarrow \sqrt{\frac{2\mu}{\alpha^2}} \int_{y_1}^{y_2} \frac{dy}{y(1+y)} \left[E y^2 - D_e y^2 + 2D_e b y - D_e b^2 - \frac{\left(l + \frac{1}{2} \right)^2 \hbar^2 y^2 \alpha^2 c_0 - \frac{\hbar^2 \alpha^2 \left(l + \frac{1}{2} \right)^2}{2\mu} - \frac{y \hbar^2 \alpha^2 \left(l + \frac{1}{2} \right)^2}{2\mu} \right]^{\frac{1}{2}} = \pi \hbar \left(n + \frac{1}{2} \right) \quad (15)$$

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

$$\sqrt{\frac{2\mu}{\alpha^2}} \int_{y_1}^{y_2} \frac{dy}{y(1+y)} \sqrt{-N y^2 + W y - T} = \pi \hbar \left(n + \frac{1}{2} \right), \quad (16)$$

where

$$N = D_e - E + \frac{\hbar^2 \alpha^2}{2\mu} \left(l + \frac{1}{2} \right)^2 c_0 \quad (17)$$

$$W = 2b D_e - \frac{\hbar^2 \alpha^2}{2\mu} \left(l + \frac{1}{2} \right)^2 \quad (18)$$

$$T = D_e b^2 + \frac{\hbar^2 \alpha^2}{2\mu} \left(l + \frac{1}{2} \right)^2 \quad (19)$$

Equation (16) can further be simplified as

$$\sqrt{\frac{2\mu N}{\alpha^2}} \int_{y_1}^{y_2} \frac{dy}{y(1+y)} \sqrt{-y^2 + B y - C} = \pi \hbar \left(n + \frac{1}{2} \right), \quad (20)$$

where

$$B = \frac{W}{N}. \quad (21)$$

$$C = \frac{T}{N} \quad (22)$$

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

$$z = 1 + 2y \quad z \in (1, \infty) \quad (23)$$

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

$$\sqrt{\frac{2\mu N}{\alpha^2}} \int_{z_1}^{z_2} \frac{dz}{z^2 - 1} \sqrt{-z^2 + F z - G} = \pi \hbar \left(n + \frac{1}{2} \right), \quad (24)$$

where

$$F = 2 + 2B \quad (25)$$

$$G = 1 + 2B + 4C \quad (26)$$

The turning points z_2 and z_1 are given by

$$z_1 = \frac{F - \sqrt{F^2 - 4G}}{2} \quad (27)$$

$$z_2 = \frac{F + \sqrt{F^2 - 4G}}{2} \quad (28)$$

We can write Eq. (24) in a regular form as

$$\sqrt{\frac{2\mu N}{\alpha^2}} \int_{z_1}^{z_2} \frac{dz}{z^2 - 1} \sqrt{(z_2 - z)(z - z_1)} = \pi \hbar \left(n + \frac{1}{2} \right), \quad (1 < z_1 < z_2) \quad (29)$$

With the help of the semi-classical quantization integral standard given in Hruska et al. [20] we have

$$\int_{z_1}^{z_2} \frac{dz}{z^2 - 1} \sqrt{(z_2 - z)(z - z_1)} = \frac{\pi}{2} \left[\sqrt{(1 + z_2)(1 + z_1)} - \sqrt{(z_2 - 1)(z_1 - 1)} - 2 \right] \quad (30)$$

By comparing Eq. (29) and (30), implies that

$$\sqrt{\frac{2\mu N}{\alpha^2}} \left[\sqrt{(1 + z_2)(1 + z_1)} - \sqrt{(z_2 - 1)(z_1 - 1)} - 2 \right] = 2\hbar \left(n + \frac{1}{2} \right) \quad (31)$$

With the help of Eqs. (27) and (28), Eq. (31) becomes

$$\sqrt{\frac{2\mu N}{\alpha^2}} \left[\sqrt{1 + F + G} - \sqrt{1 - F + G} - 2 \right] = 2\hbar \left(n + \frac{1}{2} \right) \quad (32)$$

Next we substitute F and G given in the respective Eqs. (25) and (26) into Eq. (32) to obtain

$$\sqrt{\frac{2\mu N}{\alpha^2}} \left[\sqrt{1 + B + C} - \sqrt{C} - 1 \right] = \hbar \left(n + \frac{1}{2} \right) \quad (33)$$

Recalling the notations B and C given in Eqs. (21) and (22), Eq. (33) can be written as

$$\sqrt{\frac{2\mu N}{\alpha^2}} \left[\sqrt{1 + \frac{W}{N} + \frac{T}{N}} - \sqrt{\frac{T}{N}} - 1 \right] = \hbar \left(n + \frac{1}{2} \right) \quad (34)$$

Finally, substituting the notations N, W and T in Eqs. (17-19) into Eq. (34) with some algebraic simplifications, we obtained the energy eigenvalues equation of the Deng-Fan Potential as

$$\sqrt{\frac{2\mu(D_e(b+1)^2 - E_{nl})}{\hbar^2 \alpha^2} + c_0 \left(l + \frac{1}{2} \right)^2} - \sqrt{\frac{2\mu D_e b^2}{\hbar^2 \alpha^2} + \left(l + \frac{1}{2} \right)^2} - \sqrt{\frac{2\mu(D_e - E_{nl})}{\hbar^2 \alpha^2} + c_0 \left(l + \frac{1}{2} \right)^2} = \left(n + \frac{1}{2} \right) \quad (35)$$

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_e , r_e , and α 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 $(E_{nl} - D_e)$ 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 $\hbar c = 1973.29 \text{ eV}\text{\AA}$, $1 \text{ amu} = 931.494028 \text{ Mev}/c^2$ reported in Falaye et al. [24].

Table 1. Spectroscopic parameters for HCl, LiH and ScH diatomic molecules taken from Oyewumi et al. [3]

Molecules	D_e (eV)	r_e (\AA)	α (\AA ⁻¹)	μ (a. m. u)
HCl	4.619061175	1.2746	1.8677	0.9801045
LiH	2.515283695	1.5956	1.1280	0.8801221
ScH	2.25	1.776	1.41113	0.986040

Table 2. Comparison of ro-vibrational energy eigenvalues E_{nl} (eV) for the DFP with spectroscopic parameters $r_e = 0.40$ and $D_e = 15$ a. u with $\hbar = \mu = 1$

State	α	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	8.045333800	8.045099870	8.045099635	8.04724	8.04322	8.04508	8.045097775
	0.20	8.136619920	8.136203772	8.136203356	8.13842	8.13287	8.13613	
	0.25	8.227279483	8.226629167	8.226628516	8.22892	8.22142	8.22655	8.226613566
	0.30	8.317325475	8.316389030	8.316388092	8.31874	8.30889	8.31629	
3p	0.05	10.99778906	10.99776305	10.99776302	10.9998	10.9976	10.99776	10.997762943
	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	11.324240817
	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	11.638278167
	0.30	11.79169146	11.79075502	11.79075408	9.67565	11.7833	11.79066	
3d	0.05	10.21600623	10.21598027	10.21598019	10.21651	10.2154	10.21597	10.215980103
	0.10	10.35364341	10.35353947	10.35353916	10.35409	10.351	10.35350	
	0.15	10.48958790	10.48935439	10.48935369	10.48992	10.4837	10.48928	10.489341948
	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	10.755814653
	0.30	10.88765606	10.88672151	10.88671869	10.88719	10.8642	10.88644	
4p	0.05	12.49762844	12.49760242	12.49760240	12.4992	12.4974	12.49760	12.497602157
	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	12.888327591
	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	13.248318043
	0.30	13.42558070	13.42492049	13.42491984	13.42651	13.4197	13.42480	13.424716043
4d	0.05	12.09831623	12.09829027	12.09829019	12.0989	12.0977	12.09828	12.098289743
	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	12.466379229
	0.20	12.64298290	12.64256756	12.64256631	12.64324	12.6326	12.64244	
	0.25	12.82932285	12.82890751	12.82890626	12.82951	12.8233	12.82880	12.828716043
	0.30	13.01486280	13.01444746	13.01444621	13.01501	13.0088	13.01430	13.014216043
4f	0.05	11.82081212	11.82078623	11.82078608	11.8209	11.8195	11.82077	11.820785582
	0.10	11.99806481	11.99796121	11.99796058	11.9981	11.993	11.99790	
	0.15	12.17192945	12.17169661	12.17169520	12.1718	12.1604	12.17156	12.171646579
	0.20	12.34248626	12.34207217	12.34206967	12.3421	12.3221	12.34182	
	0.25	12.51792690	12.51751280	12.51751149	12.5176	12.5072	12.51744	12.517456043

State	α	This work	NU [3]	AIM [9]	Numerical [5]	Approx. [5]	FIM[6]	GPS [1]
5p	0.10	13.54224659	13.54214250	13.54214240	13.5434	13.5413	13.54213	13.542133643
	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		
5f	0.10	13.14770129	13.14759771	13.14759709	13.1478	13.1426		13.147569396
	0.20	13.53385635	13.53344225	13.53343975	13.5333	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	13.42667	13.3938		

Table 3. Comparison of ro-vibrational energy eigenvalues E_{nl} (eV) for the DFP with spectroscopic parameters $r_e = 0.8$ and $D_e = 15$ a. u with $\hbar = \mu = 1$

State	α	This work	NU [3]	AIM [9]	Numerical [5]	Approx. [5]	GPS [1]
2p	0.05	4.140913461	4.140887263	4.140887237	4.14208	4.14068	4.140887222
	0.10	4.219284120	4.219180128	4.219180023	4.2204	4.21835	
	0.15	4.297627357	4.297393199	4.297392964	4.2987	4.29552	4.297390050
	0.20	4.375962693	4.375546508	4.375546092	4.3769	4.37221	
	0.25	4.454309954	4.453659654	4.453659003	4.4551	4.44845	4.453636191
	0.30	4.532688242	4.531751791	4.531750853	4.5332	4.52425	
3p	0.05	7.532817713	7.532791561	7.532791535	7.5350	7.53258	7.532791457
	0.10	7.724868277	7.724764274	7.724764169	7.7271	7.72393	
	0.15	7.915412795	7.915178655	7.915178421	7.9177	7.9133	7.915170747
	0.20	8.104456816	8.104040627	8.104040211	8.1066	8.10071	
	0.25	8.292004474	8.291354169	8.291353518	8.2941	8.28615	8.291296319
	0.30	8.478057760	8.477121312	8.477120373	8.4799	8.46962	
3d	0.05	5.739777356	5.739751228	5.739751150	5.7404	5.73913	5.739751067
	0.10	5.845874062	5.845770281	5.845769968	5.8465	5.84327	
	0.15	5.950911804	5.950678133	5.950677430	5.9515	5.94505	5.950665807
	0.20	6.054948991	6.054533598	6.054532348	6.0553	6.04453	
	0.25	6.158044321	6.157395321	6.157393368	6.1582	6.14177	6.157304825
	0.30	6.260256322	6.259321745	6.259318933	6.2601	6.23682	
4p	0.05	9.613039208	9.613013087	9.613013061	9.6156	9.6128	9.613012874
	0.10	9.883627711	9.883523698	9.883523594	9.8862	9.88269	
	0.15	10.14878985	10.14855572	10.14855549	10.1514	10.1467	10.148539652
	0.20	10.40847394	10.40805775	10.40805734	10.4111	10.4047	

State	α	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	
	0.15	8.918041256	8.917807599	8.917806896	8.9194	8.91218	8.917778045
4f	0.20	9.125920478	9.125505093	9.125503844	9.1272	9.11551	
	0.05	7.434731843	7.434705812	7.434705654	7.4351	7.43346	7.434705351
	0.10	7.586522280	7.586418806	7.586418181	7.5868	7.58142	
	0.15	7.735965234	7.735732273	7.735730867	7.7361	7.72448	7.735697652
5p	0.20	7.883171622	7.882757512	7.882755012	7.8831	7.86276	
	0.10	11.30217646	11.30207244	11.30207233	11.3047	11.3012	11.302066518
5d	0.20	11.91363994	11.91322375	11.91322333	11.9161	11.9099	
	0.10	10.52018988	10.52008608	10.52008576	10.5219	10.5176	10.520074121
5f	0.20	11.06978698	11.06937161	11.06937036	11.0713	11.0594	
	0.10	9.796761519	9.796658033	9.796657408	9.7975	9.79166	9.796641911
5g	0.20	10.27345118	10.27303707	10.27303457	10.2738	10.253	
	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	

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 Oyewumi et al. [3]

State		HCL		LiH		ScH	
n	l	This work	NU [3]	This work	NU [3]	This work	NU [3]
0	0	0.2021391349	0.201984174	0.1033975959	0.103334650	0.1049386464	0.104850694
0	1	0.2050090357	0.204854248	0.1052996075	0.105236729	0.1064375371	0.106349671
1	0	0.5909027875	0.590747827	0.3020689011	0.302005955	0.3063344892	0.306246538
1	1	0.5936924013	0.593537612	0.3039015316	0.303838653	0.3077919933	0.307704129
2	0	0.9601660040	0.960011044	0.4907488062	0.490685861	0.4970386372	0.496950687
2	1	0.9628763805	0.962721591	0.4925136380	0.492450759	0.4984552600	0.498367397
2	2	0.9682961369	0.968141645	0.4960417607	0.495978997	0.5012880020	0.501200316
3	0	1.310182826	1.310027865	0.6696639648	0.669601019	0.6771811469	0.677093198
3	1	1.312814994	1.312660203	0.6713625275	0.671299648	0.6785573840	0.678469522
3	2	1.318078347	1.317923855	0.6747581514	0.674695388	0.6813093620	0.681221677
3	3	1.325970803	1.325816775	0.6798477705	0.679785205	0.6854361001	0.685348677

State		HCL		LiH		ScH	
<i>n</i>	<i>l</i>	This work	NU [3]	This work	NU [3]	This work	NU [3]
4	0	1.641202203	1.641047243	0.8390335090	0.838970564	0.8468896201	0.846801673
4	1	1.643757170	1.643602379	0.8406672816	0.840604402	0.8482259576	0.848138097
4	2	1.648866136	1.648711644	0.8439333635	0.843870601	0.8508981441	0.850810460
4	3	1.656527052	1.656373023	0.8488287687	0.848766203	0.8549052130	0.854817791
4	4	1.666736911	1.666583499	0.8553490912	0.855286782	0.8602456962	0.860158632
5	0	1.953468116	1.953313156	0.9990693464	0.999006401	1.006289259	1.006201313
5	1	1.955946871	1.955792078	1.000639759	1.00057688	1.007586174	1.007498315
5	2	1.960903424	1.960748932	1.003779159	1.003716397	1.010179523	1.010091841
5	3	1.968335762	1.968181734	1.008484637	1.008422072	1.014068354	1.013980933
5	4	1.978240925	1.978087513	1.014751899	1.014689589	1.019251220	1.019164157
5	5	1.990614950	1.990462308	1.022575209	1.022513206	1.025726220	1.025639693

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

<i>n</i>	<i>l</i>	This work	AP [10]	NU [10]	AIM [9]	GPS [1]
0	0	4.416922040	4.41705	4.41705	4.417077001	4.4170494559
	5	4.373910853	4.37843	4.37403	4.374065784	
	10	4.259606994	4.27591	4.25973	4.259761948	
5	0	2.665593059	2.66574	2.66574	2.665748019	2.6657422481
	5	2.628446225	2.63411	2.62859	2.628601192	2.6341202067
	10	2.529750732	2.55027	2.52989	2.529905688	2.5502777586
7	0	2.096369842	2.09652	2.09652	2.096524802	2.0965250897
	5	2.061465054	2.06768	2.06161	2.061620020	2.0676862795
	10	1.968737082	1.99127	1.96888	1.968892038	1.9912752181

Table 6. Comparison of the shifted DFP eigenvalues $-(E_{nl} - D_e)$ 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	2.411886099	2.41195	2.41195	2.411949045	2.41193395635
	5	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	1.492708486	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	1.201724343	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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