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BOUND STATE SOLUTIONS OF NON-RELATIVISTIC SCHRÖDINGER EQUATION WITH HELLMANN POTENTIAL WITHIN THE FRAMEWORKS OF GENERALIZED PEKERIS APPROXIMATION OF THE CENTRIFUGAL TERM POTENTIAL

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Abstract

In this paper we have solved the Schrödinger equation using the Hellmann potential and obtained bound state solutions for the energy eigenvalues and normalized radial wave functions using the recently proposed generalized Pekeris approximation model to the centrifugal term potential. We have also obtained the s-wave energy eigenvalues for 2s quantum state, our result showed excellent agreement with existing literature results for small values of potential screening parameter C. We have also studied the variation of energy eigenvalues, $E_{n\ell}$ ***with energy determining parameter*** α ***where our result showed that*** $E_{n\ell}$ ***remains fairly constant for given values of C and*** α ***with increase in principal quantum number,*** n. $E_{n\ell}$ ***also decreases with increase in*** α ***for given values of C and*** n. ***The study also reveal the existence of threshold value of*** α ***at which bound state exists for all quantum states*** $n\ell$

Keywords: Hellmann potential, Schrödinger equation, energy eigenvalues, energy determining parameter, Pekeris approximation

1.0 Introduction

Solutions of the wave equation are indispensable in quantum mechanics because of the significant information they convey about the quantum system under consideration, such information contained in the wave function include: energy, momentum, frequency, wavelength and the speed of the quantum system [1-5]. The solution of wave equation depends on the type of potential energy function used to solve the Schrödinger equation, potentials such as: harmonic oscillator, pseudoharmonic oscillator and Deng-Fan potential amongst others give exact analytical solution for all quantum states $|n\ell\rangle$ [6-9]. On the other hand, few other potentials give exact solutions only for the state $|n0\rangle$ (s-wave) [10-12]. However, for many potential functions, exact analytical solutions are not possible for all quantum states, in such a situation, one has to resort to approximate analytical solutions, the approximation is usually applied to the centrifugal term of the Schrödinger equation, various approximation models have been proposed some decades ago [1,2 13-16]. The proposed approximation models are limited to short potential range and/or screening parameter of the potential and are mostly applicable to exponential type potentials only. Recently [17] have proposed a new approximation model which is based on Taylor series expansion of the centrifugal term, the model was applied to solve the Schrödinger equation for the Rosen-Morse and the Manning-Rosen potentials. Various solution methods were used to solve the Schrödinger equation analytically, some of these methods include: standard method [6, 18, 19]. Supersymmetric quantum mechanics [20-22], Nikiforov-Uvarov method [23-26], asymptotic (and improved asymptotic) iteration method [27-29], exact (and proper) quantization rules [30-32], generalized

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pseudospectral method [33-35]. The Schrödinger equation has been solve by researchers using a number of potential models, these potentials include: Manning-Rosen potential [36-39], Eckart potential [40-41] among others.

2.0 Theoretical Approach

2.0.1 The Hellmann Potential

The Hellmann potential [35] is a superposition of Coulomb potential and Yukawa (or screened Coulomb) potential, it is given by:

$$V(r) = -\frac{A}{r} + \frac{Be^{-Cr}}{r} \tag{1}$$

where $A\,(>0)$and B are the depths of the Coulomb and Yukawa potentials respectively, r is the internuclear separation between two interacting particles and $C\,(>0)$ is the screening parameter. Like most other potentials, the Hellmann potential does not offer exact analytical solution with the Schrödinger equation, thus, the need for approximate analytical solution. Various methods have been used to solve the Schrödinger equation with Hellmann potential [35, 42-43]. Encouraged by the results and successes of the recently proposed generalized Pekeris approximation scheme [17, 19], we are motivated to solve the Schrödinger equation with the Hellmann potential via the generalized Pekeris approximation to the centrifugal term and to compare results with available data in the literature.

2.0.2 Energy Eigenvalues and Radial Wave Functions

The radial Schrödinger equation [19], for a molecule of reduced mass μ with the Hellmann potential is given by:

$$\frac{d^2R_{n\ell}}{dr^2} + \frac{2\mu}{\hbar^2}\left\{E_{n\ell} + \frac{1}{r_e}\left(A - Be^{-Cr}\right)\frac{r_e}{r} - \frac{\ell(\ell+1)\hbar^2}{2\mu r_e^2}\left(\frac{r_e}{r}\right)^2\right\}R_{n\ell} = 0\cdot \tag{2}$$

where $E_{n\ell}$ is the energy eigenvalue of the molecule, n and ℓ are the principal vibrational quantum number and the principal angular momentum quantum number respectively and r_e is the equilibrium internuclear distance.

Letting

$$z = e^{-Cr}. \tag{3}$$

Eq. (2) transforms to:

$$z^2R''_{n\ell}(z) + zR'_{n\ell}(z) + \frac{2\mu}{C^2\hbar^2}\left\{E_{n\ell} + \frac{1}{r_e}(A - Bz)\frac{r_e}{r} - \frac{\ell(\ell+1)\hbar^2}{2\mu r_e^2}\left(\frac{r_e}{r}\right)^2\right\}R_{n\ell} = 0\cdot \tag{4}$$

where prime denotes derivative with respect to z. Following [19], r_e/r and $(r_e/r)^2$ can be approximated by terms of a Taylor series expansion. In this paper we have used:

$$\frac{r_e}{r} \approx a_0 + a_1(y - \alpha)\cdot \tag{5}$$

where y and its inverse $y^{=1}$ are appropriately chosen functions, and α is an element in the domain of $y^{=1}$. The coefficients, $a_N\,(N = 0,1,2,\ldots)$ are given by:

$$a_N = \left.\frac{d^NF}{dy^N}\right|_{y=\alpha}. \tag{6}$$

with the function F given by [17]

$$F(y) \equiv \left(\frac{r_e}{r}\right)^m = \left(1 - \frac{y^{-1}}{\alpha r_e}\right)^{-m}\cdot \tag{7}$$

In the present work, we have chosen:

$$y = e^{-\alpha(Cr/\alpha - r_e)} \equiv e^{\alpha r_e}z. \tag{8}$$

And

$$y^{=1} = \ln y. \tag{9}$$

By taking $m = 1$, Eq. (6) and Eq. (7) gives:

$$a_0 = \frac{\alpha r_e}{\alpha r_e - \ln\alpha}. \tag{10}$$

and

$$a_1 = \frac{r_e}{(\alpha r_e - \ln\alpha)^2}. \tag{11}$$

Similarly, $(r_e / r)^2$ can be approximated by:

$$\left(\frac{r_e}{r}\right)^2 \approx b_0 + b_1(y-\alpha) + \tfrac{1}{2}b_2(y-\alpha)^2. \tag{12}$$

By taking $m = 2$, $b_N \equiv a_N$ in Eq. (6), Eq.(7)gives

$$b_0 = \frac{\alpha^2 r_e^2}{(\alpha r_e - \ln\alpha)^2}. \tag{13}$$

$$b_1 = \frac{2\alpha r_e^2}{(\alpha r_e - \ln\alpha)^3}. \tag{14}$$

$$b_2 = \frac{2r_e^2(3 - \alpha r_e + \ln\alpha)}{(\alpha r_e - \ln\alpha)^4}. \tag{15}$$

where $\alpha \in [1, \infty)$

Substitute Eq. (5) and Eq. (12) in Eq. (4) to obtain:

$$z^2 R''_{n\ell}(z) + z R'_{n\ell}(z) + \left(-\varepsilon_1 z^2 + \varepsilon_2 z - \varepsilon_3\right)R_{n\ell} = 0 \tag{16}$$

where

$$\varepsilon_1 = \frac{2\mu B e^{\alpha r_e}}{C^2\hbar^2 r_e}a_1 + \frac{\ell(\ell+1)e^{2\alpha r_e}}{2C^2 r_e^2}b_2. \tag{17}$$

$$\varepsilon_2 = \frac{2\mu A e^{\alpha r_e}}{C^2\hbar^2 r_e}a_1 - \frac{2\mu B}{C^2\hbar^2 r_e}(a_0 - \alpha a_1) - \frac{\ell(\ell+1)e^{\alpha r_e}}{C^2 r_e^2}(b_1 - \alpha b_2). \tag{18}$$

$$-\varepsilon_3 = \frac{2\mu E_{n\ell}}{C^2\hbar^2} + \frac{2\mu A}{C^2\hbar^2 r_e}(a_0 - \alpha a_1) - \frac{\ell(\ell+1)}{C^2 r_e^2}\left(b_0 - \alpha b_1 + \tfrac{1}{2}\alpha^2 b_2\right). \tag{19}$$

To solve Eq. (16), consider the ansatz:

$$R_{n\ell}(z) = N_n e^{-\frac{1}{2}az} z^{\frac{1}{2}b} F_{n\ell}(z). \tag{20}$$

From which we obtained:

$$R'_{n\ell}(z) = \left[-\tfrac{1}{2}a + \frac{b}{2z} + \frac{F'_{n\ell}(z)}{F_{n\ell}(z)}\right]R_{n\ell}(z). \tag{21}$$

and

$$R''_{n\ell}(z) = \left[\frac{F''_{n\ell}(z)}{F_{n\ell}(z)} + \left(-a + \frac{b}{z}\right)\frac{F'_{n\ell}(z)}{F_{n\ell}(z)} + \tfrac{1}{4}a^2 - \frac{ab}{2z} + \frac{b^2}{4z^2} - \frac{b}{2z^2}\right]R_{n\ell}(z). \tag{22}$$

Eq. (21) and Eq. (22) when used in Eq. (16) and slight simplification gives:

$$z F''_{n\ell}(z) + (b+1-az)F'_{n\ell}(z) + \left\{\varepsilon_2 - \tfrac{1}{2}ab - \tfrac{1}{2}a + \left(\tfrac{1}{4}a^2 - \varepsilon_1\right)z + \frac{\frac{1}{4}b^2 - \varepsilon_3}{z}\right\}F_{n\ell}(z) = 0. \tag{23}$$

Eq. (23) is of hypergeometric-type if the last-two terms of the coefficient of $F_{n\ell}(z)$ separately varnishes, this is true iff:

$$a = 2\varepsilon_1^{\frac{1}{2}}. \tag{24}$$

and

$$b = 2\varepsilon_3^{\frac{1}{2}}. \tag{25}$$

Putting Eq. (24) and Eq. (25) in Eq. (23), we obtain the associated Laguerre differential equation given by:

$$u F''_{n\ell}(u) + (b+1-au)F'_{n\ell}(u) + \left(\frac{\varepsilon_2}{a} - \tfrac{1}{2}b - \tfrac{1}{2}\right)F_{n\ell}(u) = 0. \tag{26}$$

where

$$u = a\,z\,. \tag{27}$$

The solution of Eq. (26) is the associated Laguerre polynomial:

$$F_{n\ell}(u) = {}_1F_1(-n, b+1, u) \equiv \frac{\Gamma(b+1+n)}{\Gamma(b+1)} \quad . \tag{28}$$

where the polynomial condition is given by:

$$\frac{\varepsilon_2}{a} - \tfrac{1}{2}b - \tfrac{1}{2} = n\,. \tag{29}$$

Energy Eigenvalues

Using Eq. (24) and Eq. (25) in Eq. (29), we obtained

$$\varepsilon_3 = \left(n + \tfrac{1}{2} - \frac{\varepsilon_2}{2\varepsilon_1^{\frac{1}{2}}} \right)^2. \tag{30}$$

Furthermore, by inputting Eq. (17), Eq. (18) and Eq. (19) in Eq. (30), we obtained:

$$E_{n\ell} = -\frac{C^2\hbar^2}{2\mu}\left\{ n + \tfrac{1}{2} - \frac{\dfrac{\mu A e^{\alpha r_e}}{C^2\hbar^2 r_e}a_1 - \dfrac{\mu B}{C^2\hbar^2 r_e}(a_0 - \alpha a_1) - \dfrac{\ell(\ell+1)e^{\alpha r_e}}{2C^2 r_e^2}(b_1 - \alpha b_2)}{\left[\dfrac{2\mu B e^{\alpha r_e}}{C^2\hbar^2 r_e}a_1 + \dfrac{\ell(\ell+1)e^{2\alpha r_e}}{2C^2 r_e^2}b_2 \right]^{\frac{1}{2}}} \right\}^2 . \tag{31}$$

$$- \frac{A}{r_e}(a_0 - \alpha a_1) + \frac{\ell(\ell+1)\hbar^2}{2\mu r_e^2}\left(b_0 - \alpha b_1 + \tfrac{1}{2}\alpha^2 b_2\right)$$

2.0.3 Normalization Constant

The normalization condition for the wave functions requires that:

$$\int_0^\infty \left| R_{n\ell}(r) \right|^2 d\,r = 1\,. \tag{32}$$

This can be expressed in terms of the variable z by inserting Eq. (3) in Eq. (32), giving:

$$\int_0^1 z^{-1} \left| R_{n\ell}(z) \right|^2 d\,z = C\,. \tag{33}$$

Substituting Eq. (20) in Eq. (33), get:

$$N_n^2 \int_0^1 e^{-a\,z} z^{b-1} \left| F_{n\ell}(z) \right|^2 d\,z = C\,. \tag{34}$$

Thus, we obtain:

$$N_n^2 \int_0^1 e^{-u} u^{b-1} \left| F_{n\ell}(u) \right|^2 d\,u = C\,a^b\,. \tag{35}$$

when Eq. (27) is used in Eq. (34). The hypergeometric function given by Eq. (28) when used in Eq. (35) leads to:

$$N_n = \left\{ \frac{C\,a^b}{\int_0^a e^{-u} u^{b-1} \left[{}_1F_1(-n, b+1, u) \right]^2 d\,u} \right\}^{\frac{1}{2}} . \tag{36}$$

3.0 Discussions

For the special case of s-wave ($\ell = 0$), Eq. (31) gives the energy eigenvalues as:

$$E_{n\ell} = -\frac{C^2\hbar^2}{2\mu}\left\{ n + \tfrac{1}{2} - \frac{\dfrac{\mu A e^{\alpha r_e}}{C^2\hbar^2 r_e}a_1 - \dfrac{\mu B}{C^2\hbar^2 r_e}(a_0 - \alpha a_1)}{\left[\dfrac{2\mu B e^{\alpha r_e}}{C^2\hbar^2 r_e}a_1 \right]^{\frac{1}{2}}} \right\}^2 - \frac{A}{r_e}(a_0 - \alpha a_1)\,. \tag{37}$$

Table 1 shows the computed energy eigenvalues (in atomic units) for $A=1$ as a function of B and C, the result shows that our computed energy eigenvalues E_{20} are in excellent agreement with those in the literature [35] for small values of screening parameter C. We have also studied the variation of the energy eigenvalue as a function of α at ($A=B=1$). The entries in Tables 2 and 3 indicates the energy eigenvalues for different quantum states $n\ell$. For a given value of α and C, E_{nl} remains fairly constant with increasing n. However, for a given n and C, E_{nl} decreases with α. Fig. 1 shows the plot of E_{nl} versus α for states $n\ell$ for the screening parameters $C=0.025$, this plot also shows the suitability of $\alpha \approx 4.625$ as a common point for computing energy eigenvalues at $A=B=1$.

Table 1 $2s$ **State Energy Eigenvalues (Atomic Units) As a Function of B and C**

B	C	α	$-E_{20}$	$-E_{20}$ [35]
0.5	0.001	1.031284	0.03174842320931	0.03174701400990
0.5	0.005	1.03194359	0.03367672591288	0.03367675354994
0.5	2	…	…	0.11290716132278
0.5	10	…	…	0.12339007950313
-0.5	0.001	1.26064	0.28074610197219	0.2807509984473
-0.5	0.005	1.257771	0.278774972576687	0.2787748073142
-0.5	2	…	…	0.1406129511670
-0.5	10	…	…	0.1268366598878
-2	0.001	2.347042	1.123009050761709	1.1230019984462
-2	0.005	2.327844	1.115049734644538	1.1150498066913
-2	2	…	…	0.2010044938456
-2	10	…	…	0.1342619146710

Table 2 Computed Energy Eigenvalues (atomic unit) as a Function of α for $A=B=1$

$n\ell$	C \ $-E_{n\ell}(\alpha)$ \ α	4.500	4.525	4.550	4.575	4.600	4.625	4.650	4.675	4.700	4.725
$2p$	0.025	0.613385	0.737126	0.862407	0.989224	1.117570	1.247443	1.378837	1.511749	1.646175	1.782109
	0.050	0.614322	0.738064	0.863345	0.990161	1.118508	1.248381	1.379775	1.512687	1.647112	1.783046
	0.075	0.615885	0.739626	0.864907	0.991724	1.120070	1.249943	1.381337	1.514249	1.648675	1.784609
	0.100	0.618072	0.741814	0.867095	0.993911	1.122258	1.252131	1.383525	1.516437	1.650862	1.786796
$3p$	0.025	0.613385	0.737126	0.862407	0.989224	1.117570	1.247443	1.378837	1.511749	1.646175	1.782109
	0.050	0.614322	0.738064	0.863345	0.990161	1.118508	1.248381	1.379775	1.512687	1.647112	1.783046
	0.075	0.615885	0.739626	0.864907	0.991724	1.120070	1.249943	1.381337	1.514249	1.648675	1.784609
	0.100	0.618072	0.741814	0.867095	0.993911	1.122258	1.252131	1.383525	1.516437	1.650862	1.786796
$3d$	0.025	…	…	…	0.185739	0.570847	0.960575	1.354907	1.753830	2.157330	2.565392
	0.050	…	…	…	0.186676	0.571785	0.961513	1.355845	1.754768	2.158267	2.566330
	0.075	…	…	…	0.188239	0.573347	0.963075	1.357407	1.756330	2.159830	2.567892
	0.100	…	…	…	0.190426	0.575535	0.965263	1.359595	1.758518	2.162017	2.570080
$4p$	0.025	0.613385	0.737126	0.862407	0.989224	1.117570	1.247443	1.378837	1.511749	1.646175	1.782109
	0.050	0.614322	0.738064	0.863345	0.990161	1.118508	1.248381	1.379775	1.512687	1.647112	1.783046
	0.075	0.615885	0.739626	0.864907	0.991724	1.120070	1.249943	1.381337	1.514249	1.648675	1.784609
	0.100	0.615885	0.739626	0.864907	0.991724	1.120070	1.249943	1.381337	1.514249	1.648675	1.784609
$4d$	0.025	…	…	…	0.185739	0.570847	0.960575	1.354907	1.753830	2.157330	2.565392
	0.050	…	…	…	0.186676	0.571785	0.961513	1.355845	1.754768	2.158267	2.566330
	0.075	…	…	…	0.188239	0.573347	0.963075	1.357407	1.756330	2.159830	2.567892
	0.100	…	…	…	0.190426	0.575535	0.965263	1.359595	1.758518	2.162017	2.570080
$4f$	0.025	…	…	…	…	…	0.530273	1.319012	2.116951	2.924062	3.740318
	0.050	…	…	…	…	…	0.531211	1.319950	2.117889	2.925000	3.741255
	0.075	…	…	…	…	…	0.532773	1.321512	2.119451	2.926562	3.742818
	0.100	…	…	…	…	…	0.534961	1.323700	2.121639	2.928750	3.745005
$5p$	0.025	0.613385	0.737126	0.862407	0.989224	1.117570	1.247443	1.378837	1.511749	1.646175	1.782109
	0.050	0.614322	0.738064	0.863345	0.990161	1.118508	1.248381	1.379775	1.512687	1.647112	1.783046
	0.075	0.615885	0.739626	0.864907	0.991724	1.120070	1.249943	1.381337	1.514249	1.648675	1.784609
	0.100	0.618072	0.741814	0.867095	0.993911	1.122258	1.252131	1.383525	1.516437	1.650862	1.786796

Table 3 Computed Energy Eigenvalues (atomic unit) as a function of α for $A = B = 1$

$-E_{n\ell}(\alpha)$

α

$n\ell$	C	4.500	4.525	4.550	4.575	4.600	4.625	4.650	4.675	4.700	4.725
$5d$	0.025	…	…	…	0.185739	0.570847	0.960575	1.354907	1.753830	2.157330	2.565392
	0.050	…	…	…	0.186676	0.571785	0.961513	1.355845	1.754768	2.158267	2.566330
	0.075	…	…	…	0.188239	0.573347	0.963075	1.357407	1.756330	2.159830	2.567892
	0.100	…	…	…	0.190426	0.575535	0.965263	1.359595	1.758518	2.162017	2.570080
$5f$	0.025	…	…	…	…	…	0.530273	1.319012	2.116951	2.924062	3.740318
	0.050	…	…	…	…	…	0.531211	1.319950	2.117889	2.925000	3.741255
	0.075	…	…	…	…	…	0.532773	1.321512	2.119451	2.926562	3.742818
	0.100	…	…	…	…	…	0.534961	1.323700	2.121639	2.928750	3.745005
$5g$	0.025	…	…	…	…	…	…	1.271152	2.601113	3.946372	5.306885
	0.050	…	…	…	…	…	…	1.272089	2.602050	3.947310	5.307822
	0.075	…	…	…	…	…	…	1.273652	2.603613	3.948872	5.309385
	0.100	…	…	…	…	…	…	1.275839	2.605800	3.951060	5.311572
$6p$	0.025	0.613385	0.737126	0.862407	0.989224	1.117570	1.247443	1.378837	1.511749	1.646175	1.782109
	0.050	0.614322	0.738064	0.863345	0.990161	1.118508	1.248381	1.379775	1.512687	1.647112	1.783046
	0.075	0.615885	0.739626	0.864907	0.991724	1.120070	1.249943	1.381337	1.514249	1.648675	1.784609
	0.100	0.618072	0.741814	0.867095	0.993911	1.122258	1.252131	1.383525	1.516437	1.650862	1.786796
$6d$	0.025	…	…	…	0.185739	0.570847	0.960575	1.354907	1.753830	2.157330	2.565392
	0.050	…	…	…	0.186676	0.571785	0.961513	1.355845	1.754768	2.158267	2.566330
	0.075	…	…	…	0.188239	0.573347	0.963075	1.357407	1.756330	2.159830	2.567892
	0.100	…	…	…	0.190426	0.575535	0.965263	1.359595	1.758518	2.162017	2.570080
$6f$	0.025	…	…	…	…	…	0.530273	1.319012	2.116951	2.924062	3.740318
	0.050	…	…	…	…	…	0.531211	1.319950	2.117889	2.925000	3.741255
	0.075	…	…	…	…	…	0.532773	1.321512	2.119451	2.926562	3.742818
	0.100	…	…	…	…	…	0.534961	1.323700	2.121639	2.928750	3.745005
$6g$	0.025	…	…	…	…	…	…	1.271152	2.601113	3.946372	5.306885
	0.050	…	…	…	…	…	…	1.272089	2.602050	3.947310	5.307822
	0.075	…	…	…	…	…	…	1.273652	2.603613	3.948872	5.309385
	0.100	…	…	…	…	…	…	1.275839	2.605800	3.951060	5.311572

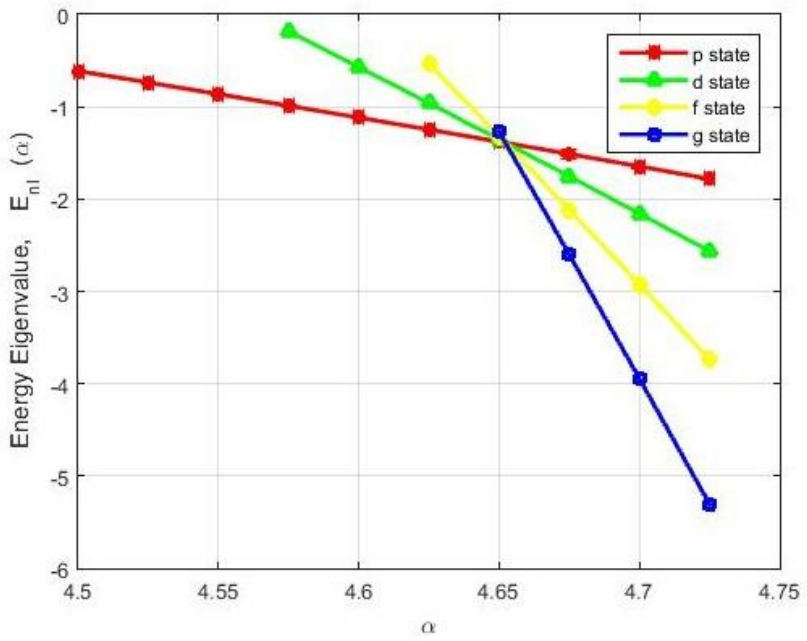

Figure.1 plot of Energy Eigenvalues versus α

4.0 Conclusion

We have obtained analytical solution of the schrodinger equation with Hellmann potential and obtained bound state solutions of energy eigenvalues and normalized radial wave functions in closed forms.we have also obtained energy eigenvalues for the case of s-wave . we have also considered the variation of the energy eigenvalues with potential screening parameter, principal quantum number and energy determinig parameter for different qunatum states.

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