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Approximate Eigensolutions of the Schrödinger Equation of a Particle in the Field of the Frost-Musulin Energy Potential Model and its Application to Diatomic Molecules

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Abstract

The approximate analytical bound state solutions of the Schrödinger equation for the Frost-Musulin potential is found by using a suitable approximation scheme to the orbital centrifugal barrier via parametric Nikiforov-Uvarov method and supersymmetric approach. We have also calculated some expectation values. The ro-vibrational energy states for some diatomic molecules are calculated for arbitrary quantum numbers n and l with the model values of some parameters. The present results are in excellent agreement with the previous result obtained by Adepoju and Eweh.

Key words: Frost-Musulin potential; approximate scheme; Schrödinger equation; centrifugal term
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1.0 Introduction

There has been a growing interest in the investigation of the analytical solutions of the Schrödinger equation for various physical potential models because the analytical solutions contain all the necessary information for the quantum system under consideration. As a result, the solutions of the wave equations in the non-relativistic quantum mechanics have received great attention in the past decades. Whether in the relativistic or non-relativistic regime, there are only few potentials that can be exactly solved in the three dimensional space due to the inverse square centrifugal term appearing in some potentials. If we intend to use analytical techniques, using approximation scheme is inevitable [1].

Moltivated by the recent work about the improved Greene-Aldrich approximation scheme [2] and the expression for the Frost-Musulin molecular energy potential model [3], we attempt to study approximately the Schrödinger equation with Frost-Musulin molecular energy potential for arbitrary angular momentum bound states. The Frost-Musulin diatomic potential function was proposed by Frost and Musulin in 1954 [4] and by 2012, Jia et al. [3], produced an improved expression for the potential using equilibrium bound length and dissociation energy. As an important physical diatomic molecular potential, the Frost-Musulin potential can be used to describe molecular vibration of a particle. The Frost-Musulin potential is written in the form [3, 5]

$$U_{FM}(r) = D_e\left[1-\frac{(r+\delta r_e(r-r_e))\,\mathrm{e}^{-\delta(r-r_e)}}{r}\right], \qquad (1)$$

where δ is the potential range, r_e is the equilibrium bound length and D_e is disociation energy. The minimum value for this potential was found by Jia et al. [3] at $r_e = \frac{1}{2}\frac{\delta p_1\sqrt{\delta p_1(\delta p_1+4p_2)}}{\delta p_2}$

where $p_1 = \frac{\delta D_e r_e^2}{e^{-\delta r_e}}$ and $p_2 = \frac{D_e(1+\delta r_e)}{e^{-\delta r_e}}$. There are several traditional techniques used to solve the Schrödinger-like differential equation with various quantum potential models [6-8]. Few of these methods are SUSY [9-19], Nikiforov-Uvarov (N.U) method [20-30], asymptotic iteration method (AIM) [31- 42], exact/proper quantization rule [43-46] etc.

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The scheme of our work is as follow: In section 2, we obtain the bound state solutions. In section 3, we present numerical result. In section 4, we calculate some expectation values. In section 5, we present result and discussion and in the final section, we give the concluding remark.
The aim of this paper is to present analytical bound state solutions of the Schrödinger equation with Frost-Musulin potential and then calculate the energy eigenvalues for some diatomic molecules. Currently, these results appear lacking in the literature.

Table 1: Model parameters used in this work for the diatomic molecules

Molecules (state)	$\mu/10^{-23}(g)$	r_e	$D_e(\mathrm{cm}^{-1})$
$O_2\left(X^3\sum_g^+\right)$	1.337	1.207	42041
$I_2\left(X(\mathrm{O}_g^+)\right)$	10.612	2.666	12547
$H_2\left(X^1\sum_g^+\right)$	0.084	0.741	38318
$N_2\left(X^1\sum_g^+\right)$	1.171	1.097	79885
$NO^+\left(X^1\sum^+\right)$	1.239	1.063	88694
$CO\left(X^1\sum^+\right)$	1.146	1.128	90531

2.0 Eigensolutions

In this section, we obtain the bound state solutions of the Schrödinger equation with the Frost-Musulin diatomic molecular potential model. Given the radial Schrödinger equation of the form

$$\frac{d^2U_{n,\ell}(r)}{dr^2}+\frac{2\mu}{\hbar^2}\left[E_{n,\ell}-V(r)-\frac{\ell(\ell+1)\hbar^2}{2\mu r^2}\right]U_{n,\ell}(r)=0, \qquad (2)$$

where μ is the reduced mass, n and ℓ denote the radial and orbital angular momentum quantum numbers, $V(r)$ is the interacting potential, r is the internuclear seperation of the diatomic molecules and $E_{n,\ell}$ is non-relativistic bound state energy. It is noted that Eq. (2) cannot be solved for $\ell\neq 0$ due to the centrifugal term. Thus, we need to employ a suitable approximation scheme to deal with the centrifugal barrier. It is found that the following Greene-Aldrich approximation type [47, 48]

$$\frac{1}{r^2}\approx\frac{\delta^2}{\left(1-e^{-\delta r}\right)^2}, \qquad (3)$$

is a good approximation to the centrifugal term $\frac{1}{r^2}$ for short range potential.

2.1 Bound State Solutions of the Schrödinger Equation using Nikiforov-Uvarov method.

To use Nikiforov-Uvarov method, we substitute potential (1) and approximation (3) into Eq. (2) and by defining a variable of the form $y=e^{-\delta r}$, we obtain

$$\frac{d^2U_{n,\ell}(\mathrm{y})}{dy^2}+\frac{1-y}{y(1-y)}\frac{dU_{n,\ell}(\mathrm{y})}{dy}+\frac{Ay^2+By+C}{y^2(1-\mathrm{y})^2}U_{n,\ell}(\mathrm{y})=0, \qquad (4)$$

where $A=\frac{2\mu E_{n,\ell}}{\delta^2\hbar^2}+\frac{2\mu D_e}{\delta^2\hbar^2}\left[b\delta r_e(1+r_e)+b-1\right]$, $B=-\frac{2\mu}{\delta^2\hbar^2}\left[2E_{n,\ell}-2D_e(1-b)+D_er_e\delta b(2+r_e)\right]$,

$C=\frac{2\mu E_{n,\ell}}{\delta^2\hbar^2}+\frac{2\mu D_e}{\delta^2\hbar^2}\left[b+b\delta r_e-1\right]-\ell(\ell+1)$ and $b=e^{\delta r_e}$.

For solving Eq. (4) using Nikiforov-Uvarov method, we first consider the following differential equation [48]

$$\frac{d^2U_{n,\ell}(\mathrm{s})}{ds^2}+\frac{\alpha_1-\alpha_2 s}{\mathrm{s}(1-\alpha_3 s)}\frac{dU_{n,\ell}(\mathrm{s})}{dy}+\frac{\zeta_1 s^2+\zeta_2 s+\zeta_3}{s^2(1-s)^2}U_{n,\ell}(\mathrm{s})=0. \quad (5)$$

The condition for energy equation is given as [48]

$$n\alpha_2-(2n+1)\alpha_5+\left[n(n-1)+2\alpha_8\right]\alpha_3+\sqrt{4\alpha_8\alpha_9}+(2n+1)\left(\sqrt{\alpha_9}+\alpha_3\sqrt{\alpha_8}\right)=0. \quad (6)$$

and the wave function is

$$U(s)=N_{n,\ell}s^{\alpha_{12}}(1-\alpha_3 s)^{\alpha_{13}}P_n^{(\alpha_{10},\alpha_1)}(1-2\alpha_3 s), \quad (7)$$

where $\alpha_4=\frac{1-\alpha_1}{2}$, $\alpha_5\frac{\alpha_2-2\alpha_3}{2}$, $\alpha_6=\alpha_5^2+C_1$, $\alpha_7=2\alpha_4\alpha_5-C_2$, $\alpha_8=\alpha_4^2+C_3$, $\alpha_9=\alpha_3(\alpha_7+\alpha_3\alpha_8)+\alpha_6$, $\alpha_{10}=\alpha_1+2\alpha_4+2\sqrt{\alpha_8}$, $\alpha_{11}=\alpha_2+2\alpha_3\sqrt{\alpha_8}+2\sqrt{\alpha_9}-2\alpha_5$, $\alpha_3\neq 0$, $\alpha_{12}=\alpha_4+\sqrt{\alpha_8}>0$ and $\alpha_{13}=\alpha_5-\left(\sqrt{\alpha_9}+\alpha_3\sqrt{\alpha_8}\right)$.

Now comparing Eq. (4) with Eq. (5), we deduce the following

$$\alpha_1=\alpha_2=\alpha_3=1,\ \alpha_4=\alpha_2-\alpha_1,\ \alpha_5=\frac{-\alpha_1}{2},\ \alpha_6=\frac{\alpha_2}{4}-\frac{2\mu D_e b\left[\delta r_e(r_e+1)+1\right]}{\delta^2\hbar^2}+\frac{2\mu(D_e-E_{n,\ell})}{\delta^2\hbar^2},$$

$$\alpha_7=\frac{2\mu D_e b\left[\delta r_e(r_e+2)+2\right]}{\delta^2\hbar^2}-\frac{4\mu(D_e-E_{n,\ell})}{\delta^2\hbar^2},\ \alpha_8=\ell(\ell+1)-\frac{2\mu D_e b(1+\delta r_e)}{\delta^2\hbar^2}+\frac{2\mu(D_e-E_{n,\ell})}{\delta^2\hbar^2},$$

$$\alpha_9=\left(\frac{1}{2}+\ell\right)^2,$$

Substituting for the parameters in Eq. (6), we obtain the energy spectrum for the Frost-Musulin potential function as

$$E_{n,\ell}=D_e(1-b\delta^2 r_e^2)-bD_e(1+\delta r_e)-\frac{\delta^2\hbar^2}{2\mu}\left[\frac{(\ell+n+1)^2+\ell(\ell+1)+\frac{2\mu b D_e r_e^2}{\hbar^2}}{2(\ell+n+1)}\right]^2. \quad (8)$$

2.2: Bound State Solutions of the Schrödinger Equation using supersymmetric approach.

In this part, the eigensolutions are obtain using the method of supersymmetric quantum mechanics. Substituting Eqs. (1) and (3) into Eq. (2), we have a differential equation of the form:

$$\frac{d^2U_{n,\ell}(r)}{dr^2}=\left[V_{eff}-E_{eff}\right]U_{n,\ell}(r), \quad (9)$$

where we have used the following for mathematical simplicity $V_{eff}=\frac{\frac{2\mu b\delta^2 r_e^2 e^{-\delta r}}{\hbar^2}}{1-e^{-\delta r}}-\frac{2\mu b D_e(1+\delta r_e)e^{-\delta r}}{\hbar^2}+\frac{\ell(\ell+1)\delta^2}{\left(1-e^{-\delta r}\right)^2}$ and $E_{eff}=\frac{2\mu(D_e-E_{n,\ell})}{\hbar^2}$. Using the basic concepts of the supersymmetric quantum mechanics and formalism [49] and shape invariance techneque [50] to solve Eq. (9). The ground – state function is written as follows

$$U_{0,\ell}(r)=exp\left(-\int W(r)\,dr\right), \quad (10)$$

where $W(r)$ is called a superpotential in supersymmetric quantum mechanics [51, 52]. Proceeding to the next level of this approach, we proposed a superpotential function of the form [53]

$$W(r)=\rho_1-\frac{\rho_2}{1-e^{-\delta r}}. \quad (11)$$

Following the shape invariance formalism, the superpotential function relates to the differential equation (9) as follows:

$$W^2(r)-\frac{dW(r)}{dr}=V_{eff}-E_{eff}. \qquad (12)$$

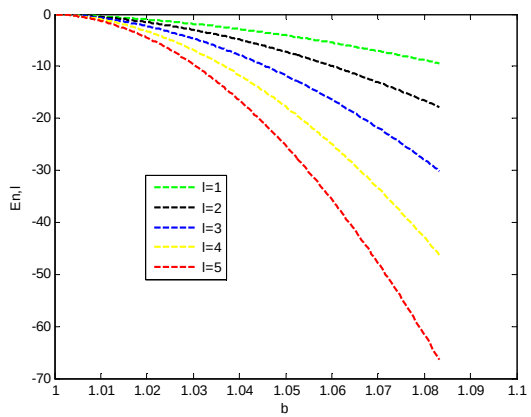

Figure 1: Energy $E_{n,\ell}$ against $b(e^{\delta r_e})$ with $\mu=\hbar^2=1,\ r_e=0.04$ and $D_e=15.$

Substituting Eq. (11) into Eq. (12) leads us to the following relations where the two constants in Eq. (11) are deduced. In this deduction, $\rho_2<1$. Hence

$$\rho_1^2=\frac{2\mu\left(D_e-E_{n,\ell}\right)}{\hbar^2}-\frac{2\mu bD_e(1+r_e\delta+r_e\delta^2)}{\hbar^2}, \qquad (13)$$

$$\rho_2=-(\ell+1)\delta, \qquad (14)$$

$$\rho_1=-\frac{\left(\rho_2^2+\ell(\ell+1)+\frac{2\mu bD_e r_e^2}{\hbar^2}\right)}{2\rho_2}. \qquad (15)$$

Having obtained the values of ρ_1 and ρ_2 using Eqs. (11) and (12), it is now convinient to construct the supersymmetric partner potentials $V_\pm(r)=W^2(r)\pm\frac{dW(r)}{dr}$ [54, 55] in view of the superpotential function

$$V_+(r)=W^2(r)+\frac{dW(r)}{dr}=\rho_1^2+\frac{\rho_2\left(\rho_2-2\rho_1\right)}{1-e^{-\delta r}}+\frac{\rho_2\left(\rho_2+\delta\right)e^{-\delta r}}{\left(1-e^{-\delta r}\right)^2}, \qquad (16)$$

$$V_-(r)=W^2(r)-\frac{dW(r)}{dr}=\rho_1^2+\frac{\rho_2\left(\rho_2-2\rho_1\right)}{1-e^{-\delta r}}+\frac{\rho_2\left(\rho_2-\delta\right)e^{-\delta r}}{\left(1-e^{-\delta r}\right)^2}. \qquad (17)$$

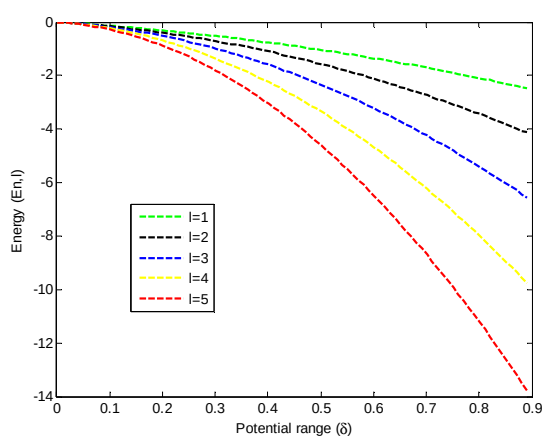

Figure 2: Energy $E_{n,\ell}$ against potential range δ with $\mu=\hbar^2=1,\ r_e=0.04$ and $D_e=15.$

Putting $\rho_2 = a_0$, we can easily show that the two partner potentials $V_+(r)$ and $V_-(r)$ are shape invariant and thus satisfied the following shape invariant condition

$$V_+(r,a_0) = V_-(r,a_1) + R(a_1), \tag{18}$$

where a_1 is a function of a_0, i.e. $a_1 = f(a_0) = \rho_2 - \delta$ and the remainder $R(a_1)$, is independent of the variable r. Using recurent relation, we have $a_2 = \rho_2 - 2\delta$, $a_3 = \rho_2 - 3\delta$ and subsequently, $a_n = \rho_2 - n\delta$. Thus, the relationship leads to the following extension

$$R(a_1) = -\frac{\left(a_0^2 + \ell(\ell+1) + \frac{2\mu b D_e r_e^2}{\hbar^2}\right)}{2a_0} + \frac{\left(a_1^2 + \ell(\ell+1) + \frac{2\mu b D_e r_e^2}{\hbar^2}\right)}{2a_2}. \tag{19}$$

$$R(a_2) = -\frac{\left(a_1^2 + \ell(\ell+1) + \frac{2\mu b D_e r_e^2}{\hbar^2}\right)}{2a_1} + \frac{\left(a_2^2 + \ell(\ell+1) + \frac{2\mu b D_e r_e^2}{\hbar^2}\right)}{2a_2}. \tag{20}$$

$$R(a_3) = -\frac{\left(a_2^2 + \ell(\ell+1) + \frac{2\mu b D_e r_e^2}{\hbar^2}\right)}{2a_2} + \frac{\left(a_3^2 + \ell(\ell+1) + \frac{2\mu b D_e r_e^2}{\hbar^2}\right)}{2a_3}. \tag{21}$$

$$\vdots \qquad\qquad \vdots$$

$$R(a_n) = -\frac{\left(a_{n-1}^2 + \ell(\ell+1) + \frac{2\mu b D_e r_e^2}{\hbar^2}\right)}{2a_{n-1}} + \frac{\left(a_n^2 + \ell(\ell+1) + \frac{2\mu b D_e r_e^2}{\hbar^2}\right)}{2a_n}. \tag{22}$$

Using Eqs.(13), (14) and (15), we calculate the energy spectral as

$$E_{n,\ell} = D_e(1 - b\delta^2 r_e^2) - bD_e(1 + \delta r_e) - \frac{\delta^2\hbar^2}{2\mu}\left[\frac{(\ell+n+1)^2 + \ell(\ell+1) + \frac{2\mu b D_e r_e^2}{\hbar^2}}{2(\ell+n+1)}\right]^2. \tag{23}$$

Eq. (23) is identical to our Eq. (8) and Eq. (9) of [5].

To obtain the corresponding wave function, we use formular method derived by Falaye et al. [56]

$$U(s) = N_n s^{k_4}(1-\alpha_3 s)^{k_5}\ {}_2F_1\left(-n, n + 2(k_4+k_5) + \frac{\alpha_2}{\alpha_3} - 1; 2k_4 + \alpha_1, \alpha_3 s\right), \tag{23a}$$

where $k_4 = \frac{(1-\alpha_1) + \sqrt{(1-\alpha_1)^2 - 4C}}{2}$ and $k_5 = \frac{1}{2} + \frac{\alpha_1}{2} - \frac{\alpha_2}{2\alpha_3} + \sqrt{\left(\frac{1}{2} + \frac{\alpha_1}{2} - \frac{\alpha_2}{2\alpha_3}\right)^2 - \left(\frac{A}{\alpha_3\alpha_3} + \frac{B}{\alpha_3} + C\right)}$, From Eq. (4), the values of α_1, α_1, α_1, A, B and C are obtain. Using the parameters above, we have $k_4 = \sqrt{\frac{-2\mu E_{n,\ell}}{\delta^2\hbar^2} - 2\mu D_e(b + b\delta r_e - 1) + \ell(\ell+)}$ and $k_5 = \frac{1}{2} + \frac{1}{2}\sqrt{\frac{8\mu b D_e r_e}{\delta^2\hbar^2} - 8\mu b D_e(\delta r_e + 1) + 4\ell(\ell+)}$.

Thus, the wave function is given as

$$U(\mathrm{y}) = N_n y^{k_4}(1-y)^{k_5}\ {}_2F_1(-n, n + 2(k_4+k_5); 2k_4 + 1, \mathrm{y}). \tag{24b}$$

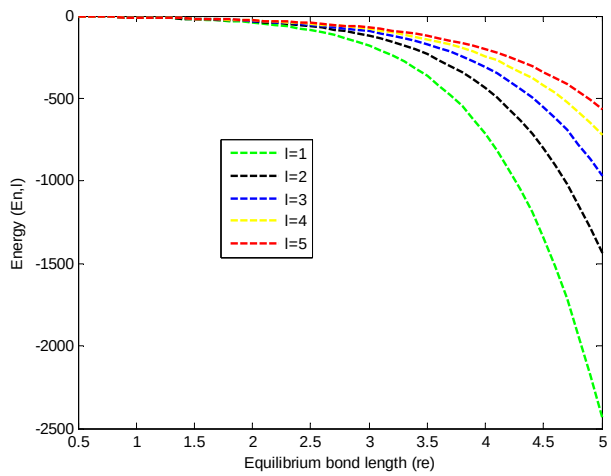

Figure 3: Energy $E_{n,\ell}$ against equilibrium length r_e with $\mu = \hbar^2 = 1,\ \delta = 0.2$ and $D_e = 15.$

3: Some expectation values for the Frost-Musulin molecular energy potential :

In this section, we calculate the some expectation values of the Frost-Musulin energy molecular potential function using Hellmann Feynman theorem [57]. If the Hamiltonian H for a particular quantum system is a function of some parameters $q,$ and then denote $E_{n,\ell}(q)$ for eigenvalue and $U_{n,\ell}(q)$ for eigenfunctions of H. Then, according to Hellmann Feynman Theorem (HFT),

$$\frac{\partial E_{n,\ell}(q)}{\partial q} = \left\langle U_{n,\ell}(q) \left| \frac{\partial H(q)}{\partial q} \right| U_{n,\ell}(q) \right\rangle, \qquad (25)$$

where the effective Hamiltonian is given by

$$H = \frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} + \frac{\hbar^2 \ell(\ell+1)}{2\mu r^2} + D_e\left[1 - \frac{(r+\delta r_e(r-r_e)\,\mathrm{e}^{-\delta(r-r_e)}}{r}\right]. \qquad (26)$$

I: The expectation value of U_1. Setting $q = D_e$, we obtain

$$\langle U_1 \rangle_{n,\ell} = 1 - b\left[\delta r_e(\delta r_e + 1) + 1\right] - \frac{\delta^2 r_e^{\,2}}{2}\left[\frac{(\ell+n+1)^2 + \ell(\ell+1) + \frac{2\mu D_e r_e^2}{\hbar^2}}{(\ell+n+1)^2}\right]. \qquad (27)$$

II: The expectation value of U_2. Setting $q = \mu,$ we have

$$\langle U_2 \rangle_{n,\ell} = -b\delta D_e\left[1 + 2r_e\right] - D_e r_e \delta^2\left[\frac{(\ell+n+1)^2 + \ell(\ell+1) + \frac{2\mu D_e r_e}{\hbar^2}}{(\ell+n+1)^2}\right]. \qquad (28)$$

III: The expectation value of U_3. Setting $q = \delta,$ we have

$$\langle U_3 \rangle_{n,\ell} = -bD_e r_e(1 + 2\delta r_e) - \frac{\delta\hbar^2}{4\mu}\left[\frac{(\ell+n+1)^2 + \ell(\ell+1) + \frac{2\mu D_e r_e^2}{\hbar^2}}{2(\ell+n+1)}\right]^2. \qquad (29)$$

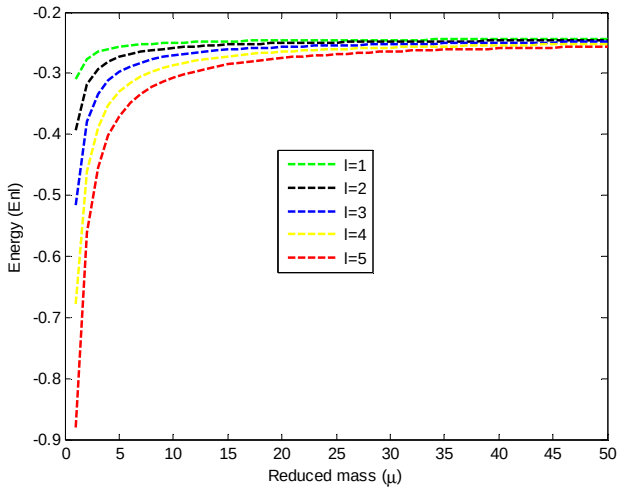

Figure 4: Energy $E_{n,\ell}$ against reduced mass μ with $r_e = 0.04,\ \hbar^2 = 1,\ \delta = 0.2$ and $D_e = 15.$

Table 2: Bound State energy eigenvalues in (eV) for various n and ℓ quantum numbers in Frost-Musulin potential with $\hbar = \mu = 1,\ \delta = 0.1$ and $D_e = 15$.

$r_e = 0.4$				$r_e = 0.8$	
n	ℓ	Present	Adepoju and Eweh	Present	Adepoju and Eweh
0	0	-1.306565933	-1.306565933	-3.247247643	-3.247247643
1	0	-1.286916932	-1.286916932	-2.845432286	-2.845432286
	1	-1.297164835	-1.297164835	-2.793688208	-2.793688208
2	0	-1.288833784	-1.288833784	-2.776577591	-2.776577591
	1	-1.302940898	-1.302940898	-2.770853170	-2.770853170
	2	-1.326412747	-1.326412747	-2.787403453	-2.787403453
3	0	-1.296067182	-1.296067182	-2.759040947	-2.759040947
	1	-1.312814390	-1.312814390	-2.767483809	-2.767483809
	2	-1.338315516	-1.338315516	-2.790181070	-2.790181070
	3	-1.372736151	-1.372736151	-2.823937246	-2.823937246
4	0	-1.306615212	-1.306615212	-2.758123986	-2.758123986
	1	-1.325816658	-1.325816658	-2.773292428	-2.773292428
	2	-1.353451695	-1.353451695	-2.799815068	-2.799815068
	3	-1.389759069	-1.389759069	-2.836255196	-2.836255196
	4	-1.435009157	-1.435009157	-2.882181604	-2.882181604
5	0	-1.319983895	-1.319983895	-2.765264773	-2.765264773
	1	-1.341615798	-1.341615798	-2.784754025	-2.784754025
	2	-1.371478782	-1.371478782	-2.814271029	-2.814271029
	3	-1.409824986	-1.409824986	-2.853095404	-2.853095404
	4	-1.456927198	-1.456927198	-2.901050928	-2.901050928
	5	-1.513019253	-1.513019253	-2.958152406	-2.958152406

Table 3: Bound state energy eigenvalues for $O_2\left(X^3\sum_g^+\right)$, $I_2\left(X(\mathrm{O}_g^+)\right)$ and $H_2\left(X^1\sum_g^+\right)$ molecules for various n and ℓ in the Frost-Musulin diatomic moecular potential.

n	ℓ	$O_2\left(X^3\sum_g^+\right)$	$I_2\left(X(\mathrm{O}_g^+)\right)$	$H_2\left(X^1\sum_g^+\right)$
0	0	-1.535690919	-2.986849670	-0.651520223
1	0	-1.299066834	-2.793156331	-0.694545926
	1	-1.271236326	-1.808307281	-0.837306330
2	0	-1.259402798	-1.794847748	-0.768651215
	1	-1.258721248	-1.453835269	-0.937373235
	2	-1.272518254	-1.300850879	-1.209312076
3	0	-1.250428763	-1.446058147	-0.872713066
	1	-1.258313745	-1.290443844	-1.069404202
	2	-1.275955464	-1.209922884	-1.365597788
	3	-1.301491712	-1.164647314	-1.767342813
4	0	-1.251660257	-1.285296867	-1.006593123
	1	-1.263805841	-1.202407843	-1.232063881
	2	-1.283981011	-1.155846189	-1.554585330
	3	-1.311361488	-1.128590987	-1.979646890
	4	-1.345733477	-1.112668258	-2.511388384
5	0	-1.258042672	-1.198689586	-1.170257245
	1	-1.273070418	-1.150074928	-1.424894724
	2	-1.295325371	-1.121521338	-1.774901763
	3	-1.324407204	-1.104661980	-2.225143077
	4	-1.360250106	-1.095194564	-2.779627564
	5	-1.402898670	-1.090737210	-3.441446871
6	0	-1.267844084	-1.147218145	-1.363693736
	1	-1.285218956	-1.116881858	-1.647705607
	2	-1.309382055	-1.098779425	-2.025891196
	3	-1.340133641	-1.088351393	-2.502530770
	4	-1.377481186	-1.083083730	-3.081400006
	5	-1.421501634	-1.081507584	-3.765578479
	6	-1.472289130	-1.080723742	-4.557517704

Table 4: Bound state energy eigenvalues for $N_2\left(X^1\sum_g^+\right)$, $NO^+\left(X^1\sum^+\right)$ and $CO\left(X^1\sum^+\right)$ molecules for various n and ℓ in the Frost-Musulin diatomic molecular potential.

n	ℓ	$N_2\left(X^1\sum_g^+\right)$	$NO^+\left(X^1\sum^+\right)$	$CO\left(X^1\sum^+\right)$
0	0	-2.740002210	-2.981163785	-3.371362626
1	0	-2.237811440	-2.406952142	-2.660099470
	1	-2.166221765	-2.321969108	-2.552406833
2	0	-2.149557432	-2.305100555	-2.533231850
	1	-2.135514463	-2.286003208	-2.507249365
	2	-2.145938459	-2.293446609	-2.513068380
3	0	-2.124272714	-2.274749110	-2.494554623
	1	-2.127449959	-2.275167272	-2.492630630
	2	-2.145041222	-2.290606582	-2.508214447
	3	-2.173027661	-2.316472394	-2.535620555
4	0	-2.118718092	-2.266511865	-2.482935315
	1	-2.129592631	-2.275446451	-2.491355286
	2	-2.151297128	-2.295318012	-2.512232865
	3	-2.182002364	-2.324030467	-2.542972958
	4	-2.221075461	-2.360822825	-2.582606238
5	0	-2.122224156	-2.268202678	-2.483289289
	1	-2.137681506	-2.282038664	-2.497531480
	2	-2.162362683	-2.304996674	-2.521999023
	3	-2.195324529	-2.335987933	-2.555339275
	4	-2.236258592	-2.374625016	-2.597047684
	5	-2.285096241	-2.420793201	-2.649655412
6	0	-2.131135114	-2.275646062	-2.490447911
	1	-2.149936727	-2.292938026	-2.508698118
	2	-2.177118330	-2.318408008	-2.536020202
	3	-2.212155247	-2.351441764	-2.571645562
	4	-2.254902884	-2.391840859	-2.615304872
	5	-2.305366055	-2.439575905	-2.666936100
	6	-2.363605592	-2.494685013	-2.726563061

4.0 Results and Discussion

In Table 2, we numerically compared our results with the results obtained using Functional Analysis method by Adepoju and Eweh [5]. It is seen that our results are in excellent agreement with the results in [5]. From Table 2, as ℓ increases, $E_{n,\ell}$ decreases (increases negatively). However, the values obtained with $r_e = 0.4$ are lesser than their counterpart with $r_e = 0.8$. In Tables 3 and 4, we computed energy values for six diatomic molecules using model parameters for equilibrium bound length and dissociation energy for various n and ℓ as given in Table 1. In Figures 1, 2 and 3, we examined the energy behaviour with b, δ and r_e respectively. It is observed that the energy is more negative as each of the parameters (b, δ, r_e) increases. This shows that a particle with these system tends to be very attractive. In Figure 4, we plottd energy against the reduced mass μ, energy increases as μ increases to 5. After this value, energy at different quantum number tends towards the same constant constant level. Thus different particles within the system exhibit similar characteristic.

5.0 Conclusion

In this research work, we obtained the bound state solutions of the Schrödinger equation with the improved expression for the Frost-Musulin diatomic molecular potential using both parametric Nikiforov-Uvarov method and supersymmetric approach. The energy equation obtained from the two methods and that of the previous result obtained are exactly the same. This energy equation is used to generate numerical values for some diatomic molecules. We have also calculated some expectation values usnig Hellmann Feynman Theorem. It is therefore, worth mentioning that the results obtained are accurate and our method is highly efficient and less cumbersome compared to the Functional analysis method used in [5].

6.0 References

[1] H. Hassanabadi, H.B. Yazarloo and L.L.Lu: Chin. Phys. Lett. **29** (2012) 020303.

[2] R L Greene and C Aldrich: Phys. Rev. A **14** (1976) 2363.

[3] P Q Wang, L H Zhang C S Jia and J Y Liu: J. Mol. Spectroscopy **274** (2012) 5.

[4] A A Frost and B Musulin: J. Chem. Phys. **22** (1954) 1017.

[5] A G Adepoju and E J Eweh: Can. J. Phys. **92** (2014) 18.

[6] S M Ikhdair and B J Falaye: JAAUBAS **16** (2014) 1.

[7] A N Ikot, E Maghsoodi, S Zarrinkamar and H Hassanabadi: Indian J. Phys. **88** (2014) 283.

[8] W A Yahya and K J Oyewumi: JAAUBAS: doi 10.1016/j.jaubas..2015.04.001.

[9] H Hassanabadi, E Maghsoodi, S Zarrinkamar and H Rahimov: Can. J. Phys. **90** (2012) 633.

[10] H Hassanabadi, L L Lu, S Zarrinkamar G Liu and H Rahimov: Acta Phys. Polo.. **122** (2012) 1111

[11] G F Wei and S H Dong: Phys. Lett. B **686** (2010) 288.

[12] G F Wei and S H Dong: EPL **87** (2009) 40004.

[13] G F Wei and S H Dong: Eur. Phys. J. A. **43** (2010) 185.

[14] C S Jia, P. Guo, Y F Diao, L Z Yi and X J Xie: Eur. Phys. J. A. **34** (2007) 41.

[15] H Hassanabadi, S Zarrinkamar and H Rahimov: Commun. Theor. Phys. **56** (2011) 423.

[16] C S Jia, T Chen and S He: Phys. Lett. A **377** (2013) 682.

[17] C A Onate: SOP Trans. Theor. Phys. **1** (2014) 118.

[18] K J Oyewumi and C O Akoshile: Eur. Phys. J. A **45** (2010) 311.

[19] F Cooper, J N Ginocchio and A Khare: Phys. Rev. D **36** (1987) 2458.

[20] H Hassanabadi, H B Yazarloo and L L Lu: Chin. Phys. Lett. **29** (2012) 020303.

[21] S M Ikhdair, M Hamzavi and B I Ita: Phys. Scr. **85** (2012) 045009.

[22] S M Ikhdair and R Sever: J. Phys. A: Math. Theor. **44** (2011) 355301.

[23] Y F Cheng and T Q Dai: Commun. Theor. Phys. **48** (2007) 431.

[24] M Hamzavi, A A Rajabi and H Hassanabadi: Int. J. Mod. Phys. A. **26** (2011) 1363.

[25] M R Setare and S Haidari: Phys. Scr. **81** (2010) 065201.

[26] M R Setare and S Haidari: Int. J. Theor. Phys. **48** (2009) 3249.

[27] W C Qiang and S H Dong: Phys. Lett. A. **372** (2008) 4789.

[28] H Hassanabadi, E Maghsoodi, S Zarrinkamar and H Rahimov: J. Math. Phys. **53** (2013). 022104.

[29] M Hamzavi and S M Ikhdair: Few-Body Syst. **53** (2012) 461

[30] S M Ikhdair: Phys. Scr. **83** (2011) 015010.

[31] A D Antia, A N Ikot and O A Awoga: Indian J. Phys. **87** (2013) 155

[32] B J Falaye: Few-Body Syst. **53** (2012) 557.

[33] A Soylu, O Bayrak and I Boztosun: J. Phys. A: Math. Theor. **41** (2008) 065308.

[34] O Bayrak and I Boztosun: J. Phys. A: Math. Theor. **40** (2007) 11119.

[35] A Soylu, O Bayrak and I Boztosun: J. Math. Phys. **48** (2007) 082302.

[34] O Bayrak and I Boztosun: Phys. Scr. **76** (2007) 92.

[35] E Ateser H Ciftci and M Uğurlu: Chin. J, Phys. **45** (2007) 346.

[36] B J Falaye, K J Oyewumi, T T Ibrahim, M A Punyasena and C A Onate: Can. J. Phys. **91** (2013) 98.

[37] K J Oyewumi, B J Falaye, C A Onate, O J Oluwadare and W A Yahya: Int. J. Mod. Phys. E.**23** (2014) 1450005.

[38] O Bayrak, I Boztosun and H Ciftci: Int. J. Quant. Chem. **107** (2007) 540.

[39] M Aygun, O Bayrak and I Boztosun: J. Phys. B. At. Mol. Opt. **40** (2007) 537.

[40] K J Oyewumi, B J Falaye, C A Onate, O J Oluwadare and W A Yahya: Mol. Phys. **112** (2014) 127.

[41] B J Falaye, K J Oyewumi, S M Ikhdair and M Hamzavi: Phys. Scr. **89** (2014) 115204.

[42] B J Falaye, S M Ikhdair and M Hamzavi: Zeitsch. Naturrf. A **70** (2015) 85.

[43] B J Falaye, S M Ikhdair and M Hamzavi: J. Math. Chem. **53** (2015) 1325.

[44] Z A Ma, A G Cisneros, B W Xu and S H Dong: Phys. Lett. A. **371** (2007) 180.

[45] X Y Gu, S H Dong and Z Q Ma: J. Phys. A: Math. Theor. **42** (2009) 035303.

[46] S M ikhdair and J A Hasna: Phys. Scr.**83** (2011) 025002.

[47] S H Dong, D Morales and J G Ravelo: Int. J. Mod. Phys. E. **16** (2007) 189.

[48] R L Greene and C Aldrich: Phys. Rev. A **14** (1976) 2363.

[49] M Hamzavi, K E Thylwe and A A Rajabi: Commun. Theor. Phys. **60** (2013) 1

[50] C A Onate: Chin. J. Phys. **53** (2015) 060002.

[51] E Witten: Nucl. Phys. B **185** (1981) 513

[52] F Cooper and B Freedman: Ann. Phys. **146** (1983) 262.

[53] L E Gendenshtein: Sov. Phys. JETP Lett. **38** (1983) 356.

[54] C A Onate and J O ojonubah: Int. J. Mod. Phys. E **24** (2015) 1550020.

[55] C A Onate, K J Oyewumi and B J Falaye: Few-Body Syst. **55** (2014) 61.

[56] B J Falaye, K J Oyewumi, S M Ikhdair and M Hamzavi: Few-Body Syst. **99** (2014)

[57] R P Feymann: Phys. Rev. **56** (1939) 340.