Bound eigenstates for two truncated Coulomb potentials

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The eigenvalue problem for two particles interacting through the attractive truncated Coulomb potential, $V(r) = -Ze^2/(r^p+\beta^p)^{1/p}$, for $p=1$ and 2 is solved numerically. Energy eigenvalues accurate to within eight to six significant figures for the states $1s$ to $4f$ are calculated as a function of the truncation parameter β. It is found that the level ordering satisfies $E_{nl} > E_{nl'}$ for $l < l'$. Systematics of the eigenvalues are studied and it is found that for each l value the energies are well represented by a Ritz type of formula.

I. INTRODUCTION

Patil[1] has made a detailed study of the analytic behavior of the phase shifts and scattering lengths for the potential

$$V(r) = \frac{-Ze^2}{(r^p+\beta^p)^{1/p}} , \tag{1}$$

where $p = 1, 2, 3, \ldots$ and β is a truncation parameter (>0) in the $\beta \to 0$ limit. The cases $p=1$ and 2 are of special physical significance. For $p=1$, Eq. (1) becomes

$$V(r) = \frac{-Ze^2}{r+\beta}, \quad \beta > 0 . \tag{2}$$

This potential[2] avoids the singularity at $r=0$ in the Coulomb potential. It is known that in the quantum-field theory, the singularity at $r=0$ in the Coulomb potential is the crux of divergence difficulties. Indeed it has been suggested[3] that if gravitational interactions of elementary particles are taken into account, there would be a gravitational cutoff of Coulomb interactions resulting in a finite theory of quantum fields. Equation (2) represents a nonrelativistic expression of this idea. This potential may also serve as an approximation to the potential due to a smeared charge rather than a point charge. Mehta and Patil[2] have analytically studied the s-state eigenvalues for the potential (2); however, no numerical results were obtained.

When $p=2$, Eq. (1) becomes

$$V(r) = -\frac{Ze^2}{(r^2+\beta^2)^{1/2}} . \tag{3}$$

Such a potential is useful for scattering by a finite-charge distribution. In particular, for scattering by a uniform spherical charge distribution, the effective potential is well simulated by $V(r)$ given in Eq. (3). The Coulomb potential of the nucleus experienced by a muon in a muonic atom is modified due to the finite size of the nucleus. The shape of this modified potential[4,5] is very similar to that given by Eq. (3) and this equation can serve as a model potential for such, and allied problems like isotope shift in atomic spectra. The truncated Coulomb potential (3) has also been found to be pertinent in the study of the energy levels of hydrogenlike atoms exposed to intense laser radiation.[6–10] Several authors[7–9] have shown that under Kramers-Henneberger transformation,[11] the laser-dressed binding potential for the hydrogenic system may be well approximated by Eq. (3). In such a situation, the truncation parameter β is related to the strength of the irradiating laser field.

Thus it was of interest to carry out a systematic study of the bound-state energy levels of potentials (2) and (3). We report the results of such a study in the present paper. As the Schrödinger equation for neither of the potentials is amenable to a general analytical solution, we employ a numerical method to calculate the energy eigenvalues for the $1s$–$4f$ states with accuracy varying from eight significant figures for low levels to six significant figures for higher levels. The numerical algorithm is discussed in Sec. II. The eigenvalues are presented and discussed in Sec. III.

II. NUMERICAL CALCULATION

In reduced units the radial Schrödinger equation for the potential (1) is

$$\left[-\frac{1}{2}\frac{d^2}{dr^2} + \frac{l(l+1)}{2r^2} - \frac{1}{(r^p+\beta^p)^{1/p}}\right] u = Eu . \tag{4}$$

In order to avoid the problems associated with a boundary condition at $r=\infty$ and the need for variable grid sizes in the numerical integration we used the transformation

$$r = \frac{x}{1-x} , \tag{5}$$

yielding

$$\left\{(1-x)^3\frac{d}{dx} - \frac{1}{2}(1-x^4)\frac{d^2}{dx^2} + \frac{(1-x)^2}{2x^2}l(l+1) - \left[\left(\frac{x}{1-x}\right)^p + \beta^p\right]^{-1/p}\right\} u = Eu . \tag{6}$$

This was converted to a differential equation and solved for E using an iterative method. In some cases in order to obtain better convergence the transformation was slightly

TABLE I. Bound-state energies $(-E)$ in reduced units for $1s$ to $4f$ states of the potential $V(r)=-1/(r+\beta)$ as a function of the parameter β.

β	$1s$	$2s$	$3s$	$4s$	$2p$	$3p$	$4p$	$3d$	$4d$	$4f$
0.1	0.387 543 65	0.109 508 05	0.050 809 14	0.029 213 49	0.117 535 35	0.053 309 30	0.030 294 97	0.054 136 57	0.030 648 45	0.030 813 60
0.2	0.331 014 27	0.100 410 58	0.047 863 78	0.027 913 68	0.111 391 71	0.051 405 26	0.029 473 37	0.052 829 67	0.030 089 10	0.030 396 14
0.3	0.293 545 28	0.093 762 04	0.045 628 85	0.026 907 70	0.106 173 51	0.049 745 58	0.028 747 71	0.051 618 83	0.029 566 14	0.029 996 10
0.5	0.244 531 44	0.084 154 89	0.042 264 18	0.025 359 20	0.097 655 62	0.046 946 07	0.027 502 66	0.049 436 96	0.028 611 81	0.029 243 11
1.0	0.180 367 05	0.069 580 66	0.036 814 20	0.022 756 98	0.082 862 42	0.041 787 66	0.025 134 40	0.045 010 01	0.026 625 06	0.027 588 16
2.0	0.125 000 00	0.054 474 04	0.030 640 35	0.019 651 19	0.065 732 01	0.035 263 92	0.021 986 76	0.038 787 14	0.023 706 66	0.024 972 05
3.0	0.098 215 64	0.045 979 04	0.026 884 27	0.017 668 20	0.055 555 56	0.031 054 60	0.019 854 09	0.034 479 64	0.021 590 82	0.022 960 24
5.0	0.070 670 28	0.036 119 25	0.022 212 32	0.015 088 44	0.043 458 40	0.025 658 95	0.016 987 44	0.028 705 69	0.018 616 11	0.020 000 00
10.0	0.043 438 72	0.024 810 36	0.016 341 47	0.011 638 31	0.029 446 52	0.018 798 15	0.013 060 94	0.021 024 30	0.014 373 46	0.015 576 60
20.0	0.025 669 94	0.016 184 16	0.011 381 02	0.008 501 27	0.018 846 22	0.012 896 36	0.009 460 83	0.014 387 21	0.010 386 93	0.011 278 29
35.0	0.016 388 67	0.011 079 59	0.008 180 24	0.006 340 88	0.012 685 92	0.009 157 17	0.006 992 37	0.010 135 72	0.007 635 02	0.008 268 68
50.0	0.012 194 69	0.008 579 24	0.006 518 35	0.005 167 08	0.009 717 59	0.007 237 44	0.005 661 48	0.007 962 80	0.006 153 63	0.006 643 88
100.0	0.006 742 08	0.005 074 63	0.004 053 13	0.003 344 14	0.005 633 74	0.004 429 79	0.003 617 22	0.004 812 49	0.003 891 90	0.004 168 78
200.0	0.003 653 17	0.002 907 08	0.002 422 39	0.002 069 59	0.003 169 53	0.002 608 78	0.002 210 90	0.002 798 56	0.002 353 65	0.002 498 27

TABLE II. Bound-state energies $(-E)$ in reduced units for $1s$ to $4f$ states of the potential $V(r)=-1/(r^2+\beta^2)^{1/2}$ as a function of the parameter β.

	$1s$	$2s$	$3s$	$4s$	$2p$	$3p$	$4p$	$3d$	$4d$	$4f$
0.1	0.474 171 71	0.121 820 90	0.054 614 51	0.030 852 79	0.124 795 93	0.055 495 23	0.031 224 57	0.055 543 22	0.031 244 80	0.031 248 14
0.2	0.439 693 76	0.117 445 99	0.053 305 44	0.030 296 99	0.124 217 22	0.055 324 99	0.031 152 91	0.055 506 41	0.031 229 28	0.031 242 57
0.3	0.408 256 72	0.113 273 28	0.052 039 11	0.029 755 38	0.123 329 14	0.055 065 07	0.031 043 65	0.055 445 60	0.031 203 67	0.031 233 30
0.5	0.357 125 77	0.106 013 61	0.049 790 42	0.028 783 55	0.120 886 65	0.054 353 89	0.030 745 04	0.055 255 40	0.031 123 73	0.031 203 79
1.0	0.274 391 35	0.092 679 33	0.045 488 94	0.026 886 37	0.113 024 19	0.052 060 38	0.029 779 94	0.054 436 21	0.030 781 50	0.031 068 46
2.0	0.193 042 20	0.076 320 17	0.039 841 73	0.024 311 02	0.097 508 10	0.047 368 34	0.027 775 33	0.051 882 47	0.029 722 44	0.030 569 37
3.0	0.151 049 16	0.066 051 42	0.036 032 10	0.022 511 13	0.085 215 23	0.043 393 55	0.026 030 50	0.048 904 38	0.028 482 08	0.029 850 50
5.0	0.107 081 37	0.053 170 56	0.030 875 39	0.019 978 65	0.068 187 16	0.037 360 53	0.023 274 75	0.043 257 55	0.026 067 67	0.028 105 24
10.0	0.063 738 92	0.037 154 40	0.023 668 23	0.016 205 55	0.046 199 04	0.028 313 69	0.018 823 38	0.033 158 59	0.021 412 57	0.023 806 74
20.0	0.036 198 55	0.024 172 96	0.016 897 67	0.012 327 01	0.028 830 11	0.019 716 23	0.014 108 39	0.022 787 16	0.015 990 34	0.017 928 61
35.0	0.022 334 28	0.016 306 06	0.012 211 73	0.009 384 42	0.018 810 95	0.013 909 02	0.010 557 94	0.015 761 48	0.011 816 98	0.013 152 44
50.0	0.016 260 72	0.012 450 96	0.009 699 65	0.007 694 78	0.014 088 38	0.010 879 00	0.008 554 01	0.012 158 71	0.009 476 02	0.010 458 42
100.0	0.008 629 78	0.007 118 61	0.005 918 95	0.004 964 73	0.007 800 13	0.006 458 83	0.005 393 70	0.007 035 19	0.005 849 63	0.006 332 73
200.0	0.004 502 86	0.003 923 03	0.003 430 34	0.003 011 75	0.004 193 07	0.003 659 49	0.003 206 25	0.003 900 20	0.003 410 24	0.003 623 85

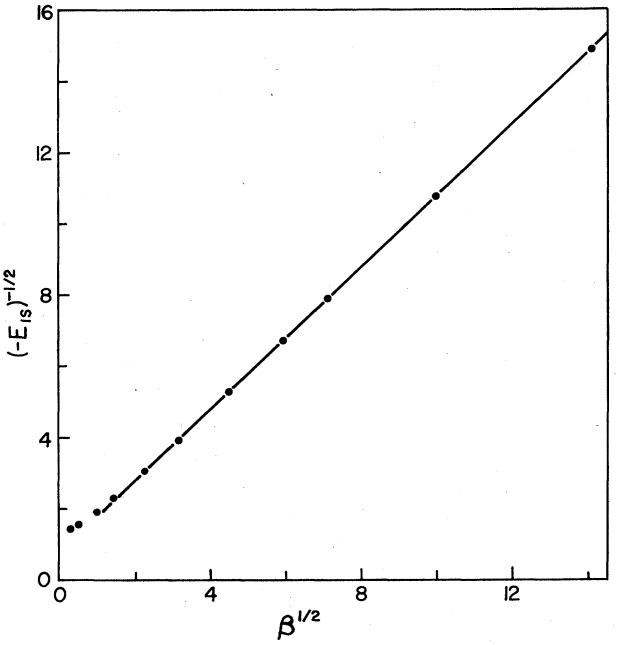

FIG. 1. The quantity $(-E)^{1/2}$ as a function of $\beta^{1/2}$ for the $1s$ state of potential (3).

modified to

$$r=\alpha\left(\frac{x}{1-x}\right) , \tag{7}$$

where α was a parameter chosen to improve the convergence.

III. RESULTS AND DISCUSSION

In Tables I and II we show the energy eigenvalues in reduced units for the $1s$–$4f$ states of potentials (2) and (3), respectively, for a wide range of values of β.

An interesting result that emerges from an examination of the results is the fact that for a fixed n and β, the state with orbital angular momentum $(l+1)$ is more strongly bound than the one with l. This level ordering is opposite to what is observed in ordinary atoms but it is analogous to the level ordering in muonic atoms. For instance, $2p$ level is lower than $2s$, which makes the $2s$ level nonmetastable. While both the potentials (2) and (3) show level ordering similar to that of muonic atoms, the shape of the potential (3) is closer to the potential experienced by a muon in a muonic atom, and thus this potential appears to be a suitable model potential for studying muonic atoms.

Next we study the systematics of the eigenvalues for these two potentials.

In Fig. 1 we show $(-E)^{-1/2}$ vs $\beta^{1/2}$ for the $1s$ state of potential (3). It will be noticed that for $\beta \geq 4$, the relationship is almost linear. For a laser-dressed hydrogenlike atom, β is proportional to $I^{1/2}/\omega^2$, where ω is the laser frequency and I is the intensity. The relationship shown in Fig. 1 suggests that for a hydrogenlike atom in the presence of an intense nonresonant laser field, the quantity (ionization potential)$^{-1/2}$ should vary linearly with $I^{1/4}/\omega$ for medium and large values of the latter quantity.

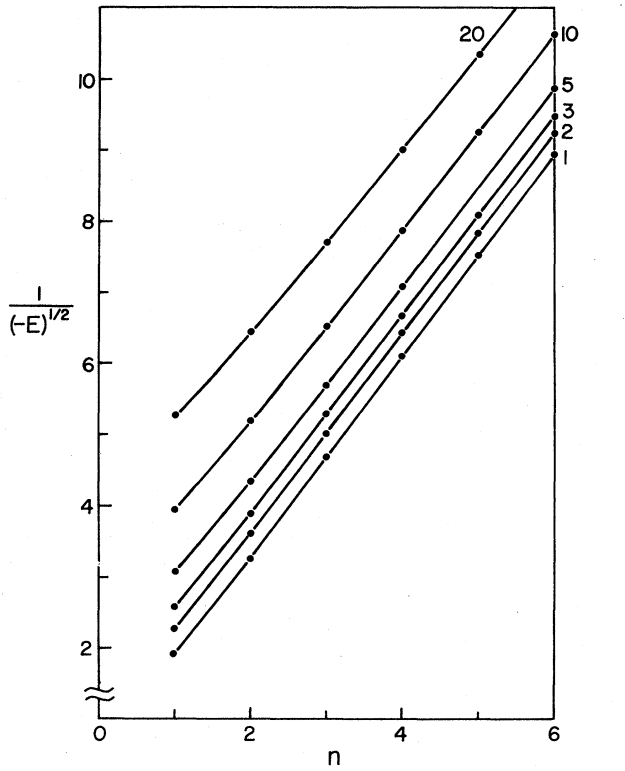

FIG. 2. The quantity $(-E)^{-1/2}$ as a function of the quantum number n for the s states of the potential (3). The numbers by the side of the curves denote β values.

In Fig. 2 we show $(-E)^{-1/2}$ as a function of the quantum number n for the s states of the potential (3) for several values of β. It will be noticed that the relationship is practically linear. The p and d states also show a similar behavior. Thus, to a first approximation,

$$(-E)^{-1/2}=a+bn \ . \tag{8}$$

It turns out that b is almost $\sqrt{2}$. Thus,

$$E=\frac{-1}{2(n+\mu)^2} , \tag{9}$$

TABLE III. Values of the parameters a, b, and c in Eq. (10) for the s states of potential (2).

β	a	b	c
1	0.968 264 3	1.415 464	−0.029 240 28
2	1.465 265 2	1.417 537	−0.054 705 06
3	1.846 272 7	1.419 797	−0.075 720 16
5	2.445 988 8	1.424 400	−0.109 597 54
10	3.530 785 8	1.435 331	−0.169 736 09
20	5.030 926 6	1.454 183	−0.246 348 07
35	6.649 839 2	1.477 263	−0.319 563 78
50	7.925 53	1.496 445	−0.371 113 3
100	11.108 07	1.545 374	−0.481 203 5
200	15.527 78	1.611 869	−0.603 344 7

TABLE IV. Values of the parameters a, b, and c in Eq. (10) for the s states of potential (3).

β	a	b	c
1	0.446 159 1	1.412 585	0.048 755 38
2	0.774 951 1	1.408 889	0.092 765 74
3	1.044 095 0	1.404 471	0.125 466 19
5	1.492 371 5	1.395 128	0.170 242 23
10	2.364 414 9	1.373 211	0.226 552 37
20	3.659 340 8	1.336 752	0.262 597 28
35	5.124 267 3	1.302 591	0.270 020 41
50	6.306 35	1.276 862	0.264 631 2
100	9.308 77	1.224 770	0.236 808 7
200	13.535 74	1.175 198	0.196 475 1

where μ is a constant. Equation (9) is similar to the well-known expression used for representing atomic terms for alkali-metal atoms. However, either of Eqs. (2) or (3) is not a suitable model potential for alkali-metal atoms because the ordering of s,p,d . . . levels is opposite to that in alkali-metal atoms.

As β increases, there is a slow departure from linearity for small n (see Fig. 2). The departure from linearity in the $(-E)^{-1/2}$, n relationship can be allowed for by a Ritz type of dependence of μ on n. Thus,

$$(-E)^{-1/2} = a + bn + c/n^2 \ , \tag{10}$$

where a, b, and c are constants. The values of these constants for potentials (2) and (3) are shown in Tables III and IV, respectively, for s states. These constants were determined by a least-squares fit of Eq. (10) to the calculated values for $n = 1$ to $n = 6$.

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