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Vibrational-rotational analysis of the Hulthén potencial using hydrogenic eigenfunction bases*

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Hulthén's potential admits analytical solutions for its energy eigenvalues and eigenfunctions corresponding to zero orbital angular momentum states, but its non zero angular momentum states are not equally known. This work presents a vibrational-rotational analy sis of Hulthén's potential using hydrogenic eigenfunction bases, which may be of interest and useful to students of quantum mechanics at different stages.

Keywords: Quantum mechanics; Hulthén's potential; variational solutions

El potencial de Hulthén admite soluciones analíticas para sus eigenvalores de la energía y eigenfunciones correspondientes a estados con momento angular orbital cero, pero sus estados con momento angular diferente de cero no son igualmente conocidos. Este trabajo presenta un análisis vibracional-rotacional del potencial de Hulthén usando bases de eigenfunciones hidrogénicas, el cual puede ser de interés y utilidad para estudiantes de mecánica cuántica en diferentes etapas.

Descriptores: Mecánica cuántica; potencial de Hulthén; soluciones variacionales

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1. Introduction

Lamek Hulthén introduced the potential

$$V^{\mathrm{H}}(r) = -V_0 \frac{e^{-\lambda r}}{1-e^{-\lambda r}} \tag{1}$$

in an article with the title " On the Eigensolution of the Schrödinger Equation of the Deuteron" published in the *Arkiv för Mathematik, Astronomi och Fysik* in 1942 [1]. The short distance behavior of the potential is like that of the Yukawa potential,

$$V^{\mathrm{Y}}(r) = -V_0 \frac{e^{-\lambda r}}{\lambda r}, \tag{2}$$

and asymptotically it becomes the exponential potential,

$$V^{\mathrm{E}}(r) = -V_0 e^{-\lambda r} \tag{3}$$

While the Schrödinger equation does not admit analytical solutions for both potentials V^{Y} and V^{E}, Hulthén showed in Ref. 1 that V^{H} has analytical expressions for the energy eigenvalues and eigenfunctions of its zero angular momentum states. In fact, he used these eigensolutions of the V^{H} potential to construct perturbative solutions of the Yukawa potential in the case of the deuteron.

On the other hand, the Schrödinger equation does not admit analytical solutions for the non-zero angular momentum states of the Hulthén potential either. Correspondingly, the study of such states has been the subject of research and the testing ground of different theoretical approaches in the last few decades. References 2–7, limited to the eighties, illustrate the methods and results of different approximation schemes and also contain references to previous works.

This work is a didactic study of both zero and non-zero angular momentum states of Hulthén's potential, which may be of interest and useful to students of quantum mechanics at different stages. For completeness sake, our own version of the exact eigensolution for s states is included in Sect. 2. Variational solutions for any angular momentum l states are formulated using hydrogenic eigenfunctions, and numerical results are presented in Sect. 3. The formulation and numerical evaluation are carried out in two successive stages. Section 3.1 is limited to the states with no radial excitation and allows the optimization of the nuclear charge variational parameter in the hydrogenic trial functions for each value of l In Sect. 3.2 the linear variational method is implemented in its matrix form using the complete hydrogenic eigenfunction bases, obtaining at once the states with successive radial excitations for each l. Section 4 includes a discussion of the results and methods.

2. Exact eigensolution of the Hulthén potential for $\ell = 0$ states

The Schrödinger equation for the relative motion of two particles interacting via the Hulthén potential is written as

$$\left[-\frac{\hbar^2}{2\mu}\nabla^2 - V_0\frac{e^{-\lambda r}}{1-e^{-\lambda r}}\right]\psi(\vec{r}) = E\psi(\vec{r}) \qquad (4)$$

in terms of the reduced mass μ. Because of the central nature of the potential the problem admits the separable solutions in terms of the spherical harmonics

$$\psi(r,\theta,\varphi) = R(r)Y_{lm}(\theta,\varphi), \qquad (5)$$

which are eigenfunctions of the energy and angular momentum. The radial function must satisfy the equation

$$\begin{aligned}\Bigg[-\frac{\hbar^2}{2\mu}\left(\frac{1}{r^2}\frac{d}{dr}r^2\frac{d}{dr} - \frac{l(l+1)}{r^2}\right)& \\ -V_0\frac{e^{-\lambda r}}{1-e^{-\lambda r}}\Bigg] R(r) &= ER(r). \qquad (6)\end{aligned}$$

The remainder of this section is restricted to s states with $l = 0$ for which we make the standard change

$$R(r) = \frac{f(r)}{r} \qquad (7)$$

obtaining the radial equation,

$$\left[-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} - V_0\frac{e^{-\lambda r}}{1-e^{-\lambda r}}\right] f(r) = Ef(r). \qquad (8)$$

The square integrability condition is translated into the boundary conditions on the radial function

$$f(r) \underset{r\to 0}{\longrightarrow} 0 \qquad \text{and} \qquad f(r) \underset{r\to\infty}{\longrightarrow} 0. \qquad (9)$$

The asymptotic behavior may be ensured through an exponentially decreasing factor

$$f(r) = e^{-\alpha r}g(r), \qquad (10)$$

in which case Eq. (8) becomes

$$\frac{d^2 g}{dr^2} - 2\alpha\frac{dg}{dr} + \frac{2\mu V_0}{\hbar^2}\frac{e^{-\lambda r}}{1-e^{-\lambda r}}g = 0 \qquad (11)$$

with

$$\alpha = \sqrt{-2\mu E/\hbar^2} \qquad (12)$$

and the reminder that the energy E is negative for bound states.

Hulthén found that Eq.(11) is integrable under the change of variable

$$x = 1 - e^{-\lambda r} \qquad (13)$$

which maps $0 \le r < \infty$ into $0 \le x < 1$, Here we take additionally

$$g(x) = xh(x) \qquad (14)$$

in order to ensure the correct behavior of Eq. (9) for $r \longrightarrow 0$. Then it is straightforward to establish that Eq. (11) takes the form

$$\begin{aligned}x(1-x)\frac{d^2h}{dx^2} + \left[2 - \left(3 + \frac{2\alpha}{\lambda}\right)x\right]\frac{dh}{dx}& \\ - \left[1 + \frac{2\alpha}{\lambda} - \frac{2\mu V_0}{\hbar^2\lambda^2}\right]h &= 0. \qquad (15)\end{aligned}$$

The reader can identify that Eq. (15) corresponds to the canonical form of the differential equation

$$x(1-x)\frac{d^2y}{dx^2} + [c - (a+b+1)x]\frac{dy}{dx} - aby = 0. \qquad (16)$$

for the hypergeometric function [8],

$$y = {}_2F_1(a,b;c;x) = \sum_{s=0}^{\infty}\frac{(a)_s(b)_s}{(c)_s s!}x^s, \qquad (17)$$

where $(a)_s = a(a+1)\cdots(a-1+s)$ and $(a)_0 = 1$ are the Pochhammer symbols. Also, the parameters in Eq. (15) are immediately identified as

$$\begin{aligned}a &= 1 + \frac{\alpha}{\lambda} - \sqrt{\left(\frac{\alpha}{\lambda}\right)^2 + \frac{2\mu V_0}{\hbar^2\lambda^2}},\\ b &= 1 + \frac{\alpha}{\lambda} + \sqrt{\left(\frac{\alpha}{\lambda}\right)^2 + \frac{2\mu V_0}{\hbar^2\lambda^2}},\\ c &= 2. \qquad (18)\end{aligned}$$

For arbitrary values of these parameters, the hypergeometric series of Eq. (17) is divergent for $x \longrightarrow 1$ corresponding to $r \longrightarrow \infty$, because each of its asymptotic terms has the limit value

$$\lim_{s\to\infty}\frac{(a)_s(b)_s}{(c)_s s!} \longrightarrow 1. \qquad (19)$$

The only way to avoid such a divergent behavior for the solution of Eq. (15), in the form of Eq. (17) with the parameters of Eq. (18), is to reduce the series with an infinite number of terms to a polynomial of degree $n_r = 0, 1, 2, \ldots$. This can be accomplished by restricting the values of the parameter a to the values $-n_r$:

$$-n_r = 1 + \frac{\alpha}{\lambda} - \sqrt{\left(\frac{\alpha}{\lambda}\right)^2 + \frac{2\mu V_0}{\hbar^2\lambda^2}}, \qquad (20)$$

ensuring that the coefficients $(-n_r)_s$ with $s > n_r$, vanish. According to Eq. (12), this is equivalent to the restriction of the energy to its eigenvalues

$$E_n = -\frac{\hbar^2}{2\mu}\frac{\lambda^2}{4}\left[\frac{2\mu V_0}{\hbar^2\lambda^2(n_r+1)} - (n_r+1)\right]^2, \qquad (21)$$

where $n = n_r + 1 = 1, 2, 3, \ldots$ plays the role of the total quantum number.

The corresponding radial eigenfunction takes the explicit form

$$R(r) = N\frac{1 - e^{-\lambda r}}{r}\exp\left[-\frac{\lambda}{2}\left(\frac{2\mu V_0}{\hbar^2\lambda^2 n} - n\right)r\right]$$
$${}_2F_1\left[-(n-1), \frac{2\mu V_0}{\hbar^2\lambda^2 n} + 1; 2; 1 - e^{-\lambda r}\right] \quad (22)$$

which involves power series in the exponential function.

For a given pair of particles interacting via a Hulthén potential, Eqs. (21) and (22) show that the number of bound s states is the integer part of $\sqrt{2\mu V_0}/\hbar\lambda$.

It is also instructive to view the Hulthén potential as a type of screened Coulomb potential, in which λ is the screening parameter. Eqs. (1) and (2) show that if the strength parameter is chosen as $V_0 = Ze^2\lambda$ then in the limit $\lambda \longrightarrow 0$, both the Hulthén and Yukawa potentials reduce to the Coulomb potential,

$$V^c(r) = -\frac{Ze^2}{r}. \quad (23)$$

It can be easily verified that in such a limit, Eq. (21) is reduced in turn to the Bohr formula for the atomic hydrogen energies

$$E_n^c = -\frac{Z^2e^4\mu}{2\hbar^2n^2}, \quad (24)$$

which are infinite in number, and the eigenfunctions in Eq. (27) also become hydrogenic [9]

$$R^C(r) = Ne^{-\frac{Ze^2\mu r}{\hbar^2 n}}\,{}_1F_1\left(-(n-1); 2; \frac{2Ze^2\mu r}{\hbar^2 n}\right), \quad (25)$$

recalling that the confluent hypergeometric function ${}_1F_1(a; c; x,)$ is the limit of the hypergeometric function [8]:

$$\lim_{b\to\infty} {}_2F_1\left(a, b; c; \frac{x}{b}\right) = {}_1F_1(a; c; x). \quad (26)$$

3. Variational solutions of the Hulthén Potential for any ℓ states

In this section we consider the solution of Eq. (6) for states with any angular momentum l. Since no analytical solutions are known in this case, we propose a variational analysis. The connection between the Hulthén potential and the Coulomb potential and their eigenfunctions, established in the previous Section, suggests that the atomic hydrogen eigenfunctions may be appropriate as a basis to construct variational solutions of Eq. (6). Here we consider the equivalent of Eq. (6) for a Coulomb potent with a nuclear charge parameter β

$$\left\{-\frac{1}{2}\left[\frac{1}{r^2}\frac{d}{dr}r^2\frac{d}{dr} - \frac{l(l+1)}{r^2}\right] - \frac{\beta}{r}\right\}R^C(r) = E^C R^C(r) \quad (27)$$

From here on we assume $\hbar = \mu = e = 1$ and $V_0 = Z\lambda$ in order to conform with the notation of [2–7]. The eigensolutions of Eq. (27) correspond to the well-known atomic hydrogen Bohr energies

$$E_n^C = -\beta^2/2n^2 \quad (28)$$

and eigenfunctions

$$R_{n_r l}^C(r) = N_{n_r l}r^l e^{-\beta r/n}\,{}_1F_1\left(-n_r; 2l+2; \frac{2\beta r}{n}\right) \quad (29)$$

where $n = n_r + l + 1$ [9]. The reader may recognize that Eqs. (28) and (29) reduce to Eqs. (24) and (25) for the case of $l = 0$ states.

The variational analysis of Eq. (6) to be carried out next is based on trial functions constructed with the basis of Eq. (29), and taking β as a variational parameter.

In Sect. 3.1 the analysis is restricted to the states without any radial excitation, for which it is sufficient to start with the trial functions of the type of Eq. (29) with $n_r = 0$. The analysis of Sect. 3.2 includes radial excitations and requires trial functions constructed as linear combinations of the complete basis of Eq. (29) with $n_r = 0, 1, 2, \ldots$

3.1. Variational Calculation for States without Radial Excitation

We choose the normalized hydrogenic trial functions

$$R^T(r) = \left[\left(\frac{2\beta}{n}\right)^{2l+3}\frac{1}{(2l+2)!}\right]^{1/2} r^l e^{-\beta r/n} \quad (30)$$

for the variational calculation of the energy eigenvalues of the states of the Hulthén potential without radial excitation for which $n_r = 0$ and $n = l + 1$. The calculation involves the evaluation of the expectation value of the energy using Eq. (6), and its minimization with respect to the variational parameter β. Both steps are carried out as described next.

The evaluation of the expectation value of the kinetic energy term in Eq. (6) for the trial function of Eq. (30), is the same as the corresponding evaluation in Eq. (27). In the latter we use the virial theorem for the Coulomb potential [9] to conclude that the expectation value of the kinetic energy is the negative of the expectation value of the total energy of Eq. (28). The evaluation of the expectation value of the Hulthén potential is straightforward making use of its geometric series representation:

TABLE I. Successive entries correspond to states nl without radial excitation for which $l = n - 1$, screening parameter λ, scaled variational parameter β/n, minimized energy $E_{\min}$, and exact energy E_{exact}, from Eq. (21) for s states and from [2] for other states.

nl	λ	β/n	$E_{\min}$	E_{exact}
1s	0.025	0.999921874999206	−0.487578124	−0.487578125
	0.050	0.999687499949197	−0.475312483	−0.475312500
	0.100	0.998749996759909	−0.451249740	−0.451250000
	0.150	0.997187463302950	−0.427811189	−0.427812500
	0.200	0.994999795404474	−0.404995874	−0.405000000
	0.300	0.988747717623176	−0.361229363	−0.361250000
2p	0.025	0.499478764284810	−0.112760438	
	0.050	0.497910184684437	−0.101042017	−0.101043
	0.100	0.491560051950861	−0.079172425	−0.079179
	0.150	0.480683850935646	−0.059405503	
	0.200	0.464744947741120	−0.041769513	−0.041886
	0.300	0.412514662309447	−0.013136737	−0.013790
3d	0.025	0.33168477909624	−0.043602856	−0.043603
	0.050	0.326639664406316	−0.032750023	−0.032753
	0.100	0.304639712141441	−0.014428372	−0.014484
	0.150	0.256131972358986	−0.001013290	−0.001391
4f	0.025	0.246186909018531	−0.019690293	−0.019691
	0.050	0.233865882537618	−0.010047935	−0.010062
	0.075	0.208808334469317	−0.002467821	−0.002556

$$\begin{aligned}\langle R^T|V_H|R^T\rangle &= -Z\lambda\left(\frac{2\beta}{n}\right)^{2l+3}\frac{1}{(2l+2)!}\int_0^\infty dr r^{-2l+2}e^{-\beta r}\sum_{s=0}^{\infty}e^{-\lambda(s+1)r}\\ &= -Z\lambda\left(\frac{2\beta}{n}\right)^{2l+3}\frac{1}{\lambda^{2l+3}}\sum_{s=0}^{\infty}\frac{1}{\left(s+1+\dfrac{2\beta}{n\lambda}\right)^{2l+3}} = -Z\lambda\left(\frac{2\beta}{n\lambda}\right)^{2l+3}\zeta\left(2l+3,\frac{2\beta}{n\lambda}+1\right),\end{aligned} \tag{31}$$

where $\zeta(N, a)$ is the generalized Riemann zeta function [10]. The first step is completed by writing the expectation value of the total energy,

$$E(\beta) = \frac{\beta^2}{2n^2} - Z\lambda\left(\frac{2\beta}{n\lambda}\right)^{2l+3}\zeta\left(2l+3,\frac{2\beta}{n\lambda}+1\right), \tag{32}$$

The second step consists in obtaining the derivative of this energy with respect to the variational parameter and finding its zeros,

$$\frac{dE}{d\beta} = 0. \tag{33}$$

The implementation of this step was carried out in a personal computer using the Mathematica program [11].

Illustrative numerical results are presented in Table I, where the successive columns correspond to the spectroscopic designation of the states without radial excitation, for which $l = n - 1$, to the chosen values of the screening parameter λ of the Hulthén potential, to the scaled variational parameter β/n evaluated via Eqs. (32) and (33), to the respective minimized energies $E_{\min}$ from Eq. (32), and to the exact energies from Eq. (21) for s states and from [2] for the other states. The reader may notice that the variational parameter β takes values close to $Z = 1$, with systematically increasing departures from such a value as the screening parameter increases and as we move to states with increasing rotational excitation. Correspondingly, the variational energies of the Hulthén potential, starting from the values of the hydrogen atomic energies Eq. (28) for $\lambda = 0$, show similar departures from these values as λ and l take on larger values; such a trend can be understood on the basis of Eq. (32). The exact energies are included as points of reference for numerical comparison. The overall conclusion is that the variational energies are very close to the exact energies with systematically increasing departures for larger values of λ and l.

3.2. Linear variational method for states with any radial excitation

In this section we formulate and implement the variational solution of the Schrödinger equation for states with any radial excitation of the Hulthén potential, Eq. (6), using the basis of hydrogenic functions, Eq. (29). We consider a trial function in the form of the linear superposition:

$$R_{vl}^{\mathrm{H}}(r) = \sum_{n_r=0}^{N} a_{vn_r} R_{n_r l}^{C}(r), \tag{34}$$

in which the nuclear charge parameter β in the hydrogenic functions is given the optimized values obtained in the previous section for chosen values of λ and l.

The substitution of the trial function, Eq. (34), in the Schrödinger Eq. (6), and the subsequent and successive scalar multiplication by each one of the hydrogenic eigenfuctions $R_{n_r\ell}^{C}(r)$, leads to the set of linear homogeneous equations for the expansion coefficients $a_{\nu n_r}$:

$$\sum_{n_r=0}^{N} a_{vn_r} \langle n_r\ell|(H^{\mathrm{H}} - E)|n_r\ell\rangle = 0,$$
$$n_r = 0, 1, 2, \ldots N. \tag{35}$$

The solution of these equations requires the vanishing of the determinant of the matrix ($\mathbf{H}^{\mathrm{H}} - E\mathbf{I}$), which determines the variational energy eigenvalues E_v and the optimized eigenvectors a_{vn_r}. By writing the Hulthén Hamiltonian in terms of the Coulomb Hamiltonian, Eq. (27), the secular equation becomes

$$\det\left|(E_n^C - E)\delta_{n'_r,n_r} + \langle n'_r\ell|(V^H - V^C)|n_r\ell\rangle\right| = 0 \tag{36}$$

The matrix elements of the Coulomb and Hulthén potential are constructed using the explicit forms of the hydrogenic functions of Eq. (29):

$$\langle n'_r\ell|\frac{1}{r}|n_r\ell\rangle = N_{n'_r\ell}N_{n_r\ell}\sum_{s=0}^{n'_r}\sum_{t=0}^{n_r}\frac{(-n'_r)_s(-n_r)_t}{(2\ell+2)_s s!(2\ell+2)_t t!}\frac{(2\beta/n')^s(2\beta/n)^t(2\ell+1+s+t)!}{(2\beta/n'+2\beta/n)^{2\ell+2+s+t}} \tag{37}$$

$$\langle n'_r\ell\left|\sum_{p=0}^{\infty}e^{-\lambda(p+1)r}\right|n_r\ell\rangle = N_{n'_r\ell}N_{n_r\ell}\sum_{s=0}^{n'_r}\sum_{t=0}^{n_r}\frac{(-n'_r)_s(-n_r)_t}{(2\ell+2)_s s!(2\ell+2)_t t!}\left(\frac{2\beta}{n'}\right)^s\left(\frac{2\beta}{n}\right)^t$$
$$\frac{(2\ell+2+s+t)!}{\lambda^{2\ell+3+s+t}}\,\zeta\left[2\ell+3+s+t, \frac{\beta}{\lambda}\left(\frac{1}{n'}+\frac{1}{n}\right)+1\right] \tag{38}$$

The numerical construction and diagonalization of the matrices was implemented in a personal computer with the Mathematica Program [11].

Table II contains the numerical results for the linear varational energies of the eigenstates of the Hulthén potential with successively increasing radial and rotational excitations. The entries in the two first columns, corresponding to the screening parameter and the states without radial excitations, coincide with their counterparts in Table I; the entries in the following columns correspond to the states with $n_r = 1, 2, 3$. The energies reported in each row were obtained from the diagonalization of 20×20 matrices constructed using Eqs. (37) and (38), and the corresponding values of the variational parameter β from Table I. Again, the exact energies from Eq. (21) for s states and from [2] for states with rotational excitation are included in parenthesis for numerical comparison. For the states without radial excitation the improvement of the linear variational energies of Table II relative to the simple variational energies of Table I is very small for the lower values of λ and ℓ, but it becomes quantitatively significant for the higher values of λ and ℓ as in the specific cases of $E(3d)$ for $\lambda = 0.150$, and $E(4f)$ for $\lambda = 0.050$ and 0.075. For the states with radial excitation the linear variational energies show convergence towards the exact energies with a decreasing number of digits as the values of λ, n_r and ℓ get larger. This trend of the convergence and accuracy of the linear variational energies follows the expected behavior; more accurate numerical results can be obtained by enlarging the size of the matrices, which we could not do in our personal computer due to its limitations in precision and memory capacity. In any case the reported values are good enough for our didactic purposes, and comparable with those of [2–7]. Also in our diagonalization procedure we obtain the energies of states with higher radial excitations, and the a_{vn_r} expansion coefficients of Eq. (34) for the linear variational eigenfunctions.

4. Discussion

The study of the Hulthén potential presented in this paper covers topics of interest for students of quantum mechanics. Section 2 illustrates an example of an exact analytical solution of the Schrödinger equation yielding the energy eigenvalues Eq. (21) and eigenfunctions Eq. (22) of Hulthén's potential $\ell = 0$ states, including their limiting atomic hydrogenic forms Eqs. (24) and Eq. (25) when the screening parameter becomes vanishingly small. Section 3.1 presents the simple varational calculation of the energies of the states with any angular momentum and no radial excitations using the corresponding atomic hydrogenic functions, Eq. (30), as trial

TABLE II. Successive entries correspond to screening parameter λ, linear variational energies $E(nl)$ of states with and without radial and rotational excitations. For comparison exact energies from Eq.(21) for s states and from [2] for other states are included in parenthesis.

λ	$E(1s)$	$E(2s)$	$E(3s)$	$E(4s)$
0.025	−0.4875781245	−0.1128124890	−0.043758616	−0.01999981
	(−0.4875781250)	(−0.11281250)	(−0.043758681)	(−0.02000)
0.050	−0.47531249	−0.1012498299	−0.033367177	−0.01124820682
	(−0.47531250)	(−0.101250)	(−0.033368056)	(−0.011250)
0.100	−0.4512498668	−0.0799975629	−0.016797794	−0.001246256
	(−0.4512500)	(−0.0800000)	(−0.016805556)	(−0.001250)
0.150	−0.4278118279	−0.061239729	−0.0058544125	
	(−0.4278125)	(−0.06112500)	(−0.005868056)	
0.200	−0.40499788	−0.04497502	−0.0005490027	
	(−0.4050000)	(−0.0450000)	(−0.0005556)	
0.300	−0.3612394377	−0.0199444		
	(−0.3612500)	(−0.0200000)		

λ	E(2p)	E(3p)	E(4p)
0.025	−0.1127604501	−0.04370687	−0.0199488
		(−0.043707)	(−0.019949)
0.050	−0.1010422	−0.03316428	−0.01105728
	(−0.101043)	(−0.033165)	(−0.011058)
0.100	−0.07917547	−0.01605176	−0.00075387
	(−0.079179)	(−0.016054)	(−0.000754)
0. 150	−0.059421418	−0.004462177	
		(−0.004466)	
0.200	−0.0418222		
	(−0.041886)		
0.300	−0.0134634		
	(-0.013790)		

λ	$E(3d)$	$E(4d)$
0.025	−0.04360294	−0.01984620
	(−0.043603)	(−0.019846)
0.050	−0.0327515	−0.010666642
	(−0.032753)	(−0.010667)
0.100	−0.01445634	
	(−0.014484)	
0.150	−0.00124455	
	(−0.001391)	

λ	$E(4f)$
0.025	−0.01969075
	(−0.019691)
0.050	−0.01005618
	(−0.010062)
0.075	−0.00252351
	(−0.002556)

functions. The numerical values of the variational energies are quite accurate, comparing favorably with the exact energies for the lower values of λ and ℓ, and showing increasing deviations as these parameters become larger. In Sect. 3.2 the linear variational method is formulated for states with both radial and rotational excitations, using the matrix formulation with the complete atomic hydrogenic eigenfunction basis, Eq. (29). For each value of ℓ, the energy eigenvalues of the states with successively increasing radial excitations are obtained simultaneously in the same numerical diagonalization process. The energies of the states with no radial excitation show an improvement when going from their values of Table I to those of Table II, the improvement being more appreciable for higher values of λ and ℓ. The linear variational energies of the states with both radial and rotational excitations show reasonable convergence and accuracy when compared with their values reported in the research literature [2–7]. Students of quantum mechanics may complement their study of topics on problems with analytical solutions, simple variational calculations and linear variational calculations by working the details of Sects. 2, 3.1 and 3.2. While the first two topics are covered and illustrated in standard courses, the last one is usually treated only formally. The availability of computers makes the latter workable and instructive for students.

Apart from the specific study of the Hulthén potential of Sect. 3, it may be pointed out that the simple variational method and the linear variational method as formulated in Sects. 3.1 and 3.2 can be systematically applied to other potentials. For instance, the Yukawa and exponential potentials, Eqs. (2) and (3), can be investigated using the same atomic hydrogenic eigenfunctions basis, Eqs. (30) and (29); in both cases the evaluation of the matrix elements is straightforward, involving factorials instead of generalized Riemann zeta functions in the counterparts of Eqs. (32) and (38). Of course, other basis of functions may be used for these and other potentials trying to improve the convergence and accuracy of the results in each specific situation. Also, the reader may become aware of the approximate perturbative methods of [1–7], and be interested in comparing them among themselves and with the variational methods.

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