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Analytical and Numerical Study of the Bound State Energy Eigenvalues of the Schrödinger Equation in D – dimensions

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ABSTRACT

In this work, we present the analytical and numerical study of the bound state energy eigenvalues using the Nikiforov-Uvarov method. The Hulthen plus Yukawa potentials were combined to solve the approximate bound state solutions of the radial part of the Schrödinger wave equation. The NU method is used to solve hypergeometric-type second-order differential equations having special orthogonal functions. We presented graphically the behavior of the Hulthen and the Yukawa potentials at different screening parameters, α, and potential strength, V_o. The investigation of how the energy eigenvalues respond or behave when plotted against the screening parameter and the potential depth was done. And from our results, it was observed in table 1 that as the quantum state or quantum number increased, the energy eigenvalues became more bounded. That means that the energy eigenvalues increased as the quantum number increased. Also, that the energy eigenvalues decreased when the values of the screening parameter are increased. For Table 1 and 2, we noticed the degeneracies of the energy levels in quantum numbers n = 2, 3, 4 and 5 for dimensions, D = 3 and 5. Also, as the values of the potential depth were increased, the energy eigenvalues reduced. The results are consistent with existing literatures referenced in the work.

***Keywords*:** Eigenvalues, Nikiforov-Uvarov method, D-dimensions, Hulthen plus Yukawa Potentials

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1. INTRODUCTION

The knowledge of Schrödinger equation (SE) and its solution for a quantum mechanical system enables one to predict the physical properties like the quantum state amongst others when details of the energy eigenvalue and wave function are known [1,2,3]. There are few important potentials- harmonic oscillator, Coulomb, Kratzer potentials etc that one can obtain their exact solution analytically with SE. For potentials that cannot be solved exactly, approximation or numerical methods are adopted [4]. However, for SE that are hypergeometric in nature, possessing exponential and radial terms, one can only solve it analytically with an approximation approach [2]. The centrifugal term is handled by the introduction of a suitable approximation scheme. Exponential-type potentials like the Eckart, Hylleraas, Hulthen, Manning-Rosen, Rosen-Morse, Wood-Saxon, Yukawa etc are being researched by several researchers with various analytical methods to obtain bound state solutions. The NU method, asymptotic iteration method (AIM), the exact quantization rule, factorization method, supersymmetric shape invariance approach (SUSYQM), Path integral solution, variational method, the shifted 1/N expansion, the hypervirial perturbation, the algebraic approach, etc are some of these methods [5-7].

Recently, Ahmadov *et al* investigated the bound state solutions of temperature-dependent Schrödinger equation for Cornell, inverse quadratic and harmonic oscillator-type potentials. The energy eigenvalues and wave function expressed analytically by them, were used to study heavy quarkonia and B_c meson masses for various quantum states [8]. Also, B.I Ita *et al*, used Wentzel-Kramers-Brillouin Jeffery (WKBJ) approximation method to obtain the bound state energy eigenvalues for Manning-Rosen plus class of Yukawa potentials [9].

In this work, within the framework of NU method, the Hulthen plus Yukawa potentials will be used to solve approximate bound state solution of the radial part of SE. In a situation when the quantum state of a particle confined in a potential in a way the particle exhibits the tendency of being localized in one or more region of space, such situation is referred to as bound state. In such a case, the energy eigenvalues ($E<0$) in a field vanish at infinity. The energy is quantized or in discrete manner [10]. We will also investigate how the screening parameters and potential depth affect the structure of the eigenvalues and wave function of the system. Okon *et al* [11] in their study of the bound state solution with Hulthen plus exponential Coulombic potential showed that the bound state energy decreased as the screening parameter was increased.

In atomic physics, condensed matter physics, nuclear physics and solid state physics, Hulthen potential plays a vital role in the description of the molecular structure of an atom and nuclear interaction. As a short-range potential, it shows a Coulomb-like behavior for small values of the screening parameter, α with an exponential decrease for large values of α [12, 13, 14]. Yukawa potential, a non-relativistic potential and also a screened version of the Coulomb potential is used in the description of the interactions between nucleons. The value of the screening parameter of this potential tells more of the physics behind it [15].

The organization of the rest of this paper is as follows; we give a brief concept of the NU method and its parametric form in section 2. The illustration of the graphical behavior of the Hulthen and Yukawa potentials will be shown in section 3. The analytical solution of the radial part of the SE and wave function in D-dimension for the Hulthen plus Yukawa potential will feature in section 4. In section 5, we will present the numerical values, plots for the screening parameter, r and potential depth V_1. In section 6 and 7, we will discuss the results and conclude respectively. Meanwhile, the Maple software will be used for all graphical illustration and numerical computations.

2. THE NU METHOD AND ITS PARAMETRIC FORM

The NU method was formulated by A.F Nikiforov and V.B Uvarov to solve the hypergeometric-type second order differential equations having special orthogonal functions. By using appropriate coordinate transformation r → s, the Schrödinger or Schrödinger-like equations can be reduced to hypergeometric-type depending on the particular potential. Such hypergeometric second-order differential equation is given below [2].

$$\psi''_{(s)}+\frac{\tilde{\tau}_{(s)}}{\sigma_{(s)}}\psi'_{(s)}+\frac{\tilde{\sigma}_{(s)}}{\sigma^2_{(s)}}\psi_{(s}=0 \tag{1}$$

In eq (1) $\sigma_{(s)}$ and $\check{\sigma}_{(s)}$are polynomials at most second degree, $\check{\tau}_{(s)}$ is a first-degree polynomial and $\psi_{(s)}$ is a function of the hypergeometric-type. In order to obtain the particular solution of eq. (1), one can carry out the following transformation

$$\psi_{(s)}=\phi_{(s)}y_{(s)} \tag{2}$$

This transformation yields an equation of the hypergeometric–type given as:

$$\sigma_{(s)}y''\psi_{(s)}+\tau_{(s)}y'_{(s)}+\lambda y_{(s)}=0 \tag{3}$$

where: $y_n(s)$ satisfy the Rodrigues relation [16] and can be written as

$$y_n(s)=\frac{Dn}{\rho(s)}\frac{d^n}{ds^n}\left(\sigma^n(s)\rho(s)\right) \tag{4}$$

where, D_n is the normalization constant and $\rho(s)$ is the weight function which must satisfy the condition

$$\frac{d}{d(s)}[\sigma(s)\rho(s)=\tau(s)\rho(s)] \tag{5}$$

Also,

$$\frac{\phi'(s)}{\phi(s)}=\frac{\pi(s)}{\sigma(s)} \tag{6}$$

$$\tau(s)=\tilde{\tau}(s)+2\pi(s),\quad \tau(s)<0 \tag{7}$$

Bear in that the derivative of $\tau(s)$ with respect to s, is negative.

$$\Lambda_n = -n\tau''(s) - \frac{n(n-1)}{2}\sigma'(s), n = 0, 1, 2 \tag{8}$$

where $\pi(s) = \frac{\sigma'(s)-\tilde{\tau}(s)}{2} \pm \sqrt{\frac{\sigma'(s)-\tilde{\tau}(s)-\tilde{\sigma}(s)+k\sigma(s)}{2}}$ (9)

where

$$k = \Lambda - \pi'(s) \tag{10}$$

For the constant k, to be determined, the discriminant of the quadratic of equation (9) must be set to zero. Bear in mind that since $\pi(s)$ is a polynomial of degree at most one, the expression under the square root sign must be the square of that polynomial. Having met this requirement, and the value of k, obtained, the polynomial $\pi(s)$ is gotten from the Eq. (8) [2, 6, 17].

However Cevdet Tezcan and Ramazan Sever went ahead to formulate the parametric form of the NU method that can be employed for central, non-central and hypergeometric-type potential. This can be obtained when we compare the hypergeometric-type Schrödinger equation written as [18, 19]

$$[\frac{d^2}{ds^2} + \frac{\delta_1-\delta_2}{s(1-\delta_3 s)}\frac{d}{ds} + \frac{-\varsigma_1 s^2+\varsigma_2 s-\varsigma_3}{s^2(1-\delta_3 s)^2}]\,\psi = 0 \tag{11}$$

with Eq.(1) and the following parametric polynomials will be obtained [19]

$$\tilde{\tau} = \delta_1 - \delta_2 s \tag{12}$$

$$\sigma = s(1-\delta_3) \tag{13}$$

$$\tilde{\sigma} = -\varsigma_1 + \varsigma_2 - \varsigma_3 \tag{14}$$

Eq. (15) is obtained when Eq. (12)-(14) are substituted into Eq. (9)

$$\pi = \delta_4 + \delta_5 \pm \sqrt{(\delta_6 - \delta_5)s^2(\delta_7 + k)s + \delta_8} \tag{15}$$

where the following parameters are written as

$$\delta_4 = \frac{1}{2}(1-\delta_1) \tag{16}$$

$$\delta_5 = \frac{1}{2}(\delta_2 - 2\delta_3) \tag{17}$$

$$\delta_6 = \delta_5 + \varsigma_1 \tag{18}$$

$$\delta_7 = 2\delta_4\delta_5 - \varsigma_2 \tag{19}$$

$$\delta_8 = \delta^2{}_4 + \varsigma_3 \tag{20}$$

In accordance to the NU method, the parameters k is obtained from the expression given in Eq.(9). Therefore,

$$K\pm = -(\delta_7 + 2\delta_3\delta_8) \pm \sqrt{\delta_8\delta_9} \tag{21}$$

where we define

$$\delta_9 = \delta_3\delta_7 + \delta^2{}_3\delta_8 + \delta_6 \tag{22}$$

The function π represented in Eq. (15) becomes

$$\pi = \delta_4 + \delta_5 s - [(\sqrt{\delta_9} + \delta_3\sqrt{\delta_8})s - \sqrt{\delta_8}\,] \tag{23}$$

For the k- value that is negative, it is obtained as

$$k = -(\delta_7 + 2\delta_3\delta_8) - 2\sqrt{\delta_8\delta_9} \tag{24}$$

and τ from Eq. (7) we have

$$\tau = \delta_1 + 2\delta_4 - (\delta_2 - \delta_5)s - 2[(\sqrt{\delta_9} + \delta_3\sqrt{\delta_8})s - \sqrt{\delta_8}\,] \tag{25}$$

whose derivative is less than zero, that is negative. So,

$$\tau = -2\delta_3 - 2[\sqrt{\delta_9} + \delta_3\sqrt{\delta_8} < 0 \tag{26}$$

From Eqs. (10), (23) and (25) the parametric energy eigenvalue equation is obtained as

$$\delta_2 n - (2n+1)\delta_5 + (2n+1)[\sqrt{\delta_9} + \delta_3\sqrt{\delta_8}\quad] + n(n-1)\delta_3 + \delta_7 + 2\delta_3\delta_8 + 2\sqrt{\delta_8\delta_9} = 0$$
(27)

With Eq. (4), the weight function is obtained as

$$\rho_{(s)} = s^{\delta_{10}-1}(1 - \delta_3 s)^{\frac{\delta_{11}}{\delta_3} - \delta_{10} - 1} \tag{28}$$

and when Eq. (28) is used in Eq. (5), we obtained Eq. (29) written as

$$\gamma_n = P_n^{\left(\delta_{10}-1,\ \frac{\delta_{11}}{\delta_3}-\delta_{10}-1\right)}(1-2\delta_3 s) \tag{29}$$

where

$$\delta_{10} = \delta_1 + 2\delta_4 + 2\sqrt{\delta_8} \tag{30}$$

$$\delta_{11} = \delta_2 - 2\delta_5 + 2(\sqrt{\delta_9} + \delta_3\sqrt{\delta_8}) \tag{31}$$

and $P_n^{(\delta_{10},\delta_{11})}$ are Jacobi polynomial [18]. By using Eq. 6 we obtain

$$\psi = S^{\delta_{12}}(1-\delta_3 S)^{-\delta_{12}-\frac{\delta_{13}}{\delta_3}} \tag{32}$$

where

$$\delta_{12} = \delta_4 + \sqrt{\delta_8} \tag{33}$$

$$\delta_{13} = \delta_5 - (\sqrt{\delta_9} + \delta_3\sqrt{\delta_8}) \tag{34}$$

So, the general solution or wave function is

$$\psi = S^{\delta_{12}}(1-\delta_3 S)^{-\delta_{12}-\frac{\delta_{13}}{\delta_3}} P_n^{\left(\delta_{10}-1,\ \frac{\delta_{11}}{\delta_3}-\delta_{10}-1\right)}(1-2\delta_3 s) \tag{35}$$

There are some problems $\delta_3 = 0$, Eq. (35) becomes

$$\psi = S^{\delta_{12}} e^{\delta_{13} s} P_n^{\delta_{10}-1}(\delta_{11} S) \tag{36}$$

2 .1. Graphical behavior of Hulthen Plus Yukawa Potential

We choose our confining potential $V_{(r)}$ to be that of Hulthen and Yukawa [21,22] which will shall termed Hulthen plus Yukawa potential written as:

$$V_{(r)} = -\left(\frac{\mathrm{V_o} e^{-\alpha r}}{(1-e^{-\alpha r})} + V_1\left(\frac{e^{-\alpha r}}{r}\right)\right) \tag{37}$$

This is a combination of two different potentials. Eq. (37) becomes our confining potential. Here, V_o represents the strength, V_1 , α are the potential depth and the screening parameter. Let us have a look at the graphical behavior of the Hulthen plus Yukawa potential. If $V_1 = 0$ Eq. (37) reduces to the Hulthen potential which is of the form:

$$V_{(r)} = -\frac{\mathrm{V_o} e^{-\alpha r}}{(1-e^{-\alpha r})} \tag{38}$$

The plot is shown in Figure.1

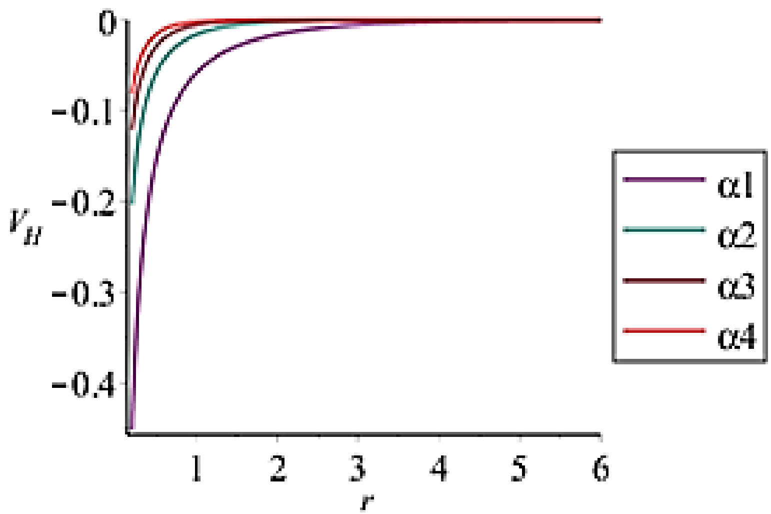

Figure 1. Hulthen potential versus r with V_0 = 0.1meV, for **α** = 1, 2, 3 and 4

when $V_o = 0$ Eq. (37) reduces to the Yukawa potential written as

$$V_{(r)} = -V_1\left(\frac{e^{-\alpha r}}{r}\right) \tag{39}$$

The plot is shown in Figure 2

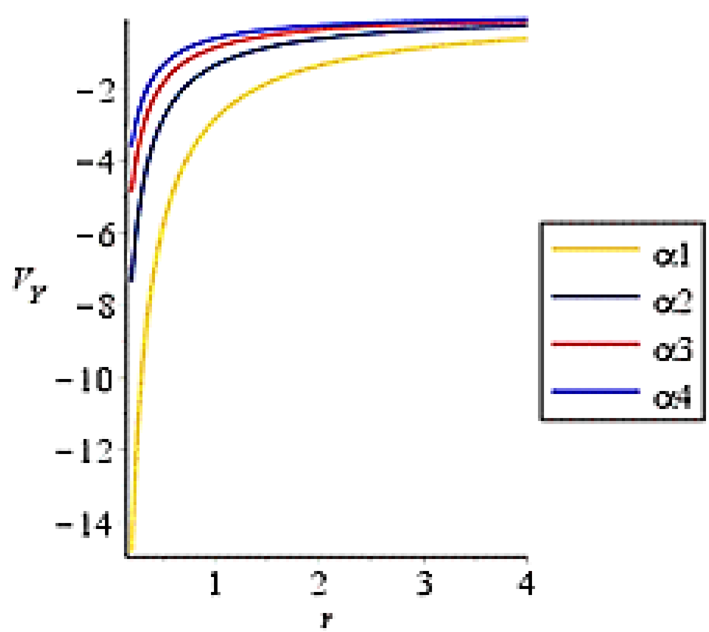

Figure 2. Yukawa potential versus r with V_1 = 0.3meV for **α** = 0.1, 0.2, 0.3 and 0.4

3. ANALYTICAL SOLUTIONS OF THE SE IN D-DIMENSIONS

The SE in D- dimension is written as [7]

$$\frac{d^2U_{n,l}(r)}{dr^2} + \frac{2\mu}{\hbar^2}\left[E - V_{(r)}\right]U_{n,l} - \frac{1}{r^2}\left[\frac{(D-1)(D-3)}{4} + l(l+D-2)U_{n,l}(r) = 0 \quad (40)$$

Now, we want to solve the radial part of the SE in D-dimensions given in Eq. (40) for the Hulthen and Yukawa potential given in Eq.(37) as our confining potential.

Substituting Eq. (37) into Eq. (40) we will obtain the following equation given as

$$\frac{d^2U_{n,l}(r)}{dr^2} + \frac{2\mu}{\hbar^2}\left(E + \frac{Voe^{-\alpha r}}{(1-e^{-\alpha r})^2} + V_1\left(\frac{e^{-\alpha r}}{r}\right)\right) - \frac{1}{r^2}\left(\frac{(D-1)(D-3)}{4} + l(l+D-2)\right)U_{n,l} = 0 \quad (41)$$

In order to solve Eq. (41), we employ the approximation scheme given in Eq. (42) [12]. This approximation scheme is for short range potential to enable us handle the centrifugal term of Eq. (40)

$$\frac{1}{r^2} \approx \frac{\alpha^2}{(1-e^{-\alpha r})^2}, \frac{1}{r} \approx \frac{\alpha}{(1-e^{-\alpha r})} \quad (42)$$

With this approximation scheme of Eq. (42), Eq. (41) can be re-written as

$$\frac{d^2U_{n,l}(r)}{dr^2} + \frac{2\mu}{\hbar^2}\left(E - \frac{Voe^{-\alpha r}}{(1-e^{-\alpha r})} + \frac{V_1\alpha}{(1-e^{-\alpha r})}\right) - \frac{\alpha^2}{(1-e^{-\alpha r})^2}\left(\frac{(D-1)(D-3)}{4} + l(l+D-2)\right)U_{n,l} = 0 \quad (43)$$

By using the coordinate transformation, $s = e^{-\alpha r}$ Eq. (43) yields the following hypergeometric equation given as

$$\frac{d^2U_{n,l}(s)}{ds^2} + \frac{(1-s)}{s(1-s)}\frac{dU_{n,l}}{ds} + \frac{1}{s^2(1-s)^2}\left[-\varepsilon(1-s)^2 + \chi(1-s)s + \tau(1-s)s - \vartheta\right]U_{n,l}(s) = 0 \quad (44)$$

Subsequently Eq. (44) can be evaluated further to obtain an equation of the form

$$\frac{d^2U_{n,l}(s)}{ds^2} + \frac{(1-s)}{s(1-s)}\frac{dU_{n,l}}{ds} + \frac{1}{s^2(1-s)^2}\left[-(\varepsilon+\chi+\tau)s^2 + (2\varepsilon+\chi+\tau)s - (\varepsilon+\vartheta)\right]U_{n,l}(s) = 0 \quad (45)$$

where

$$-\varepsilon = \frac{2\mu E}{\hbar^2\alpha^2} \quad (46)$$

$$\chi = \frac{2\mu V_o}{\hbar^2\alpha^2} \quad (47)$$

$$\tau = \frac{2\mu V_1}{\hbar^2\alpha} \quad (48)$$

$$\vartheta = \frac{1}{r^2}\left(\frac{(D-1)(D-3)}{4} + l(l+D-2)\right) \quad (49)$$

Comparing Eq. (45) with the parametric form of the NU equation written as:

$$\psi^{"} + \frac{\delta_1-\delta_2 s}{s(1-\delta_3)s}\psi' + \left[\frac{-\varsigma_1 s^2+\varsigma_2-\varsigma_3}{s^2(1-\delta_3 s)^2}\right]\psi_{(s)} = 0 \tag{50}$$

the following parameters can be found:

$$\delta_1 = \delta_2 = \delta_3 = 1, \delta_4 = \frac{1}{2}(1-\delta_1) = 0,\ \delta_5 = \frac{1}{2}(\delta_2 - 2\delta_3) = -\frac{1}{2} \tag{51}$$

$$\varsigma_1 = \varepsilon + \chi + \tau\, , \varsigma_2 = 2\varepsilon + \chi + \tau\, ,\ \varsigma_3 = \varepsilon + \vartheta \tag{52}$$

$$\delta_6 = \delta^2{}_5 + \varsigma_1 = \frac{1}{4} + \varepsilon + \chi + \vartheta \tag{53}$$

$$\delta_7 = 2\delta_4\delta_5 - \varsigma_2 = -(2\varepsilon + \chi + \tau) \tag{54}$$

$$\delta_8 = \delta^2{}_4 + \varsigma_3 = \varepsilon + \vartheta \tag{55}$$

$$\delta_9 = \delta_3\delta_7 + \delta^2{}_3\delta_8 + \delta_6 = \frac{1}{4} + \vartheta \tag{56}$$

The NU energy eigenvalues equation is written as:

$$\delta_2 n-(2n + 1)\ \delta_5 + (2n + 1)\ [\sqrt{\delta_9} + \delta_3\sqrt{\delta_8}] + n\ (n\ -1)\ \delta_3+\delta_7+2\delta_3\delta_8+\ 2\sqrt{\delta_8\delta_9} = 0 \tag{57}$$

With Eq. (51-57) the energy eigenvalues of the Hulthen plus Yukawa potentials is obtained as:

$$E_{n,l} = -\frac{\hbar^2\alpha^2}{2\mu}\left\{\left[\frac{\sigma+\eta}{2(n+\sqrt{\sigma})} + \frac{(n+\sqrt{\sigma})}{2}\right]^2 - \frac{1}{r^2}\left(\frac{(D-1)(D-3)}{4} + l(l+D-2)\right)\right\} \tag{58}$$

where

$$\sigma = \frac{1}{4} + \vartheta\, , \tag{59}$$

$$\eta = \chi + \tau + 2\vartheta \tag{60}$$

The corresponding wave function is given as:

$$\psi_{(s)} = s^{\delta_{12}}(1 - \delta_3 s)^{-\delta_{12} - \delta_{13}/\delta_3}\, p_n{}^{\delta_{10}-1, \left(\frac{\delta_{11}}{\delta_3}\right)-(\delta_{10}-1)}(1-2\delta_3 s) \tag{61}$$

$$\psi_{(s)} = s^{\sqrt{\varepsilon+\vartheta}}(1 - s)^{\frac{1}{2}+\sqrt{\frac{1}{4}+\vartheta}}\, p_n{}^{2\sqrt{\varepsilon+\vartheta},\ 2\sqrt{\frac{1}{4}+\vartheta}}\ (1-2s) \tag{62}$$

4. NUMERICAL AND DISCUSSION OF RESULTS

Table 1. Energy eigenvalues (in units of me V) for different values of n, l with $\hbar = \mu = 0.1$, $\alpha = 0.1,\ Vo = 0.1\ \ V_1 = 0.3,$ for D = 3, 4 and 5

N	L	D = 3	D = 4	D = 5
0	0	-33.80000000	-8.352406250	-3.639888888
1	0	-3.698000000	-2.039632812	-1.269080000
2	0	-1.290320000	-0.8711562500	-0.6165102040
	1	-0.6165102040	-0.4500019531	-0.3350000000
3	0	-0.6275918370	-0.4628457031	-0.3486543208
	1	-0.3486543208	-0.2660862500	-0.2043388429
	2	-0.2043388429	-0.1568758680	-0.1195502959
4	0	-0.3555555556	-0.2745762500	-0.2138099174
	1	-0.2138099174	-0.1669453125	-0.1299704142
	2	-0.1299704142	-0.1002327806	-0.07592000000
	3	-0.07592000000	-0.05575830080	-0.03883044982
5	0	-0.2185950414	-0.1730703125	-0.1370355030
	1	-0.1370355030	-0.1079623724	-0.08412000000
	2	-0.08412000000	-0.06428955080	-0.04759169555
	3	-0.04759169555	-0.03337847219	-0.02116343488
	4	-0.02116343488	-0.01057531250	-0.001326430590

Table 2. Energy eigenvalues (in units of me$V$) for different values of n, l with $\hbar = \mu = 0.1$, $\alpha = 0.1,\ Vo = 0.2\ \ V_1 = 0.2,$ for D = 3, 4 and 5

N	L	D = 3	D = 4	D = 5
0	0	-98.80000000	-24.403490625	-10.55988888
1	0	-10.65800000	-5.926507810	-3.731480000
2	0	-3.767120000	-2.573656250	-1.850795918

	1	-1.850795918	-1.379533203	-1.055000000
3	0	-1.869224490	-1.400814453	-1.077543210
	1	-1.077543210	-0.8447862500	-0.6714462810
	2	-0.6714462810	-0.5387508680	-0.4348165680
4	0	-1.088888889	-0.8586762500	-0.6868677685
	1	-0.6868677685	-0.5550703125	-0.4516272188
	2	-0.4516272188	-0.3688552296	-0.3015200000
	3	-0.3015200000	-0.2459536133	-0.1995224914
5	0	-0.6946280990	-0.2459536133	-0.4629526627
	1	-0.4629526627	-0.3811766582	-0.3145200000
	2	-0.3145200000	-0.2594067383	-0.2132664360
	3	-0.2132664360	-0.1742118055	-0.1408310249
	4	-0.1408310249	-0.1120503125	-0.1408310249

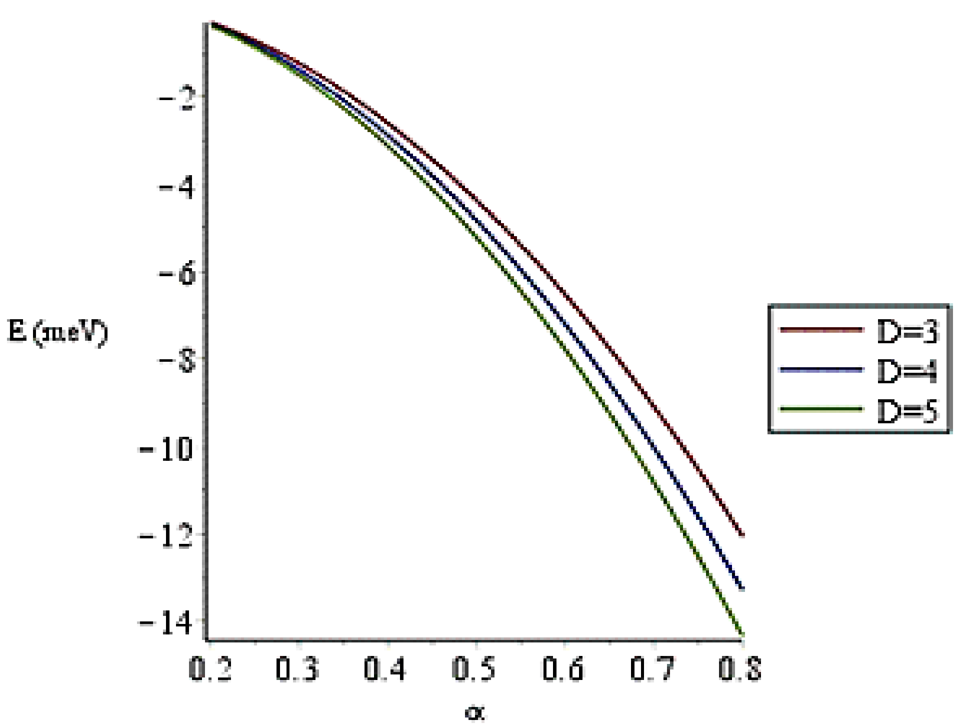

Figure 3. Energy Versus Screening parameter **α**

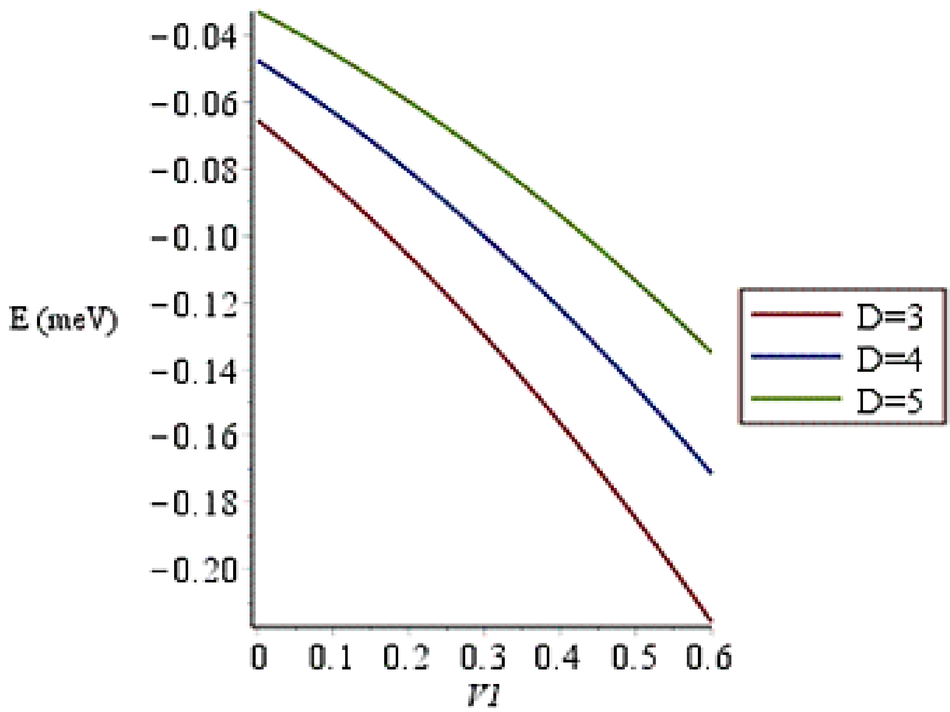

Figure 4. Energy versus potential depth V_1

The bound state energy eigenvalues are presented in Table 1 and 2 for the different quantum numbers. There is a correlation between the quantum numbers and the energy eigenvalues. As the quantum state increases, there is also a corresponding increment in the energy eigenvalues. That is, the energy eigenvalues become more bounded. Also, for table 1 and 2 one can see the degeneracy of the energy level in D = 3 and 5. Figure 3 shows us the variation of the bound state energy against the screening parameter α. It is seen that the bound state energy decreases as the screening parameter increases. This result is consistent with the work of Ref. [11]. In Figure 4, the behavior of the bound state energy with the potential depth V_1 is shown. We can see from the plot that as the bound state energy is decreasing, the potential depth is increasing. This result is in agreement with the work of Refs. [11, 12].

5. CONCLUSION

The Hulthen plus Yukawa potentials have been used to study the bound state solutions of the energy eigenvalues in the D - dimensions of the Schrödinger equation analytically and numerically. We saw the graphical behavior of the Hulthen and the Yukawa potential. And our results obtained are in good agreement with Ref. [11].

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