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Bound states of the Hulthén and Yukawa potentials

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The generalized variational method is used to compute energies for the Yukawa and Hulthén potentials for states with $n \leq 6$. This straightforward approach is based on forming trial wave functions from a linear combination of independent functions. The estimates for the energies produced by this method are considerably more accurate than previous results for a wide range of values for the screening parameter.

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I. INTRODUCTION

For many years there has been considerable interest in finding the energies of screened Coulomb potentials. These potentials are important in several contexts. For example, the Hulthén potential [1] has been used in nuclear and particle physics [2], atomic physics [3], and in solid-state physics [4]. The Yukawa potential may be used to approximate the potential experienced by electrons in an atom where the remaining atoms screen the nuclear charge. It describes the shielding effect in plasmas where it is called by Debye-Hückel potential, and is known as the Thomas-Fermi potential in solid-state physics. This potential is also important in studying hydrogen under pressure [5–7].

Numerous attempts have been made to determine the bound-state energies of these potentials [8–31]. However, exact results have only been obtained for the s states of the Hulthén potential [1,32]. In this report, energy estimates are presented which are much more accurate than all previous results for the Hulthén potential. For the Yukawa potential, results are obtained which are comparable to the very accurate results in Ref. [20] where estimates were found for the 1s, 2s, and 2p states. In this paper, a more extensive study is made in which all states with $n \leq 6$ are included.

The calculational tool employed in this study is the generalized variational method (see, for example, Ref. [33]). This technique is based on forming trial wave functions from a linear combination of N independent functions ψ_j as

$$\Psi = \sum_{k=1}^{N} c_k \psi_k \ . \tag{1.1}$$

The following matrix equation is obtained from the Schrödinger equation:

$$\mathcal{H}\phi = \mathcal{E}\mathcal{J}\phi \ , \tag{1.2}$$

where $\mathcal{H}$ is the Hamiltonian matrix and $\mathcal{J}$ is the overlap matrix. These matrices have dimensions $N \times N$ and the corresponding eigenvectors and eigenvalues are given by ϕ and $\mathcal{E}$. According to the Hylleraas-Undheim theorem [34] the ordered set of N eigenvalues will be upper bounds to the corresponding exact energies. Moreover, the exact eigenvalues are approached monotonically as N is increased.

In Secs. II and III, the variational method is applied to the Hulthén and Yukawa potentials, respectively. In these sections, the choice of the basis used is motivated by examining the short-range and long-range behavior of the radial Schrödinger equation. The results from these models are compared with the most accurate energies from previous studies. Concluding remarks are presented in Sec. IV.

II. THE HULTHÉN POTENTIAL

Throughout this paper we will use atomic units ($\hbar = e = m = 1$). The Hulthén potential written in these units is given by

$$V(r) = -Z\lambda \frac{e^{-\lambda r}}{1-e^{-\lambda r}} \ , \tag{2.1}$$

where Z is a constant and λ is the screening parameter. Since this is a central potential, Schrödinger's equation can be separated into radial and angular parts. The radial equation is given by

$$\left[-\frac{1}{2r}\frac{d^2}{dr^2} r - Z\lambda \frac{e^{-\lambda r}}{1-e^{-\lambda r}} + \frac{l(l+1)}{2r^2} \right] R(r) = ER(r) \tag{2.2}$$

and the Hamiltonian may be written as

$$H = -\frac{1}{2r}\frac{d^2}{dr^2} r - Z\lambda \frac{e^{-\lambda r}}{1-e^{-\lambda r}} + \frac{l(l+1)}{2r^2} \ . \tag{2.3}$$

The scale transformation

$$r \rightarrow r/Z \tag{2.4}$$

leads to the relation

$$E(Z,\lambda) = Z^2 E(1,\lambda/Z) \ . \tag{2.5}$$

Thus there is no loss of generality if we study only the case where $Z = 1$.

In order to effectively apply the generalized variational method to this model, an appropriate basis must first be found. This may be done by examining the short-range and long-range behavior of the radial solutions Eq. (2.2). Defining the variable

$$u=rR \tag{2.6}$$

Eq. (2.2) may be written as

$$\frac{d^2}{dr^2}u+2Z\lambda\frac{e^{-\lambda r}}{1-e^{-\lambda r}}u-\frac{l(l+1)}{r^2}u=2|E|u\ . \tag{2.7}$$

For large r this reduces to

$$\frac{d^2}{dr^2}u=2|E|u\ . \tag{2.8}$$

So u has the form

$$u\sim e^{-\beta r} \tag{2.9}$$

for large r. For small r Eq. (2.7) reduces to

$$\frac{d^2}{dr^2}u-\frac{l(l+1)}{r^2}u=0\ . \tag{2.10}$$

Substitution of the trial solution $u=r^m$ gives

$$u\sim Ar^{-l}+Br^{l+1}\ . \tag{2.11}$$

In order for u to vanish at the origin, we must have $A=0$. So

$$u\sim r^{l+1} \tag{2.12}$$

for small r. Therefore we look for solutions of the form

$$u=F(r)r^{l+1}e^{-\beta r}\ , \tag{2.13}$$

where

$$F(r)=\sum_{i=0}^{\infty}a_i r^i\ . \tag{2.14}$$

Alternatively, we may write

$$R(r)=F(r)r^l e^{-\beta r}\ . \tag{2.15}$$

We want to construct our basis vectors ψ_k in such a way that Eq. (1.1) has the same form as Eq. (2.15). So we write

$$\psi_k=r^k e^{-\beta r}\ . \tag{2.16}$$

However, the matrix elements for the Hamiltonian produce complicated functions due to the second term in Eq. (2.3). This may be mended by multiplying Eq. (2.16) by a factor to cancel the denominator of the second term in the Hamiltonian. Therefore we use a basis formed by the functions

$$\psi_k=A_k r^k e^{-\beta r}(1-e^{-\lambda r})\ , \tag{2.17}$$

where $k=-1,0,1,2,\ldots$ for the s states and $k=0,1,2,\ldots$ for the $l\neq0$ states. Here, β is a variational parameter determined by minimizing the energy for a given state and basis size. The constant

$$A_k=\frac{(2\beta+\lambda)^{k+1}}{\sqrt{(2k+2)!}} \tag{2.18}$$

is included to prevent numerical overflow. The matrix elements are given by

$$\langle\psi_j|\psi_k\rangle=\frac{1}{\tau_1}g(j,k)\left[\frac{\tau_2}{\tau_1}\right]^{p+2}-\frac{2}{\tau_2}g(j,k)+\frac{1}{\tau_3}g(j,k)\left[\frac{\tau_2}{\tau_3}\right]^{p+2}\ , \tag{2.19}$$

where

$$\tau_1=2\beta\ ,\quad \tau_2=2\beta+\lambda\ ,\quad \tau_3=2\beta+2\lambda\ ,\quad p=j+k\ , \tag{2.20}$$

and

$$g(j,k)=\frac{(j+k+2)!}{\sqrt{(2j+2)!(2k+2)!}}\ . \tag{2.21}$$

This last expression may be evaluated numerically for large j and k by noting that for two integers a and b, $g(a,a)=1$ and

$$g(a,b)=\prod_{i=0}^{b-a-1}\left[\frac{2a+3+i}{a+b+3+i}\right]^{1/2}\quad \text{for } -1\leq a<b\ . \tag{2.22}$$

The matrix elements for the Hamiltonian with $Z=1$ are given by the formula

$$\begin{aligned}\langle\psi_j|H|\psi_k\rangle={}&\frac{C_2}{p+2}g(j,k)\left[\frac{\tau_2}{\tau_1}\right]^{p+2}+\frac{C_3-C_2}{p+2}g(j,k)-\frac{C_3}{p+2}g(j,k)\left[\frac{\tau_2}{\tau_3}\right]^{p+2}\\&-\frac{C_1\tau_1}{(p+1)(p+2)}g(j,k)\left[\frac{\tau_2}{\tau_1}\right]^{p+2}+2\frac{C_1\tau_2}{(p+1)(p+2)}g(j,k)-\frac{C_1\tau_3}{(p+1)(p+2)}g(j,k)\left[\frac{\tau_2}{\tau_3}\right]^{p+2}\\&+\frac{C_4}{\tau_1}g(j,k)\left[\frac{\tau_2}{\tau_1}\right]^{p+2}+\frac{C_5-C_4-\lambda}{\tau_2}g(j,k)+\frac{\lambda-C_5}{\tau_3}g(j,k)\left[\frac{\tau_2}{\tau_3}\right]^{p+2}\\&+\frac{l(l+1)}{2}\frac{g(j,k)}{(p+1)(p+2)}\left[\tau_2\left[\frac{\tau_2}{\tau_1}\right]^{p+1}-2\tau_2+\tau_2\left[\frac{\tau_2}{\tau_3}\right]^{p+1}\right]\ .\end{aligned} \tag{2.23}$$

TABLE I. Energy eigenvalues (in a.u.) of the Hulthén potential as a function of the basis size N for the 3s state with $\lambda=\frac{1}{10}$. Here β is a nonlinear variational parameter which is present in each basis function. A negative sign before the energy has been omitted everywhere.

N	Energy	Optimal β
5	0.016 805	0.270 327 308 954
10	0.016 805 555 555	0.268 511 868 647
15	0.016 805 555 555 555 555 555	0.267 395 720 649
20	0.016 805 555 555 555 555 555 555 555	0.266 991 564 267
25	0.016 805 555 555 555 555 555 555 555 555	0.259 630 427 841
30	0.016 805 555 555 555 555 555 555 555 555	0.303 636 084 861
35	0.016 805 555 555 555 555 555 555 555 555	0.318 590 522 497
Exact	0.016 805 555 555 555 555 555 555 555 555 555. . .	

The constants are given as

$$C_1=\tfrac{1}{2}k(k+1)\ , \quad C_2=\beta(k+1)\ ,$$
$$C_3=-(\beta+\lambda)(k+1)\ , \tag{2.24}$$

$$C_4=-\tfrac{1}{2}\beta^2\ , \quad C_5=\tfrac{1}{2}[\beta^2+\beta\lambda+\lambda(\beta+\lambda)]\ . \tag{2.25}$$

The exact energies for the $l=0$ states are given by

$$\mathcal{E}_n=-\frac{\lambda^2}{8n^2}\left[\frac{2}{\lambda}-n^2\right]^2 . \tag{2.26}$$

The trial state in Eq. (2.17) with $k=-1$ gives the exact eigenfunction for the 1s state. For the higher s states, we use the exact results to check our approximate energies. In Table I we show the convergence of our results for the 3s state with $\lambda=\frac{1}{10}$. In order to minimize rounding errors, these calculations were done in quadruple precision using a VAX station 3100. It should be noted that the correct digits are stable when we increase the size of the basis. Hence the accuracy of these results may be determined by requiring that correct digits are stable if we increase the size of the basis by at least five. Although this is not a rigorous guarantee, experience has shown that it does work in practice. For example, in each case this prescription gives correct results out to the precision reported for the $l=0$ states in Table II. The accuracy of this prescription can also be seen in Table IV for the 1s and 2s states of the Yukawa potential, where for large values of the screening parameter the more accurate results in Ref. [20] may be used as a check for the results in

TABLE II. Variational estimates for the s states of the Hulthén potential. The size of the basis is indicated by the value of N and λ is the screening parameter for the model. A negative sign before the energy (in a.u.) has been omitted everywhere.

State	λ	N	Energy	Exact	Ref. [24]
2s	0.050	15	0.101 250 000 000 000 000 000 000 000 000	0.101 25	0.101 248 5
	0.100	15	0.080 000 000 000 000 000 000 000 000 000	0.08	0.079 996 9
	0.200	20	0.045 000 000 000 000 000 000 000 000 000	0.045	0.045 001 4
	0.300	30	0.020 000 000 000 000 000 000 000 000 000	0.02	0.020 001 4
	0.400	30	0.004 999 999 999 999 999 999 999 99	0.005	
	0.490	30	0.000 049 999 9	0.000 05	
3s	0.050	20	0.033 368 055 555 555 555 555 555 555 555	0.033 368 055. . .	0.033 368 7
	0.100	25	0.016 805 555 555 555 555 555 555 555 555	0.016 805 555. . .	0.016 807 0
	0.150	30	0.005 868 055 555 555 555 555 555 555 5	0.005 868 055. . .	0.005 879 7
	0.200	30	0.000 555 555 555 555	0.000 555 555. . .	0.000 555 6
4s	0.025	20	0.020 000 000 000 000 000 000 000 000 000	0.02	0.020 001 7
	0.050	25	0.011 250 000 000 000 000 000 000 000 000	0.011 25	0.011 253 3
	0.075	30	0.004 999 999 999 999 999 999 999 999 999	0.005	
	0.100	30	0.001 249 999 999 999 999 99	0.001 25	0.001 253 2
	0.120	20	0.000 049 999 9	0.000 05	
5s	0.010	20	0.015 312 500 000 000 000 000 000 000 000	0.015 312 5	
	0.025	25	0.009 453 125 000 000 000 000 000 000 000	0.009 453 125	
	0.050	30	0.002 812 499 999 999 999 999 999 999	0.002 812 5	
	0.075	30	0.000 078 124 99	0.000 078 125	
6s	0.010	25	0.009 338 888 888 888 888 888 888 888 8	0.009 338 888. . .	
	0.020	30	0.005 688 888 888 888 888 888 888 888 8	0.005 688 888. . .	
	0.030	30	0.002 938 888 888 888 888 888 888 888 88	0.002 938 888. . .	
	0.040	30	0.001 088 888 888 888 888 888 8	0.001 088 888. . .	
	0.050	30	0.001 388 888 888	0.001 388 888. . .	

this report. Therefore the author believes that all results in this paper are correct out to the number of digits reported. The largest basis that could be used in this study was for $N=35$. Consequently, the most accurate results that are reported are for $N=30$, with the $N=35$ results used as a check for stability.

In Table III the $l \neq 0$ results are compared with the most accurate energies found in the literature, the numerical integration results of Ref. [27] and the dynamical-group approach results of Ref. [24]. The dynamical-group approach is an algebraic perturbation calculation which is based on the Lie algebra of the group SO(2,1). As the screening parameter is increased, the energy for each state approaches zero. The critical screening parameter for a particular state is the value of the screening parameter that results in the energy being zero for that state. As we approach the critical screening parameter for a state the results become less accurate. This is because a bigger basis is needed to approximate the true eigenfunctions of the Hamiltonian. Nevertheless, as seen in Tables II and III, these results are considerably more accurate than previous results even near the critical screening parameter.

III. THE YUKAWA POTENTIAL

The Yukawa potential in atomic units is given by

$$V(r) = -Z\frac{e^{-\lambda r}}{r} . \tag{3.1}$$

TABLE III. Variational estimates for the $l \neq 0$ states of the Hulthén potential. The size of the basis is indicated by the value of N and λ is the screening parameter for the model. The result from Ref. [27] was obtained by numerical integration. A negative sign before the energy (in a.u.) has been omitted everywhere.

State	λ	N	Energy	Ref. [27]	Ref. [24]
2*p*	0.025	10	0.112 760 465 559 343 425 619 752 170 155	0.112 760 5	0.112 760 4
	0.050	15	0.101 042 452 072 357 836 879 339 073 587	0.101 042 5	0.101 042 5
	0.075	15	0.089 847 752 885 906 144 304 385 693 159	0.089 847 8	
	0.100	15	0.079 179 439 105 145 937 524 790 404 026	0.079 179 4	0.079 179 4
	0.150	20	0.059 441 517 852 607 600 646 996 227 124	0.059 441 5	0.059 441 5
	0.200	25	0.041 886 049 217 867 004 860 632 106 240	0.041 886 0	0.041 886 0
	0.250	30	0.026 611 051 350 910 183 726 258 733 021	0.026 611 1	
	0.300	30	0.013 790 034 782 404 699 158 753 65	0.013 790 0	0.013 790 0
	0.350	30	0.003 793 098 147 021 733 958	0.003 793 1	
3*p*	0.025	15	0.043 706 891 586 462 308 141 294 038 749	0.043 706 9	0.043 707 1
	0.050	20	0.033 164 501 183 867 202 344 100 104 947	0.033 164 5	0.033 165 0
	0.075	20	0.023 939 747 261 830 537 729 569 804 128	0.023 939 7	
	0.100	25	0.016 053 726 638 917 253 120 820 512 320	0.016 053 7	0.016 053 7
	0.150	30	0.004 466 308 785 352 310 813 134 770	0.004 466 3	0.004 466 4
3*d*	0.025	15	0.043 603 050 099 100 057 801 958 125 136	0.043 603 0	0.043 603 0
	0.050	20	0.032 753 184 225 127 904 255 118 098 806	0.032 753 2	0.032 753 2
	0.075	20	0.023 030 704 076 838 084 236 822 010 206	0.023 030 7	
	0.100	25	0.014 484 226 905 249 705 674 298 019 569	0.014 484 2	0.014 484 2
	0.150	30	0.001 396 592 465 736 554 737	0.001 396 6	0.001 396 5
4*p*	0.025	15	0.019 948 905 991 591 497 285 687 056 245	0.019 948 9	0.019 949 0
	0.050	30	0.011 058 170 219 449 860 057 316 743 972	0.011 058 2	0.011 058 3
	0.075	30	0.004 621 926 453 225 971 222 181 244 080	0.004 621 9	0.004 622 4
	0.100	30	0.000 754 993 385 350 572	0.000 755 0	
4*d*	0.025	20	0.019 846 254 274 766 466 787 699 765 732	0.019 846 2	0.019 846 2
	0.050	25	0.010 667 404 172 560 599 405 741 457 388	0.010 667 4	0.010 667 4
	0.075	30	0.003 834 533 076 921 216 496 412 143 50	0.003 834 5	0.003 834 6
4*f*	0.025	20	0.019 691 095 298 151 444 342 346 808 311	0.019 691 1	0.019 691 1
	0.050	25	0.010 061 964 550 932 802 432 661 352 583	0.010 062 0	0.010 061 9
	0.075	30	0.002 556 296 978 072 423 535 750 629	0.002 556 3	0.002 556 3
5*p*	0.025	20	0.009 403 557 163 486 734 175 586 234 194	0.009 303 7	
	0.050	30	0.002 649 010 790 807 918 733 598 141 5	0.002 649 0	
5*d*	0.025	25	0.009 303 717 458 026 345 334 747 579 627	0.009 303 7	
	0.050	30	0.002 313 111 821 208 130 166 125 748 7	0.002 313 1	
5*f*	0.025	25	0.009 152 143 725 161 372 680 058 181 756	0.009 152 1	
	0.050	30	0.001 783 545 794 710 618 483 506 22	0.001 015 9	
5*g*	0.025	25	0.008 946 497 371 021 501 003 395 968 061	0.008 946 5	
	0.050	30	0.001 015 881 590 452 020 711 485	0.001 015 9	
6*p*	0.025	30	0.004 154 759 470 233 324 871 44	0.004 154 8	
6*d*	0.025	30	0.004 060 553 888 060 235 634 492	0.004 060 6	
6*f*	0.025	30	0.003 916 768 896 642 590 859 760 5	0.003 916 8	
6*g*	0.025	30	0.003 720 093 464 283 440 373 336 23	0.003 720 1	
6*h*	0.025	30	0.003 465 434 587 072 453 281 320 807		

Here Z is a constant and λ is the screening parameter. The scaling relation in Eq. (2.5) also holds for this potential and following the previous analysis we look for a radial solution of the form in Eq. (2.15). Thus we choose a basis formed by the functions

$$\psi_k = B_k r^k e^{-(\beta/2)r}\ , \quad k=0,1,2,\ldots\ , \tag{3.2}$$

where the normalization constant B_k is

$$B_k = \left[\frac{\beta^{2k+3}}{(2k+2)!} \right]^{1/2}\ , \tag{3.3}$$

and β is a variational parameter. The matrix elements are given by

$$\langle \psi_j | \psi_k \rangle = g(j,k) \tag{3.4}$$

and

$$\begin{aligned}\langle \psi_j | H | \psi_k \rangle = &- \frac{g(j,k)k}{2}(k+1)\frac{\beta^2}{(p+1)(p+2)} \\ &+ g(j,k)\frac{\beta^2}{2}\frac{k+1}{p+2} - g(j,k)\frac{\beta^2}{8} \\ &+ g(j,k)\frac{l(l+1)}{2}\frac{\beta^2}{(p+1)(p+2)} \\ &- \frac{g(j,k)}{(\lambda+\beta)^{p+2}}\frac{1}{p+2}\ .\end{aligned} \tag{3.5}$$

The energies for this model are given in Tables IV and V. We compare our results with two previous reports. The study in Ref. [20] uses Rayleigh-Schrödinger perturbation theory and writes the energy as

$$E_{NLM} = -\frac{Z^2}{2N^2} + \sum_{n=1}^{\infty} E_{NLM}^{(n)}(Z)\lambda^n\ . \tag{3.6}$$

TABLE IV. Variational estimates for the lowest three states of the Yukawa potential. The size of the basis is indicated by the value of N and λ is the screening parameter for the model. A negative sign before the energy (in a.u.) has been omitted everywhere.

State	λ	N	Energy	Ref. [20]
1*s*	0.10	20	0.407 058 030 613 403 156 754 507 070 361	0.407 058 030 613 403 156 75
	0.20	25	0.326 808 511 369 193 384 882 495 419 281	0.326 808 511 369 193 384 88
	0.30	25	0.257 638 586 303 054 148 878 964 069 306	0.257 638 586 303 054 148 88
	0.40	30	0.198 376 083 361 850 216 608 413 859 925	0.198 376 083 361 850 216 61
	0.50	30	0.148 117 021 889 932 616 711 758 2	0.148 117 021 889 932 616 71
	0.60	30	0.106 135 907 505 814 193 000 73	0.106 135 907 505 814 193 00
	0.70	30	0.071 833 555 904 512 213 0	0.071 833 555 904 512 213 04
	0.80	30	0.044 704 304 497 359 66	0.044 704 304 497 359 663 20
	0.90	30	0.024 314 193 827 50	0.024 314 193 827 502 054 89
	1.00	30	0.010 285 789 9	0.010 285 789 990 017 696 80
	1.15	30	0.000 455 8	0.000 455 889 021 355 957 79
2*s*	0.01	15	0.115 293 285 167 994 256 222 045 516 170	0.115 293 285 167 994 246 22
	0.02	25	0.106 148 320 244 695 503 250 708 341 185	0.106 148 320 244 695 503 25
	0.03	30	0.097 531 786 134 660 862 770 039 060 920	0.097 531 786 134 660 862 77
	0.04	30	0.089 414 634 185 159 188 415 714 621 025	0.089 414 634 185 159 188 42
	0.05	30	0.081 771 195 795 253 124 173 489 413 770	0.081 771 195 795 253 124 17
	0.06	30	0.074 578 534 412 709 709 694 885 171 159	0.074 578 534 412 709 709 69
	0.07	30	0.067 815 959 981 462 181 222 810 363 310	0.067 815 959 981 462 181 22
	0.08	30	0.061 464 656 212 300 385 911 466 251 113	0.061 464 656 212 300 385 91
	0.09	30	0.055 507 388 553 290 736 394 798 978 073	0.055 507 388 553 290 736 39
	0.10	30	0.049 928 271 331 918 889 234 996 681 036	0.049 928 271 331 918 889 23
	0.15	30	0.027 222 190 725 688 518 250 187 26	0.027 222 190 725 688 518 25
	0.20	30	0.012 107 865 195 440 464 38	0.012 107 865 195 440 464 39
	0.25	30	0.003 395 906 283 23	0.003 395 906 283 239 307 80
2*p*	0.01	15	0.115 245 224 090 564 185 894 783 216 335	0.115 245 224 090 564 185 89
	0.02	20	0.105 963 398 179 939 904 755 731 028 037	0.105 963 398 179 939 904 76
	0.03	25	0.097 131 366 795 691 310 671 783 889 214	0.097 131 366 795 691 310 67
	0.04	30	0.088 729 373 582 879 526 287 939 141 467	0.088 729 373 582 879 526 29
	0.05	30	0.080 740 387 037 784 609 712 102 743 610	0.080 740 387 037 784 609 71
	0.06	30	0.073 149 619 385 860 625 023 805 418 420	0.073 149 619 385 860 625 02
	0.07	30	0.065 944 176 996 156 573 384 560 516 651	0.065 944 176 996 156 573 38
	0.08	30	0.059 112 804 787 031 234 635 692 332 927	0.059 112 804 787 031 234 64
	0.09	30	0.052 645 701 331 584 274 463 576 906 198	0.052 645 701 331 584 274 46
	0.10	30	0.046 534 390 486 724 608 386 600 840 395	0.046 534 390 486 724 608 39
	0.15	30	0.021 104 888 927 736 242 916 943 3	0.021 104 888 927 736 242 92
	0.20	30	0.004 101 646 530 784 0	0.004 101 646 53
	0.21	30	0.001 808 760 066 28	0.001 808 760
	0.22	30	0.000 028 69	0.000 026

TABLE V. Variational estimates for the energies (in a.u.) of the Yukawa potential. The size of the basis is indicated by the value of N and λ is the screening parameter for the model. A negative sign before the energy has been omitted everywhere.

State	λ	N	Energy	Ref. [14]
3*s*	0.025	25	0.034 329 509 911 543 775 438 062 336 055	0.034 33
	0.050	30	0.019 352 554 814 752 342 295 397 996 788	0.019 35
	0.080	30	0.007 775 877 038 957 710 092 63	0.007 78
	0.100	30	0.003 208 046 744 690 25	0.003 21
	0.120	30	0.000 727 473 19	0.000 73
3*p*	0.025	25	0.034 078 910 428 938 130 548 463 162 217	0.034 08
	0.050	30	0.018 557 751 883 405 996 604 893 993 884	0.018 56
	0.080	30	0.006 329 995 439 268 113 269	0.006 33
	0.100	30	0.001 589 001 525 867	0.001 58
3*d*	0.025	25	0.033 573 122 086 666 003 102 965 090 942	0.033 57
	0.050	30	0.016 915 570 569 815 842 886 114 758 243	0.016 92
	0.080	30	0.003 248 360 428 751 993 5	0.003 24
4*s*	0.025	30	0.012 503 238 318 007 071 505 739 698 432	0.012 50
	0.050	30	0.003 091 659 900 161 321 484	0.003 09
	0.060	30	0.001 236 719 097 035 0	0.001 24
4*p*	0.025	30	0.012 294 320 436 313 933 670 168 893 844	0.012 29
	0.050	30	0.002 598 058 852 571 853 96	0.002 60
	0.060	30	0.000 729 172 766 63	0.000 75
4*d*	0.010	30	0.022 227 792 489 804 398 453 786 853 193	
	0.025	30	0.011 870 448 936 190 599 940 851 142 013	0.011 87
	0.050	30	0.001 580 871 626 871 004	0.001 58
4*f*	0.010	30	0.022 098 770 463 802 567 552 796 834 9	
	0.020	30	0.014 491 978 017 490 743 686 655 396 719	
	0.030	30	0.008 282 152 466 779 632 959 281 124 004	
5*s*	0.010	25	0.011 661 054 230 397 962 151 615 838	
	0.020	30	0.006 030 038 507 130 855 809 946 414 5	
	0.030	30	0.002 482 776 201 983 677 88	
	0.040	30	0.000 590 704 475 90	
5*p*	0.010	25	0.011 622 036 755 969 693 601 356 199 243	
	0.020	30	0.005 910 736 541 809 108 790 145 851 07	
	0.030	30	0.002 290 415 355 742 325 98	
	0.040	30	0.000 386 829 339 3	
5*d*	0.010	30	0.011 543 695 211 053 011 928 645 361 77	
	0.020	30	0.005 669 005 190 254 584 440 116 780 89	
	0.030	30	0.001 898 003 084 809 707 76	
5*f*	0.010	30	0.011 425 400 166 089 089 065 660 934 0	
	0.020	30	0.005 297 913 897 837 897 341 850 570 7	
	0.030	30	0.001 286 301 759 146 104 1	
5*g*	0.010	30	0.011 266 164 788 451 476 673 882 577 389	
	0.020	30	0.004 784 984 511 570 123 196 068 811 64	
	0.030	30	0.000 409 879 466 872 47	
6*s*	0.010	30	0.006 176 422 150 691 064 607 767 739 5	
	0.020	30	0.001 955 646 068 966 604 941 3	
	0.030	30	0.000 194 065 818	
6*p*	0.010	30	0.006 141 621 281 428 276 706 306 968	
	0.020	30	0.001 866 293 792 266 562 918	
	0.030	30	0.000 105 967 90	
6*d*	0.005	30	0.009 474 251 021 475 242 223 013 899 58	
	0.010	30	0.006 071 656 603 180 676 415 731 809 7	
	0.020	30	0.001 685 173 401 671 858 130 7	
6*f*	0.005	30	0.009 442 748 962 862 212 124 240 756 269	
	0.010	30	0.005 965 775 123 381 422 937 208 235	
	0.020	30	0.001 406 727 545 898 197 781	
6*g*	0.005	30	0.009 400 599 086 133 379 855 529 675 467	
	0.010	30	0.005 822 774 561 765 861 856 536 178 5	
	0.020	30	0.001 020 146 540 570 374 82	
6*h*	0.005	25	0.009 347 671 582 077 595 872 354 001 364	
	0.010	30	0.005 640 900 220 362 825 894 758 261 802	
	0.020	30	0.000 503 073 278 505 243 12	

They chose a trial wave function with the form

$$\psi = e^{-r} B(r) Y_{LM}(\theta,\phi) \,, \tag{3.7}$$

where

$$B(r) = \sum_{n=0} \lambda^n B_n(r) \,, \quad B_n(r) = \sum_{j=0} b_{jn} r^j \,. \tag{3.8}$$

The perturbation coefficients $E^{(n)}$ were calculated up to $n=100$ for the 1*s*, 2*s*, and 2*p* levels. In Ref. [14], energies are estimated by forming Padé approximants to the energy perturbation series.

The results in this report for the 1*s* and 2*s* states are not as accurate as the excellent results of Ref. [20], for large values of the screening parameters. However, our results are more accurate for smaller values of λ. Also, the current energies for the 2*p* state are considerably more accurate than those in Ref. [20] for the entire range of the screening parameter. All of the present results are more accurate than the results in Ref. [14].

It was shown recently by Wang [35] that for two potentials $V_1(\mathbf{r})$ and $V_2(\mathbf{r})$, if $V_1(\mathbf{r}) \le V_2(\mathbf{r})$ everywhere in space then for the same quantum numbers the energies of $V_1(\mathbf{r})$ are less than or equal to the energies of $V_2(\mathbf{r})$. It is not hard to show that

$$-\frac{1}{r} \le -\lambda \frac{e^{-\lambda r}}{1-e^{-\lambda r}} \le -\frac{e^{-\lambda r}}{r} \quad \text{for } 0 \le r < \infty \,, \; \lambda > 0 \,. \tag{3.9}$$

So according to the result by Wang, the following relation should hold for the energies of the Coulomb, Hulthén, and Yukawa potentials:

$$\mathcal{E}_n^{\text{Coulomb}} \le \mathcal{E}_{n,l}^{\text{Hulthén}}(\lambda) \le \mathcal{E}_{n,l}^{\text{Yukawa}}(\lambda) \,. \tag{3.10}$$

It can be seen from the tables that the current results support this relation. For example, the 2*s* and 2*p* state energies for the Hulthén potential in Table II and III are all higher than the Coulomb energy of $\mathcal{E}_2^{\text{Coulomb}} = -(1/2)(1/2^2) = -0.125$. Also, the 2*s* state energies of the Hulthén potential with $\lambda = 0.05, 0.1, 0.2$ are smaller than the corresponding energies of the Yukawa potential. A similar relation can be seen for the energies of the Hulthén and Yukawa potentials for the 2*p* state with $\lambda = 0.05, 0.1, 0.15, 0.2$.

A more compelling example occurs when the screening parameter approaches zero. In this limit, the Hulthén and Yukawa potentials reduce to the Coulomb potential. Indeed, the energies for these three potentials become arbitrarily close for small λ, but Eq. (3.10) must still hold. An example of this is given by comparing energies of the $n=2$ states for $\lambda = 10^{-8}$. The energies for the 2*s* states are

$$\begin{aligned} \mathcal{E}_{2,s}^{\text{Hulthén}} &= -0.124\,999\,995\,000\,000\,050\,5 \,, \\ \mathcal{E}_{2,s}^{\text{Yukawa}} &= -0.124\,999\,990\,000\,000\,299\,999\,993\,000\,000\,303 \end{aligned} \tag{3.11}$$

and the energies for the 2*p* state are

$$\begin{aligned} \mathcal{E}_{2,p}^{\text{Hulthén}} &= -0.124\,999\,995\,000\,000\,042 \,, \\ \mathcal{E}_{2,p}^{\text{Yukawa}} &= -0.124\,999\,990\,000\,000\,249\,999\,995\,000\,000\,238 \,. \end{aligned} \tag{3.12}$$

These results were obtained with a basis of only five states. The difference in these energies is very small yet the 2*s* and 2*p* states of the Hulthén potential are still higher than the Coulomb energy and lower than the corresponding energies of the Yukawa potential. It should also be noted that the difference between the 2*s* and 2*p* states is very small for both the Hulthén and Yukawa potentials. This is due to the fact that the energy levels for different angular momentum states become degenerate in the limit where λ goes to zero, just as in the Coulomb potential.

IV. CONCLUDING REMARKS

The main interest in this paper has been to obtain an efficient method for estimating the energies of the Hulthén and Yukawa potentials. This problem has received great attention in past years and has been approached by a broad range of methods. It has been shown in this report that a linear combination of simple functions can be used to yield very accurate results for these potentials. We also point out that the results in this paper may be improved by finding a better set of basis functions and/or increasing the size of the basis. The accuracy of the upper bounds has been estimated by comparing the results of two different basis sizes. For the cases where very accurate results exist, we have demonstrated that this prescription produces very good results.

Using the general theorem derived by Wang [35], we have shown that the energies of the Hulthén potential are always between those of the Coulomb and Yukawa potentials. A stringent test of this relation occurs for small values of the screening parameters, since as the screening parameter goes to zero the energies of these three potentials become arbitrarily close together. We have given a numerical example of this relation for a very small value of the screening parameter and have shown for this extreme case that the relation still holds.

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