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APPROXIMATE ℓ-STATE SOLUTION OF TIME INDEPENDENT SCHRÖDINGER WAVE EQUATION WITH MODIFIED MÖBIUS SQUARED POTENTIAL PLUS HULTHÉN POTENTIAL

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ABSTRACT

In this work we have applied ansatz method to solve for the approximate ℓ-state solution of time independent Schrödinger wave equation with modified Möbius squared potential plus Hulthén potential to obtain closed form expressions for the energy eigenvalues and normalized radial wave-functions. In dealing with the spin-orbit coupling potential of the effective potential energy function, we have employed the Pekeris type approximation scheme, using our expressions for the bound state energy eigenvalues, we have deduced closed form expressions for the bound states energy eigenvalues and normalized radial wave-functions for Hulthén potential, modified Möbius square potential and Deng-Fan potential. Using the value 0.976865485225 for the parameter ω, we have computed bound state energy eigenvalues for various quantum states (in atomic units). We have also computed bound state energy eigenvalues for six diatomic molecules: HCl, LiH, TiH, NiC, TiC and ScF. The results we obtained are in near perfect agreement with numerical results in the literature and a clear demonstration of the superiority of the Pekeris-type approximation scheme over the Greene and Aldrich approximation scheme for the modified Möbius squares potential plus Hulthén potential.

Keywords: Ansatz solution, Deng-Fan potential, energy eigenvalues, radial wavefunction, Pekeris approximation schemes

INTRODUCTION

The need for exact solution of Schrödinger wave equation in quantum mechanics cannot be over emphasized, this is due to the vital information derivable from them (Miranda *et al*., 2010; Qiang, *et al*., 2009), information such as energy, momentum, wavelength and frequency of the system can only be obtained with the knowledge of the wave function (Eyube *et al*., 2019). Exact solution of the Schrödinger equation is restricted to only few potential models such as the Coulombic potential and harmonic oscillator potential (Hitler *et al*., 2017; Tsaur and Wang, 2014) for all quantum states $n\ell$ where n is the principal quantum number and ℓ is the angular momentum quantum number. The Hulthén, Morse, and Eckart potentials are among the few potential energy functions which give exact solution for zero angular momentum quantum number ($\ell = 0$), these solutions are often referred to as s-wave solutions (Hitler *et al*., 2017; Tsaur and Wang, 2014). Most of the known potential energy functions have no exact solutions with the Schrödinger equation for all values of n and ℓ, for such potentials, approximate solutions (numerical or analytical) can be used in place of exact solutions (Rahbar and Sadeghi,2016). In order to obtain approximate analytical solution, a very suitable approximation scheme (Wei and Dong, 2010; Chen *et al*., 2009; Jia *et al*, 2008) must be applied on the spin-orbit term of the effective potential, having applied the approximation model on the centrifugal term, a solution method must be adopted to solve the resulting equation. Researchers have developed and used various solution methods to solve the Schrödinger equation, amongst some of the methods include: ansatz method (Taskin and Kocal, 2010), Nikiforov-Uvarov method (Ikot *et al*., 2014; Yazarloo *et al*., 2012), factorization method (Pahlavani *et al*., 2013), asymptotic iteration method (Awoga and Ikot 2012), Fröbenius series solution method (Nyengeri *et al.*, 2018), exact quantization rule (Qiang *et al* 2008). Various forms of potential energy functions have been used to solve the radial Schrödinger equation. Yazarloo *et al.* (2012) have obtained the oscillator strength for the modified Möbius square potential. The Schrödinger equation was studied by an improved approximation scheme for the Hulthén potential (Ikhdair,2009), Okorie *et al*. (2018) have studied the solution of the Schrödinger equation with modified Möbius square potential, they used their results to explore the thermodynamic properties of the potential. Researchers have also used combined potentials to the radial Schrödinger equation. Recently Ita *et al*. (2018) have solved the Schrödinger equation with the Woods-Saxon plus attractive inversely quadratic potential for the bound state solution Hitler *et al*. (2017) have applied the Nikiforov-Uvarov method to solve for the s-wave solution of Schrodinger equation with Kratzer plus modified Deng-Fan potential, in another event Edet and collaborators have used modified Kratzer potential plus screened coulomb potential to study the Schrödinger equation (Edet *et al*., 2019). The list of authors who have used combined potentials seems to endless in the literature. In this paper, we are encouraged to solve for the approximate ℓ-state solution of time independent Schrödinger wave equation with modified Möbius squared potential plus Hulthén potential, which, to the best of our knowledge has never been solved in the literature. Our specific task is to obtain (i) closed form expressions for the bound state energy eigenvalues and normalized radial wave functions of the modified Möbius square potential plus Hulthén potential, (ii) use our results to derive expressions for the bound state energy eigenvalues and radial wave functions of Hulthén potential, modified Möbius square potential and Deng-Fan potential, (iii) use our results to compute bound state energy eigenvalues of Hulthén potential and Deng-fan potential for arbitrary values of quantum numbers, (iv) compare our results with existing results in the literature.

Theoretical Formalism

The modified Möbius squared potential plus Hulthén potential

The modified Mobius Squared Potential (Okorie *et al.*, 2018) plus the Hulthén potential (MMSPHP) (Jia *et al.*, 2008) is given by:

$$V(r)=-V_0\left(\frac{A+Be^{-2\delta r}}{1-e^{-2\delta r}}\right)^2-\frac{Ze^2\,\delta\, e^{-\delta r}}{1-e^{-\delta r}}\,. \tag{1}$$

where V_0, A, B and δ are the depth of the potential, the range of the potential, the length of the molecular bond and the adjustable screening parameter, Z is a constant which is related to the atomic number of an element. $V(r)$ is the modified Mobius square potential plus the Hulthén potential. The effective potential is given by

$$V_{eff}(r)=-V_0\left(\frac{A+Be^{-2\delta r}}{1-e^{-2\delta r}}\right)^2+\frac{Ze^2\,\delta\, e^{-\delta r}}{1-e^{-\delta r}}+\frac{L\hbar^2}{2\mu r^2}\,. \tag{2}$$

$L=\ell(\ell+1)$, μ is the mass of the system, r is the internuclear separation and $\hbar$ is the reduced Planck's constant.

The radial Schrödinger equation

The radial Schrödinger equation reads (Okorie *et al.*,2018)

$$\frac{d^2\psi_{nl}}{dr^2}+\frac{2\mu}{\hbar^2}\left[E_{nl}-V_{eff}(r)\right]\psi_{nl}(r)=0 \tag{3}$$

where $E_{n\ell}$ is the energy spectrum of the potential, $\psi_{nl}(r)$ is the radial wavefunction. Substituting Eq. (2) into Eq. (3) gives

$$\frac{d^2\psi_{nl}}{dr^2}+\frac{2\mu}{\hbar^2}\left[E_{nl}+V_0\left(\frac{\mathrm{A}+\mathrm{B}e^{-\delta r}}{1\text{-}e^{-\delta r}}\right)^2+\frac{Ze^2\delta e^{-\delta r}}{1\text{-}e^{-\delta r}}-\frac{L\hbar^2}{2\mu r^2}\right]\psi_{nl}(r)=0 \tag{4}$$

Eq. (4) have exact solution for the special case of the s-wave ($\ell=0$). However, if $\ell\neq 0$ only approximate solutions can be obtained due to the presence of the centrifugal term potential (spin-orbit coupling term). By employing a suitable approximation scheme to deal with the centrifugal term. In this article we will use Pekeris type approximation model proposed by Jia *et al*. (Jia *et al* 2008) given below:

$$\frac{1}{r^2}\approx\delta^2\left\{\frac{\omega e^{-\delta r}}{1-e^{-\delta r}}+\frac{e^{-2\delta r}}{\left(1-e^{-\delta r}\right)^2}\right\} \tag{5}$$

where ω is an adjustable dimensionless parameter. Inserting the approximation expression Eq. (5) into Eq. (4) now turns to:

$$\frac{d^2\psi_{nl}}{dr^2}+\frac{2\mu}{\hbar^2}\left\{E_{nl}+V_0\left(\frac{\mathrm{A}+\mathrm{B}e^{-\delta r}}{1\text{-}e^{-\delta r}}\right)^2+\frac{Ze^2\delta e^{-\delta r}}{1\text{-}e^{-\delta r}}-\frac{L\hbar^2\delta^2}{2\mu}\left[\frac{\omega e^{-\delta r}}{1-e^{-\delta r}}+\frac{e^{-2\delta r}}{\left(1-e^{-\delta r}\right)^2}\right]\right\}\psi_{nl}(r)=0 \tag{6}$$

with the approximation given by Eq. (5) substituted in Eq. (2) gives:

$$V_{eff}(r)=-V_0\left(\frac{\mathrm{A}+\mathrm{B}e^{-\delta r}}{1\text{-}e^{-\delta r}}\right)^2-\frac{Ze^2\delta e^{-\delta r}}{1\text{-}e^{-\delta r}}+\frac{L\hbar^2\delta^2}{2\mu}\left[\frac{\omega e^{-\delta r}}{1-e^{-\delta r}}+\frac{e^{-2\delta r}}{\left(1-e^{-\delta r}\right)^2}\right] \tag{7}$$

To express Eq. (6) in a more compact form, we have used the following coordinate transformation of the form

$$z=e^{-\delta r} \tag{8}$$

Eq. (6) reduces to

$$\frac{d^2\psi_{nl}(r)}{dr^2}+\frac{2\mu}{\hbar^2}+\left[E_{nl}+\frac{Ze^2\delta z}{(1-z)}+V_0\left(\frac{A+Bz}{(1-z)}\right)^2-\frac{L\hbar^2\delta^2}{2\mu}\left(\frac{\omega z}{1-z}+\frac{z^2}{(1-z)^2}\right)\right]\psi_{nl}(z)=0 \tag{9}$$

Further reduction, results to,

$$z^2\frac{d^2\psi_{nl}(z)}{dz^2}+z\frac{d\psi_{nl}(z)}{dz}+\left[-e_1+\frac{e_2}{(1-z)}-\frac{2Lz+e_3-L}{(1-z)^2}\right]\psi_{nl}(z) \tag{10}$$

where

$$-e_1=\frac{2\mu}{\delta^2\hbar^2}\left(E_{nl}-Ze^2\delta+V_0B^2\right)-L(1-\omega) \tag{11}$$

$$-e_2=\frac{4\mu V_0B(A+B)}{\delta^2\hbar^2}-\frac{2\mu Ze^2\delta}{\delta^2\hbar^2}+L\omega \tag{12}$$

$$-e_3=\frac{2\mu V_0(A+B)^2}{\hbar^2\delta^2}\ . \tag{13}$$

The boundary condition on the wave function $\psi_{nl}(z)$ is as: $r \to 0$, $z \to 1$ and as $r \to \infty$, $z \to 0$. Under this condition, for bound state solutions we can choose a reasonable physical wavefunction as follows (Dong and Gu, 2007):

$$\psi_{nl}(z)=N_{nl}\,z^a(1-z)^b f_{nl}(z). \tag{14}$$

where *a* and *b* are constants to be satisfied by Eq. (9) and $N_{n\ell}$ is the normalization constant to be determined by normalization condition. Substituting the wavefunction given by Eq. (14) into Eq. (9), we obtained

$$z(1-z)\frac{d^2f_{nl}(z)}{dz^2}+\left[2a+1-(2a+2b+1)z\right]\frac{d\,f_{nl}(z)}{d\,z}-\left[\left((a+b)^2-e_1\right)+\frac{b^2-b-L-e_3}{1-z}+\frac{a^2-e_1+e_2-e_3+L}{z}\right]f_{nl}(z)=0. \tag{15}$$

Eq. (15) is Gaussian hypergeometric (Dong and Gu, 2007) if and only if

$$a=\sqrt{e_1-e_2+e_3-L} \tag{16}$$

and

$$b=\frac{1}{2}+\sqrt{\frac{1}{4}+L+e_3} \tag{17}$$

which reduces Eq. (15) into the following form

$$z\,(1-z)\frac{d^2f_{nl}(z)}{d\,z^2}+\left[2\,a+1-(2\,a+2b+1)z\right]\frac{d\,f_{\,nl}(z)}{d\,z}-\left[(a+b)^2-e_1\right]f_{\,nl}(z)=0 \tag{18}$$

Eq. (18) has solution given by (Dong and Wei, 2008):

$$f_{nl}(z)={}_2F_1(\alpha\,,\beta\,,\gamma\,;z). \tag{19}$$

where $f_{nl}(z)$ as given by Eq. (19) is the hypergeometric function and:

$$\alpha=a+b+\sqrt{e_1}\ . \tag{20}$$

$$\beta=a+b-\sqrt{e_1} \tag{21}$$

$$\gamma=2\,a+1\,. \tag{22}$$

For a polynomial solution, the quantum condition (Jia *et al.*, 2008) must be satisfied, this requires that either α or β must be an integer, that is

$$\beta=-n \tag{23}$$

using Eq. (11) in Eqs. (21) and (23) we obtained

$$n+b+\sqrt{e_1-e_2+e_3-L}=\sqrt{e_1}\ . \tag{24}$$

and

$$E_{nl}=-\frac{\delta^2\hbar^2}{2\mu}\left\{\frac{e_2-e_3+L}{2(n+b)}-\frac{n+b}{2}\right\}^2+Z\,e^2\delta-V_0\,B^2-\frac{\delta^2\hbar^2}{2\mu}\left(e_2-e_3+L\right). \tag{25}$$

Eq. (25) transforms to:

$$E_{nl} = -\frac{\delta^2\hbar^2}{2\mu}\left\{\frac{\frac{2\mu V_0\left(A^2-B^2\right)}{\delta^2\hbar^2}+\frac{2\mu Z e^2}{\delta\hbar^2}-\ell(\ell+1)(1-\omega)}{2n+1+\sqrt{(2\ell+1)^2-\frac{8\mu V_0(A+B)^2}{\delta^2\hbar^2}}}-\frac{2n+1+\sqrt{(2\ell+1)^2-\frac{8\mu V_0(A+B)^2}{\delta^2\hbar^2}}}{4}\right\}^2$$
$$+Ze^2\delta-V_0B^2-\frac{\delta^2\hbar^2}{2\mu}\left\{\frac{2\mu V_0\left(A^2-B^2\right)}{\delta^2\hbar^2}+\frac{2\mu Ze^2\delta}{\delta^2\hbar^2}-\ell(\ell+1)(1-\omega)\right\} \tag{26}$$

Eq. (26) is the expression for the bound state energy eigenvalues of the modified Möbius square potential plus Hulthén potential.

Normalization constant

The normalization of the wave function (Saxena, 2012) requires that

$$\int_0^\infty \left|\psi_{nl}(r)\right|^2 dr = 1. \tag{27}$$

where $\left|\psi_{n\ell}(r)\right|^2 = \psi^*_{n\ell}(r)\,\psi_{n\ell}(r)$ and $\psi^*_{n\ell}(r)$ is the complex conjugate of $\psi_{n\ell}(r)$

Eq. (27) can be expressed in terms of the variable z by inserting Eqs. (8) and (14) in Eq. (27), giving rise to:

$$\int_0^1 z^{-1}\left|N_{nl}\, z^a (1-z)^b\, f_{nl}(z)\right|^2 dz = \delta. \tag{28}$$

the hypergeometric function has the form, $f_{nl}(z) = {}_2F_1(\alpha,\beta,\gamma;z)$ from Eq. (19) upon inserting the values of α, β and γ from Eq. (20), Eq. (21) and Eq. (22) results to,

$$f_{nl}(z) = {}_2F_1(-n, n+2a+2b; 2a+1; z) \tag{29}$$

Putting Eq. (29) into Eq. (28), we get,

$$N^2_{nl}\int_0^1 z^{2a-1}(1-z)^{2b}\left|{}_2F_1(-n,n+2a+2b;2a+1;z)\right|^2 dz = \delta \tag{30}$$

$$N_{n_l} = \left(\frac{\delta}{S}\right)^{\frac{1}{2}} \tag{31}$$

where

$$S = \int_0^1 z^{2a-1}(1-z)^{2b}\left|{}_2F_1(-n,n+2a+2b;2a+1;z)\right|^2 dz \tag{32}$$

Following (Miranda *et al*., 2010), we find:

$$S = \frac{n!\,(n+b)\Gamma(n+2b)\Gamma(2a)\Gamma(2a+1)}{(n+a+b)\Gamma(n+2a+1)\Gamma(n+2a+2b)} \tag{33}$$

RESULTS AND DISCUSSION

Hulthén potential

If we set *A = B = 0* in Eq. (7), we have the expression for the effective Hulthén potential (Jia *et al*., 2008)

$$V_{eff}(r) = -\frac{Ze^2\delta e^{-\delta r}}{1\text{-}e^{-\delta r}}+\frac{\ell(\ell+1)\hbar^2\delta^2}{2\mu}\left[\frac{\omega e^{-\delta r}}{1-e^{-\delta r}}+\frac{e^{-2\delta r}}{\left(1-e^{-\delta r}\right)^2}\right] \tag{34}$$

Therefore, by substituting the above values of A and B in Eq. (26), we have the energy eigenvalue for the Hulthén potential given by:

$$E_{nl} = -\frac{\delta^2\hbar^2}{2\mu}\left\{\frac{\dfrac{2\mu Z e^2}{\delta\hbar^2} - \ell(\ell+1)(1-\omega)}{2\,(n+\ell+1)} - \frac{n+\ell+1}{2}\right\}^2 \tag{35}$$

To confirm the validity of Eq. (35), we have computed the bound state energy eigenvalues as a function of screening parameter δ for arbitrary values of n and ℓ. The data in Table 1 shows the computed energy eigenvalues obtained by using Eq. (35), also shown in Table 1 are corresponding bound state energy eigenvalues of the Hulthén potential in the literature which were obtained numerically (Varshni, 1990) and by asymptotic iteration method (Bayrak *et al*., 2006). For small values of the screening parameters, our computed bound state energy eigenvalues values are almost indistinguishable from literature results. However, for larger values of the screening parameters such as $\delta = 0.035$, for 2p state, our result differs significantly from numerically computed result but in total agreement with those obtained by Bayrak *et al*. (2006), this trend also applies for the other quantum states, therefore, confirming the applicability of our result for the bound state energy eigenvalues for the Hulthén potential.

Table 1: Energy eigenvalues of the Hulthén potential as a function of screening parameter for 2p, 3p, 3d, 4p, 4d and 4f states in atomic units ($\hbar = \mu = e = 1$) for Z = 1 and ω = 0.9912122120

state	δ	PR	(Varshi, 1990)	(Bayrak et al., 2006)
2p	0.025	0.1127603	0.1127605	0.1128125
	0.050	0.1011512	0.1010425	0.1012500
	0.075	0.0901725	0.0898478	0.0903125
	0.100	0.0798243	0.0791794	0.0800000
	0.150	0.0610195	0.0594415	0.0612500
	0.200	0.0447368	0.0418860	0.0450000
	0.250	0.0309760	0.0266111	0.0312500
	0.300	0.0197372	0.0137900	0.0200000
	0.350	0.0110205	0.0037931	0.0112500
3p	0.025	0.0437370	0.0437069	0.0437590
	0.050	0.0333302	0.0331645	0.0333681
	0.075	0.0243352	0.0239397	0.0243837
	0.100	0.0167519	0.0160537	0.0168056
	0.150	0.0058206	0.0044663	0.0058681
3d	0.025	0.0436937	0.0436030	0.0437587
	0.050	0.0332546	0.0327532	0.0333681
	0.075	0.0242384	0.0230307	0.0243837
	0.100	0.0166448	0.0144842	0.0168055
	0.150	0.0057261	0.0013966	0.0058681
4p	0.025	0.0199890	0.0199625	0.0200000
	0.050	0.0112335	0.0110582	0.0112500
	0.075	0.0049835	0.0046219	0.0050000
	0.100	0.0012390	0.0007550	0.0012500
4d	0.025	0.0199671	0.0198462	0.0200000
	0.050	0.0112006	0.0106674	0.0112500
	0.075	0.0049507	0.0038345	0.0050000
4f	0.025	0.0199341	0.0196911	0.0200000
	0.050	0.0111514	0.0100620	0.0112500
	0.075	0.0049016	0.0025563	0.0050000

Modified Möbius square potential

If we let $Z = 0$ in Eqs. (7) and (26), we have for the modified Möbius square potential:

$$V_{eff}(r) = -V_0\left(\frac{\mathrm{A}+\mathrm{B}e^{-\delta r}}{1\text{-}e^{-\delta r}}\right)^2 + \frac{L\hbar^2\delta^2}{2\mu}\left[\frac{\omega e^{-\delta r}}{1-e^{-\delta r}} + \frac{e^{-2\delta r}}{\left(1-e^{-\delta r}\right)^2}\right] \tag{36}$$

$$E_{nl}=-\frac{\delta^2\hbar^2}{2\mu}\left\{\frac{\dfrac{2\mu V_0\left(A^2-B^2\right)}{\delta^2\hbar^2}-\ell(\ell+1)(1-\omega)}{2n+1+\sqrt{(2\ell+1)^2-\dfrac{8\mu V_0(A+B)^2}{\delta^2\hbar^2}}}-\frac{2n+1+\sqrt{(2\ell+1)^2-\dfrac{8\mu V_0(A+B)^2}{\delta^2\hbar^2}}}{4}\right\}^2-V_0B^2$$
$$-\frac{\delta^2\hbar^2}{2\mu}\left\{\frac{2\mu V_0\left(A^2-B^2\right)}{\delta^2\hbar^2}-\ell(\ell+1)(1-\omega)\right\} \tag{37}$$

Further, by letting $\delta = 2\alpha$ and $\omega = 0$, Eqs. (36) and (37) reduces to the effective potential and bound state energy eigenvalues derived by Okorie *et al*. (2018)

Deng-Fan potential

The Deng-Fan potential has been proposed in an attempt to finding a more suitable diatomic potential to describe the vibrational spectrum, qualitatively, it is similar to the Morse potential but has the correct asymptotic behaviour as the internuclear distance approaches zero (Oyewumi *et al.*, 2013). If we choose $A=1,\ B=-e^{\delta r_e}$, $V_0=-D_e$ and $Z=0$, where r_e is the equilibrium bond length and D_e is the dissociation energy. Eqs. (7) and (26) give respectively for the Deng-Fan potential.

$$V_{eff}(r)=D_e\left(1-\frac{e^{\delta r_e}-1}{e^{\delta r}-1}\right)^2+\frac{L\hbar^2\delta^2}{2\mu}\left\{\frac{\omega e^{-\delta r}}{1-e^{-\delta r}}+\frac{e^{-2\delta r}}{\left(1-e^{-\delta r}\right)^2}\right\} \tag{38}$$

$$E_{nl}=-\frac{\delta^2\hbar^2}{2\mu}\left\{\frac{\dfrac{2\mu D_e\left(e^{2\delta r_e}-1\right)}{\delta^2\hbar^2}-\ell(\ell+1)(1-\omega)}{2n+1+\sqrt{(2\ell+1)^2+\dfrac{8\mu D_e\left(e^{\delta r_e}-1\right)^2}{\delta^2\hbar^2}}}-\frac{2n+1+\sqrt{(2\ell+1)^2+\dfrac{8\mu D_e\left(e^{\delta r_e}-1\right)^2}{\delta^2\hbar^2}}}{4}\right\}^2$$
$$+D_e e^{2\delta r_e}-\frac{\delta^2\hbar^2}{2\mu}\left\{\frac{2\mu D_e\left(e^{2\delta r_e}-1\right)}{\delta^2\hbar^2}-\ell(\ell+1)(1-\omega)\right\} \tag{39}$$

To test the accuracy of our approximations scheme we have employed equation (39) to compute the energy eigenvalues of various quantum states *viz*: 2p, 3p, 3d, 4p, 4d, 5p, 5d, 5f, 6p, 6d, 6f and 6g states for the parameter ω = 0.97685485225. Tables 2 and 3, shows the computed energy eigenvalues (eV) in the present (PR) study, also shown in the tables are energy eigenvalues extracted in the literature which were obtained by numerical (NUM) method, Nikiforov-Uvarov(NU) method, Supersymmetric quantum mechanics(SUSY) approach and functional analysis method (FUN). From the results shown in Tables 2 and 3, it is obvious that the energy eigenvalues obtained in the present study is in near perfect agreement with values obtained numerically, thus, confirming the accuracy of the Pekeris-type approximation over the Greene and Aldrich approximation models.

Table 2: Energy eigenvalues (eV) $E_{n\ell}$ of the Deng-Fan potential in atomic units ($\hbar = \mu = 1$) with $D_e = 15$ and $r_e = 0.40$.

state	δ	PR	NUM	NU	SUSY	FUN
2p	0.05	7.86203	7.8628	7.86080	7.86080	7.86060
	0.10	7.95542	7.95537	7.95330	7.95330	7.95247
	0.15	8.04778	8.04724	8.04510	8.04510	8.04322
	0.20	8.13910	8.13842	8.13620	8.13620	8.13287
	0.25	8.22942	8.22892	8.22663	8.22663	8.22142
	0.30	8.31874	8.31874	8.31639	8.31639	8.30889
3p	0.05	10.99840	10.9998	10.99776	10.99780	10.99760
	0.10	11.16349	11.1647	11.16256	11.16260	11.16170
	0.15	11.32513	11.32647	11.32425	11.32420	11.32240
	0.20	11.48333	11.48513	11.48284	11.48280	11.47950
	0.25	11.63811	11.64068	11.63834	11.63830	11.63310
	0.30	11.78946	9.67565	11.79076	11.79080	11.78330
3d	0.05	10.21832	10.21651	10.21598	10.21598	10.21540
	0.10	10.35722	10.35409	10.35354	10.35354	10.35100
	0.15	10.49337	10.48992	10.48935	10.48935	10.48370
	0.20	10.62682	10.62403	10.62346	10.62346	10.61350
	0.25	10.75760	10.75645	10.75591	10.75591	10.74030
	0.30	10.88575	10.88719	10.88672	10.88672	10.86420
4p	0.05	12.49795	12.4992	12.49760	12.49760	12.49740
	0.10	12.69715	12.69851	12.69680	12.69680	12.69600
	0.15	12.88836	12.8901	12.88835	12.88835	12.88650
	0.20	13.07157	13.074	13.07224	13.07224	13.06890
	0.25	13.24677	13.2501	13.24847	13.24847	13.24330
4d	0.05	12.09957	12.0989	12.09829	12.09829	12.09770
	0.10	12.28654	12.2857	12.28501	12.28501	12.28250
	0.15	12.46717	12.46715	12.46642	12.46642	12.46080
	0.20	12.64152	12.64324	12.64257	12.64257	12.63260
4f	0.05	11.82365	11.8209	11.82079	11.82079	11.81950
	0.10	12.00166	11.9981	11.99796	11.99796	11.99300
	0.15	12.17420	12.1718	12.17170	12.17170	12.16040
	0.20	12.34134	12.3421	12.34207	12.34207	12.32210
5p	0.10	13.54218	13.5434	13.54214	13.54214	13.54130
	0.20	13.92767	13.9301	13.92899	13.92899	13.92570
5d	0.10	13.30717	13.3075	13.30680	13.30680	13.30430
	0.20	13.68927	13.6931	13.69266	13.69266	13.68270
5f	0.10	13.14872	13.1478	13.14760	13.14760	13.14260
	0.20	13.52741	13.5333	13.53344	13.53344	13.51340
5g	0.10	13.04026	13.0379	13.03798	13.03798	13.02960
	0.10	13.41795	13.42667	13.42711	13.42711	13.39380
6p	0.10	14.05193	14.053	14.05209	14.05209	14.05130
6d	0.10	13.90674	13.9075	13.90705	13.90705	13.90450
6f	0.10	13.81080	13.8113	13.81119	13.81119	13.80620
6g	0.10	13.74622	13.7466	13.74661	13.74661	13.73830

Table 3: Energy eigenvalues (eV) $E_{n\ell}$ of the Deng-Fan potential in atomic units (ħ = μ =1) with D_e =15 and r_e = 0.80

state	δ	PR	NUM	NU	SUSY	FUN
2p	0.05	4.14177	4.14208	4.14089	4.14089	4.14068
	0.10	4.22060	4.2204	4.21918	4.21918	4.21835
	0.15	4.29902	4.2987	4.29739	4.29739	4.29552
	0.20	4.37703	4.3769	4.37555	4.37555	4.37221
	0.25	4.45466	4.4551	4.45366	4.45366	4.44845
	0.30	4.53193	4.5332	4.53175	4.53175	4.52425
3p	0.05	7.53336	7.535	7.53279	7.53279	7.53258
	0.10	7.72556	7.7271	7.72476	7.72476	7.72393
	0.15	7.91587	7.9177	7.91518	7.91518	7.91330
	0.20	8.10428	8.1066	8.10404	8.10404	8.10071
	0.25	8.29081	8.2841	8.29135	8.29135	8.28615
	0.30	8.47546	8.4799	8.47712	8.47712	8.46962
3d	0.05	5.74196	5.7404	5.73975	5.73975	5.73913
	0.10	5.84917	5.8465	5.84577	5.84577	5.84327
	0.15	5.95427	5.9515	5.95068	5.95068	5.94505
	0.20	6.05732	6.0553	6.05453	6.05453	6.04453
	0.25	6.15836	6.1582	6.15740	6.15740	6.14177
	0.30	6.25748	6.2601	6.25932	6.25932	6.23682
4p	0.05	9.61339	9.6156	9.61301	9.61301	9.61280
	0.10	9.88394	9.8862	9.88352	9.88352	9.88269
	0.15	10.14866	10.1514	10.14856	10.14856	10.14670
	0.20	10.40752	10.4111	10.40806	10.40806	10.40470
	0.25	10.66046	10.665	10.66197	10.66197	10.65680
4d	0.05	8.49478	8.4948	8.49334	8.49334	8.49272
	0.10	8.70898	8.7087	8.70711	8.70711	8.70461
	0.15	8.91910	8.9194	8.91781	8.91781	8.91218
	0.20	9.12521	9.1272	9.12551	9.12551	9.11551
4f	0.05	7.43817	7.4351	7.43471	7.43471	7.43346
	0.10	7.59136	7.5868	7.58642	7.58642	7.58142
	0.15	7.74016	7.7361	7.73573	7.73573	7.72448
	0.20	7.88468	7.8831	7.88276	7.88276	7.86276
5p	0.10	11.30223	11.3047	11.30207	11.30207	11.30120
	0.20	11.91217	11.9161	11.91322	11.91322	11.90990
5d	0.10	10.52098	10.5219	10.52009	10.52009	10.51760
	0.20	11.06710	11.0713	11.06937	11.06937	11.05940
5f	0.10	9.79922	9.7975	9.79666	9.79666	9.79166
	0.20	10.27014	10.2738	10.27304	10.27304	10.25300
5g	0.10	9.15766	9.1524	9.15222	9.15222	9.14389
	0.10	9.55051	9.5528	9.55287	9.55287	9.51954
6p	0.10	12.27978	12.2822	12.27980	12.27980	12.27900
6d	0.10	11.73667	11.7383	11.73644	11.73644	11.73390
6f	0.10	11.24582	11.2459	11.24481	11.24481	11.23980
6g	0.10	10.81778	10.8158	10.81533	10.81533	10.80700

Having established the superiority of the Pekeris-type approximation scheme over the Greene and Aldrich model on the modified Möbius squared potential plus Hulthén potential, we have applied our derived energy eigenvalue equation to a more idealized system, here, we have considered six diatomic molecules: HCl, LiH, TiH, NiC, TiC and ScF, the choice of these diatomic molecules is to enable compare our results with those obtained by other authors. The data shown in Table 4 (Oyewumi, Oluwadare, Sen and Babalola, 2012) shows model parameters of the diatomic molecules used in our computation of the bound state energy

Table 4: Spectroscopic parameters of selected molecules, used in the present study.

molecules	De (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
TiH	2.05	1.781	1.32408	0.9873710
NiC	2.76	1.621	2.25297	9.974265
TiC	2.66	1.790	1.52550	9.606790
ScF	5.85	1.794	1.46102	13.358942

The results shown in Tables 5 and 6 are the computed bound state energy eigenvalues for HCl, LiH, TiH, NiC, TiC and ScF. We have included columns for bound state energy eigenvalues of the Deng-Fan potential computed within the frameworks of

Nikiforov-Uvarov (NU) method, comparison of the present results (PR) and that obtained by NU method shows good agreement for the state between our computed energy eigenvalues and those obtained by NU method, however, there is no available data on results obtained by numerical methods to enable further comparison. The plots in Figures 1 and 2 are the radial wave functions for 2p, 5f for HCl and 1s, 4f for LiH.

Table 5: The bound state energies E_{nl} (in eV) for HCl, LiH and TiH

state		HCl		LiH		TiH	
		PR	**NU**	**PR**	**NU**	**PR**	**NU**
0	0	0.202058236	0.201984174	0.103333625	0.103334650	0.095194192	0.095195135
	1	0.204074322	0.204854248	0.104898886	0.105236729	0.096217575	0.096647888
1	0	0.590952203	0.590747827	0.302003040	0.302005955	0.277946427	0.277949104
	1	0.592885903	0.593537612	0.303497609	0.303838653	0.278925122	0.279358078
2	0	0.960325653	0.960011044	0.490681252	0.490685861	0.450920200	0.450924416
	1	0.962178048	0.962721591	0.492106738	0.492450759	0.451854842	0.452290234
	2	0.965881747	0.968141645	0.494956099	0.495978997	0.453723485	0.455021255
3	0	1.310433982	1.310027865	0.669594907	0.669601019	0.614253922	0.614259487
	1	1.312206130	1.312660203	0.670952866	0.671299648	0.615145130	0.615582758
	2	1.315749352	1.317923855	0.673667213	0.674695388	0.616926918	0.618228694
	3	1.321061502	1.325816775	0.677734812	0.679785205	0.619598028	0.622196086
4	0	1.641527447	1.641047243	0.838963132	0.838970564	0.768082994	0.768089723
	1	1.643220385	1.643602379	0.840255067	0.840604402	0.768931376	0.769371041
	2	1.646605204	1.648711644	0.842837407	0.843870601	0.770627521	0.771933083
	3	1.651679792	1.656373023	0.846707095	0.848766203	0.773170195	0.775774658
	4	1.658440980	1.666583499	0.851859551	0.855286782	0.776557543	0.780893985
5	0	1.953851289	1.953313156	0.998997828	0.999006401	0.912539887	0.912547598
	1	1.955466034	1.955792078	1.000225194	1.000576880	0.913346036	0.913787546
	2	1.958694483	1.960748932	1.002678435	1.003716397	0.914957727	0.916266858
	3	1.963534556	1.968181734	1.006354573	1.008422072	0.917373744	0.919984364
	4	1.969983136	1.978087513	1.011249142	1.014689589	0.920592266	0.924938312
	5	1.978036066	1.990462308	1.017356201	1.022513206	0.924610865	0.931126367

Table 6: The bound state energies E_{nl} (in eV) for NiC, TiC and ScF

state		NiC		TiC		ScF	
		PR	NU	PR	NU	PR	NU
0	0	0.055343810	0.055344362	0.039112902	0.039113293	0.047569741	0.047570217
	1	0.055451873	0.055579192	0.039212882	0.039272617	0.047642645	0.047682126
1	0	0.164292441	0.164294062	0.116392271	0.116393424	0.142067832	0.142069247
	1	0.164399275	0.164527691	0.116491037	0.116551564	0.142140230	0.142180660
2	0	0.270944879	0.270947523	0.192438048	0.192439939	0.235730886	0.235733223
	1	0.271050486	0.271179952	0.192535604	0.192596892	0.235802779	0.235844142
	2	0.271261700	0.271644807	0.192730711	0.192910789	0.235946566	0.236065981
3	0	0.375304805	0.375308427	0.267253990	0.267256594	0.328560483	0.328563726
	1	0.375409188	0.375539658	0.267350339	0.267412364	0.328631873	0.328674152
	2	0.375617952	0.376002118	0.267543033	0.267723901	0.328774651	0.328895002
	3	0.375931094	0.376695804	0.267832066	0.268191197	0.328988816	0.329226276
4	0	0.477375891	0.477380444	0.340843838	0.340847133	0.420558199	0.420562331
	1	0.477479052	0.477610482	0.340938984	0.341001723	0.420629086	0.420672264
	2	0.477685371	0.478070549	0.341129272	0.341310904	0.420770858	0.420892131
	3	0.477994846	0.478760649	0.341414695	0.341774668	0.420983514	0.421221926
	4	0.478407469	0.479680772	0.341795242	0.342393002	0.421267051	0.421661649
5	0	0.577161800	0.577167239	0.413211313	0.413215272	0.511725603	0.511730608
	1	0.577263740	0.577396081	0.413305260	0.413368688	0.511795988	0.511840049
	2	0.577467619	0.577853763	0.413493149	0.413675522	0.511936756	0.512058932
	3	0.577773432	0.578540282	0.413774975	0.414135763	0.512147906	0.512387253
	4	0.578181173	0.579455631	0.414150724	0.414749401	0.512429435	0.512825013
	5	0.578690835	1.022513206	0.414620383	0.931126367	0.512781339	1.022513206

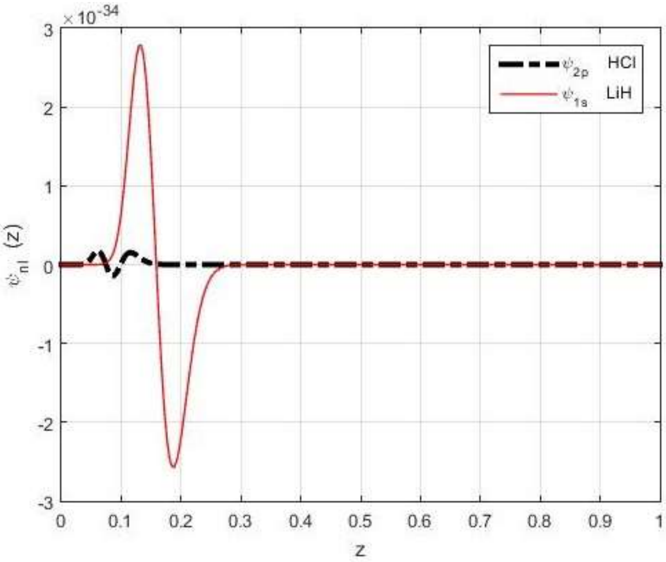

Figure 1: Plot of unnormalised radial wave functions of HCl and LiH for 2p and 1s states

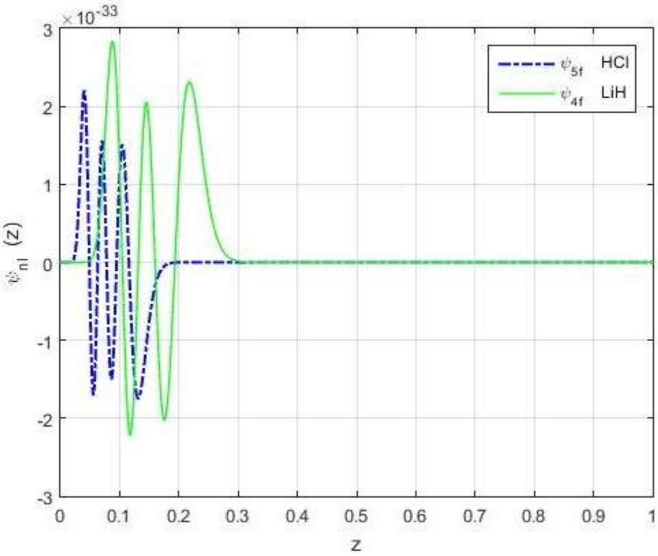

Figure 2: Plot of unnormalised radial wave functions of HCl and LiH for 5f and 4f states

CONCLUSION

We have solved for the approximate ℓ-state solution of time independent Schrödinger wave equation with modified Möbius squared potential plus Hulthén potential, the Pekeris-type approximation scheme was used to simplify the spin-orbit centrifugal term. we have obtained closed form expressions for the bound state energy eigenvalues and normalized radial wave functions of the modified Möbius squared potential plus Hulthén potential, using our results we have derived expressions for the bound state energy eigenvalues and radial wave functions of Hulthén potential, modified Möbius squared potential and Deng-Fan potential, by appropriately selecting the parameter ω, we have computed bound state energy eigenvalues for Hulthén potential and Deng-fan potential for arbitrary values of quantum numbers, we have also obtained the bound state energy eigenvalues for the Deng-fan potential for six diatomic molecules: HCl, LiH, TiH, NiC, TiC and ScF, our computed results compared favorably with existing results in the literature. The results obtained in this research work can find useful applications in the area of solid state physics, atomic physics, molecular physics and chemical physics

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