Numerical tests of the Landé subtraction method for the Coulomb potential in momentum space

John W. Norbury
Physics Department, University of Wisconsin, La Crosse, Wisconsin 54601

Khin Maung Maung
Physics Department, Hampton University, Hampton, Virginia 23668

David E. Kahana
Physics Department, Kent State University, Kent, Ohio 44242

(Received 3 February 1994)

The Landé subtraction method is a technique for removing the singularity which arises when one solves the Schrödinger equation in momentum space for the Coulomb potential. Using this technique, numerical solutions for eigenvalues and eigenfunctions are presented and compared to exact results. Approximately 50 eigenvalues can be calculated very accurately for various values of the angular momentum. Numerous eigenfunctions can also be found very accurately. In addition, it is shown how to implement the Landé subtraction method for potentials which are a linear combination of the Coulomb potential and some other potential. Using a basis-function expansion technique, it is shown how to obtain solutions in those cases where the momentum integrals must be evaluated explicitly.

PACS number(s): 03.65.Ge, 02.60.Nm, 31.15.+q, 32.30.−r

I. INTRODUCTION

Momentum-space solutions of bound-state and scattering equations are of great importance in solving relativistic quantum problems. For example, the most straightforward relativistic generalization of the kinetic-energy operator is very cumbersome in configuration space, but rather simple in momentum space [1]. In addition the handling of retardation and nonlocality is much simpler to implement in momentum space [2–4], as well as other relativistic aspects of strong-interaction physics [2–6].

Momentum-space bound-state and scattering equations [1,6] are usually written as integral equations and except for the simplest of cases must be solved by numerical techniques. Consequently, it is of importance to study numerical solutions of momentum-space equations for the many standard potentials that are widely used in physics such as the Coulomb, Yukawa [6,7], confining [8], Cornell [9], Hulthen [6,7], etc., potentials. Such solutions are far from trivial, especially when the potentials possess momentum-space singularities, as is the case for the Coulomb [10] and confining potentials [8].

Our interest in the present work is the solution of the momentum-space, nonrelativistic Schrödinger equation for the Coulomb potential. Actually, the analytic solution to this problem has already been presented [11]. Nevertheless, it is still important to obtain *numerical* solutions as well. The reason for this is that the Coulomb potential often appears in combinations with other potentials that cannot be solved analytically. One example is the Cornell potential, which consists of the Coulomb potential plus a linear confining term [9]. One must have *numerical* solutions for the pure Coulomb problem when solving the Cornell potential in momentum space [10]. Another example in which one needs numerical solutions to the Coulomb problem occurs in the study of hadronic atoms [2–4].

The most significant difficulty in obtaining numerical solutions to the Schrödinger equation is in the handling of the momentum-space singularity, which the Coulomb potential possesses. Landé [12] has suggested a technique for removing this singularity, which has become known as the Landé subtraction method. This procedure has been used by Landau [2,3] and Kwon and Tabakin [4] in their studies of hadronic atoms. It has also been used in Refs. [13,14]. In these works the Landé subtraction method was only tested numerically for a few low-energy eigenvalues and with low accuracy.

The aim of the present work is to test the Landé subtraction method by calculating a wide variety of eigenvalues and wave functions. The accuracy of these results will show that the Landé method can be used very confidently for almost any physical system that one wishes to study. We will show that the Landé subtraction method is capable of yielding of the order of 50 eigenvalues for any angular momentum and is also capable of yielding very good wave functions. This means that the method should be very suitable for the study of Rydberg atoms. We will also show that the method enables low-energy eigenvalues to be calculated with great accuracy. This particular aspect of the Landé method has not been investigated before. Being able to do this is very significant, because it means that fine-structure effects can be investigated with momentum-space techniques. For instance, it is known that relativistic kinematic corrections are of the order 10^{-4} smaller than a first-order calculation of the energy [15]. One needs to be able to calculate at least to this accuracy if relativistic effects are to be explored.

As mentioned above, the Coulomb potential often appears in combination with other potentials. If these other potentials *also* possess momentum-space singularities, then one may not be able to implement the Landé method because the integrals must be performed explicitly. (For a detailed discussion of this point, see Ref. [10].) We present a technique that gets around this problem by expanding the wave function in a certain set of known basis functions. Again we will show that this method can be used confidently for a more restricted range of studies.

II. LANDÉ SUBTRACTION METHOD

The Landé subtraction method is described in Refs. [1–4,10,13,14], to which the reader is referred to for full details. We shall follow the method outlined in Ref. [10], which provides the clearest discussion of the singularity structure for arbitrary partial waves, and we shall write down some of the equations here for completeness. We write the Coulomb potential in configuration space as

$$V(r)=\lambda \lim_{\eta\to 0}\frac{e^{-\eta r}}{r} . \tag{1}$$

This form is important in developing the Landé subtraction method. The momentum-space Schrödinger equation for the lth partial wave is

$$\frac{p^2}{2\mu}\varphi_l(p)+\int_0^\infty p'^2dp'V_l(p,p')\varphi_l(p')=E\varphi_l(p) , \tag{2}$$

where, for the Coulomb potential,

$$V_l(p,p')=\frac{\lambda}{\pi}\lim_{\eta\to 0}\frac{Q_l(y)}{pp'} , \tag{3}$$

with $p=|\mathbf{p}|$ and $y\equiv(\eta^2+p^2+p'^2)/2pp'$ and $Q_l(y)$ being the special Legendre functions of the second kind. The singularity structure for arbitrary partial waves is most easily seen by writing [10]

$$Q_l(y)=P_l(y)Q_0(y)-w_{l-1}(y) , \tag{4}$$

where

$$w_{l-1}(y)=\sum_{m=1}^{l}\frac{1}{m}P_{l-m}(y)P_{m-1}(y) . \tag{5}$$

$Q_0(y)$ is singular at $p'=p$. Substituting the Coulomb potential into the Schrödinger equation (2), we obtain

$$\frac{p^2}{2\mu}\varphi_l(p)+\frac{\lambda}{\pi p}\int_0^\infty p'^2dp'P_l(y)\frac{Q_0(y)}{p'}\varphi_l(p')$$
$$-\frac{\lambda}{\pi p}\int_0^\infty p'dp'w_{l-1}(y)\varphi_l(p')=E\varphi_l(p) . \tag{6}$$

Only the first integral possesses a singularity. The essence of the Landé subtraction method is to make use of the relation

$$\int_0^\infty dp'\frac{Q_0(y,\eta=0)}{p'}=\frac{\pi^2}{2} . \tag{7}$$

This result is then added and subtracted from Eq. (6) to obtain a singularity free equation [10],

$$\frac{p^2}{2\mu}\varphi_l(p)+\frac{\lambda}{\pi p}\left[\frac{\pi^2}{2}p^2\varphi_l(p)\right]+\frac{\lambda}{\pi p}\int_0^\infty dp'P_l(y)\frac{Q_0(y)}{p'}\left[p'^2\varphi_l(p')-\frac{p^2\varphi_l(p)}{P_l(y)}\right]-\frac{\lambda}{\pi p}\int_0^\infty p'dp'w_{l-1}(y)\varphi_l(p')=E\varphi_l(p) . \tag{8}$$

Note that now when $p'=p$ the integrand of the first integral is zero, so that the whole equation can now be cast into discretized form and solved with standard matrix techniques [1,4,10].

The new feature of the present work is the precise calculation of a very large number of eigenvalues and wave functions. Eigenvalues calculated from Eq. (8) are presented in Tables I and II together with a comparison to the exact results. Results in Table I have been given in atomic units ($\hbar=e=m=c=1$). One can see that the Landé subtraction method yields a large number of correct eigenvalues, and that the lowest ones are reproduced extremely accurately. Some of the calculated eigenfunctions are presented in Figs. 1 and 2 and compared to the exact results as discussed by Bethe and Salpeter [11]. (Our normalization is the same as theirs.)

The significance of the present work is that the extensive results presented in Tables I and II and Figs. 1 and 2 show that the Landé subtraction method yields outstanding results for energies and wave functions. As mentioned above, the fact that the energy levels can be calculated so accurately means that the Landé method can be used to investigate fine-structure effects. In addition, our demonstration that about 50 eigenvalues can be accurately calculated means that the method should be suitable for studying Rydberg atoms.

II. LANDÉ SUBTRACTION METHOD WITH BASIS-FUNCTION EXPANSION

In many physical applications, one often uses the Coulomb potential with another potential added on [2–4,9,10]. Sometimes this potential may have a singularity structure that prohibits the use of the method described above. Specifically, one may be forced to evaluate the integrals in Eq. (8) explicitly because of additional singular terms appearing in the integrands due to other potentials. This situation occurs for the Cornell potential in momentum space [10]. However, one cannot evaluate the integrals explicitly without first knowing the wave functions, which is what we wish to solve for. The way around this is to expand the wave function in a suitable set of basis functions [16], as in

$$\varphi(p)=\sum_{i}^{M} C_i g_i(p) \ . \tag{9}$$

Then instead of solving for the wave functions, one solves for the expansion coefficients. More details (but no results) can be found in Ref. [10]. Clearly, the accuracy of this technique depends very much on the choice of the expansion functions $g_i(p)$. Obviously, one will be inclined to choose functions suitable to the physical prob-

TABLE I. Energy eigenvalues (in 10^{-3} a.u.). A negative sign before the energy has been omitted everywhere. Reduced mass is equal to 1 a.u. 1700 integration points were used to generate numerical eigenvalues.

		Numerical		
n	Exact	$l=0$	$l=1$	$l=2$
1	500.000 000 0	500.000 000 3		
2	125.000 000 0	125.000 000 6	125.000 000 2	
3	55.555 555 56	55.555 557	55.555 556	55.555 554
4	31.250 000 00	31.250 002	31.250 002	31.250 006
5	20.000 000 00	20.000 004	20.000 003	20.000 002
6	13.888 888 89	13.888 89	13.888 89	13.888 89
7	10.204 081 63	10.204 09	10.204 09	10.204 09
8	7.812 500 000	7.812 51	7.812 51	7.812 51
9	6.172 839 506	6.172 86	6.172 86	6.172 85
10	5.000 000 000	5.000 02	5.000 02	5.000 02
11	4.132 231 405	4.132 26	4.132 26	4.132 26
12	3.472 222 222	3.472 26	3.472 26	3.472 25
13	2.958 579 882	2.958 62	2.958 62	2.958 62
14	2.551 020 408	2.551 07	2.551 07	2.551 07
15	2.222 222 222	2.222 29	2.222 28	2.222 28
16	1.953 131 250	1.953 19	1.953 19	1.953 19
17	1.730 103 806	1.730 19	1.730 19	1.730 19
18	1.543 209 877	1.543 3	1.543 3	1.543 3
19	1.385 041 551	1.385 2	1.385 2	1.385 2
20	1.250 000 000	1.250 1	1.250 1	1.250 1
21	1.133 786 848	1.133 9	1.133 9	1.133 9
22	1.033 057 851	1.033 2	1.033 2	1.033 2
23	0.945 179 584 1	0.945 4	0.945 4	0.945 4
24	0.868 055 555 6	0.868 3	0.868 3	0.868 3
25	0.800 000 000 0	0.800 2	0.800 2	0.800 2
26	0.739 644 970 4	0.739 8	0.739 9	0.739 9
27	0.685 871 056 2	0.686 1	0.686 1	0.686 1
28	0.637 755 102 0	0.638 1	0.638 1	0.638 1
29	0.594 530 321 0	0.594 9	0.594 9	0.594 9
30	0.555 555 555 6	0.555 9	0.555 9	0.555 9
31	0.520 291 363 2	0.520 7	0.520 7	0.520 7
32	0.488 281 250 0	0.488 7	0.488 7	0.488 7
33	0.459 136 822 8	0.459 6	0.459 6	0.459 6
34	0.432 525 951 6	0.433 0	0.433 0	0.433 0
35	0.408 163 265 3	0.408 7	0.408 7	0.408 7
36	0.385 802 469 1	0.386 4	0.386 4	0.386 4
37	0.365 230 095 0	0.365 8	0.365 8	0.365 8
38	0.346 260 387 8	0.346 9	0.346 9	0.346 9
39	0.328 731 098 0	0.329 4	0.329 4	0.329 4
40	0.312 500 000 0	0.313 2	0.313 2	0.313 2
41	0.297 441 998 8	0.298	0.298	0.298
42	0.283 446 712 0	0.284	0.284	0.284
43	0.270 416 441 3	0.271	0.271	0.271
44	0.258 264 462 8	0.259	0.259	0.259
45	0.246 913 580 2	0.248	0.248	0.248
46	0.236 294 896 0	0.237	0.237	0.237
47	0.226 346 763 2	0.227	0.227	0.227
48	0.217 013 888 9	0.218	0.218	0.218
49	0.208 246 563 9	0.209	0.209	0.209
50	0.200 000 000 0	0.201	0.201	0.201

TABLE II. Energy eigenvalues (in electron volts) for a spinless electron in an external Coulomb potential (hydrogen atom problem). A negative sign before the energy has been omitted everywhere. 1700 integration points were used to generate numerical eigenvalues.

		Numerical		
n	Exact	$l=0$	$l=1$	$l=2$
1	13.605 697 95	13.605 697 99		
2	3.401 424 489	3.401 424 50	3.401 424 49	
3	1.511 744 217	1.511 744 23	1.511 744 23	1.511 744 22
4	0.850 356 122 2	0.850 356 14	0.850 356 13	0.850 356 13
5	0.544 227 918 2	0.544 227 94	0.544 227 94	0.544 227 93
6	0.377 936 054 3	0.377 936 08	0.377 936 08	0.377 936 07
7	0.277 667 305 2	0.277 667 35	0.277 667 34	0.277 667 33
8	0.212 589 030 5	0.212 589 08	0.212 589 08	0.212 589 07
9	0.167 971 579 7	0.167 971 65	0.167 971 64	0.167 971 63
10	0.136 056 979 5	0.136 057 1	0.136 057 1	0.136 057 1
11	0.112 443 784 8	0.112 443 9	0.112 443 9	0.112 443 9
12	0.094 484 013 6	0.094 484 2	0.094 484 1	0.094 484 1
13	0.080 507 088 5	0.080 507 3	0.080 507 2	0.080 507 2
14	0.069 416 826 3	0.069 417 0	0.069 417 0	0.069 417 0
15	0.060 469 768 7	0.060 470 0	0.060 470 0	0.060 470 0
16	0.053 147 257 6	0.053 147 5	0.053 147 5	0.053 147 5
17	0.047 078 539 6	0.047 078 9	0.047 078 8	0.047 078 8
18	0.041 992 894 9	0.041 993 3	0.041 993 3	0.041 993 2
19	0.037 688 914 0	0.037 689 3	0.037 689 3	0.037 689 3
20	0.034 014 244 9	0.034 014 7	0.034 014 7	0.034 014 7
21	0.030 851 922 8	0.030 852 5	0.030 852 4	0.030 852 4
22	0.028 110 946 2	0.028 111 5	0.028 111 5	0.028 111 5
23	0.025 719 655 9	0.025 720 3	0.025 720 3	0.025 720 3
24	0.023 621 003 4	0.023 621 7	0.023 621 7	0.023 621 7
25	0.021 769 116 7	0.021 769 9	0.021 769 9	0.021 769 9
26	0.020 126 772 1	0.020 127 7	0.020 127 7	0.020 127 7
27	0.018 663 508 9	0.018 664 5	0.018 664 5	0.018 664 5
28	0.017 354 206 6	0.017 355	0.017 355	0.017 355
29	0.016 178 000 0	0.016 179	0.016 179	0.016 179
30	0.015 117 442 2	0.015 119	0.015 119	0.015 119
31	0.014 157 854 3	0.014 159	0.014 159	0.014 159
32	0.013 286 814 4	0.013 288	0.013 288	0.013 288
33	0.012 493 753 9	0.012 495	0.012 495	0.012 495
34	0.011 769 634 9	0.011 771	0.011 771	0.011 771
35	0.011 106 692 2	0.011 109	0.011 109	0.011 109
36	0.010 498 223 7	0.010 500	0.010 500	0.010 500
37	0.009 938 420 7	0.009 941	0.009 941	0.009 941
38	0.009 422 228 5	0.009 425	0.009 425	0.009 425
39	0.008 945 232 1	0.008 948	0.008 948	0.008 948
40	0.008 503 561 2	0.008 506	0.008 506	0.008 506
41	0.008 093 812 0	0.008 097	0.008 097	0.008 097
42	0.007 712 980 7	0.007 716	0.007 716	0.007 716
43	0.007 358 408 8	0.007 362	0.007 362	0.007 362
44	0.007 027 736 5	0.007 031	0.007 031	0.007 031
45	0.006 718 863 2	0.006 723	0.006 723	0.006 722
46	0.006 429 914 0	0.006 434	0.006 434	0.006 434
47	0.006 159 211 4	0.006 163	0.006 163	0.006 163
48	0.006 905 250 8	0.005 910	0.005 910	0.005 910
49	0.005 666 679 7	0.005 671	0.005 671	0.005 671
50	0.005 442 279 2	0.005 447	0.005 447	0.005 447

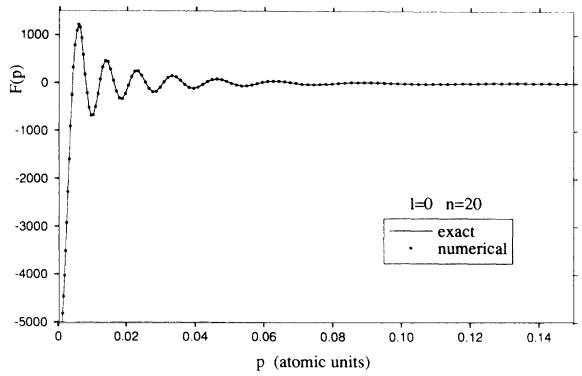

FIG. 1. Exact vs numerical radial wave function in momentum space for $l=0$ and $n=20$. Exact wave functions and normalizations are taken from Ref. [11]. All quantities are in atomic units. Reduced mass is equal to 1 a.u. 600 integration points were used to generate numerical wave functions.

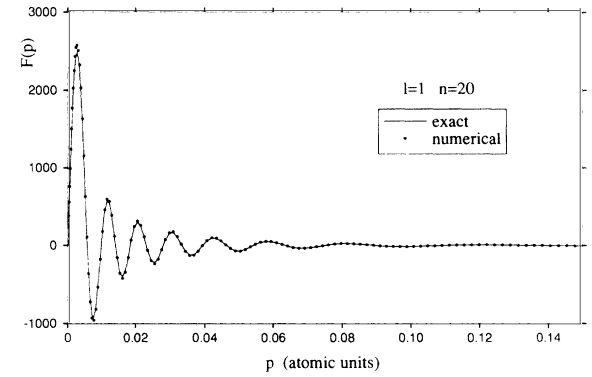

FIG. 2. Same as Fig. 1 except $l=1$.

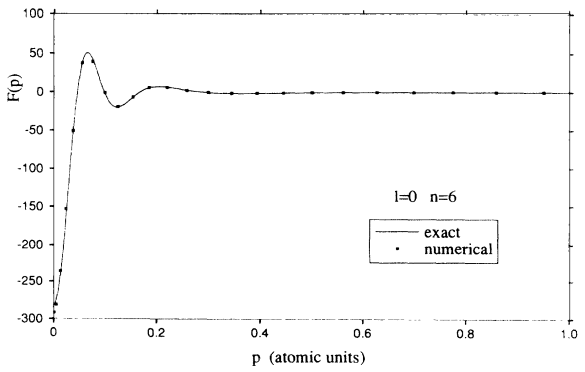

FIG. 3. Exact vs numerical radial wave function in momentum space for $l=0$ and $n=6$. Exact wave functions and normalizations are taken from Ref. [11]. All quantities are in atomic units. Numerical wave functions are calculated using a set of basis functions as explained in the text. Reduced mass is equal to 1 a.u. 14 basis functions and 48 integration points were used to generate numerical wave functions.

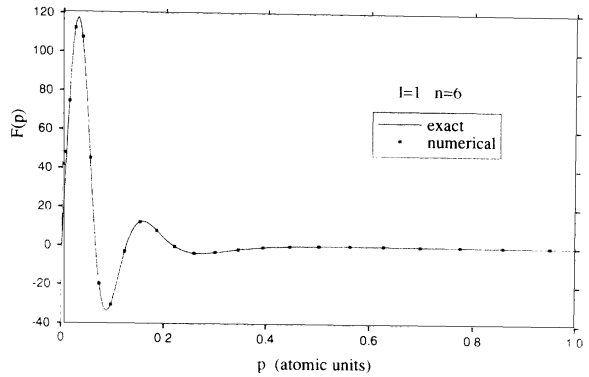

FIG. 4. Same as Fig. 3 except $l=1$.

lem being studied. Thus what is presented here is only intended to illustrate the technique and to show what accuracy one might expect.

Choosing

$$g_i(p)=\frac{1}{[(ip)^2+1]^2}\ , \tag{10}$$

we proceed to solve the corresponding matrix equations for the eigenvalues and expansion coefficients as discussed in Refs. [8,10].

The results are shown in Table III and Figs. 3 and 4. Even though the results obtained are not as extensive as those obtained without basis functions, nevertheless those eigenvalues and wave functions which are able to be calculated are seen to be very reliable. Clearly one can optimize the results by much more careful choice of the basis functions. We choose not to explore this more extensively here because the choice will more likely depend on the other potentials that one is considering. Our major point is that if other potentials force one to evaluate the integrals explicitly, the Landé subtraction method can still be used very usefully in the above modified form.

To illustrate this point for a specific potential, we consider the Cornell potential [9]:

TABLE III. Energy eigenvalues (in 10^{-3} a.u.). A negative sign before the energy has been omitted everywhere. Reduced mass is equal to 1 a.u. Numerical eigenvalues were calculated using a set of 12 basis functions and 48 integration points as explained in the text.

		Numerical		
n	Exact	$l=0$	$l=1$	$l=2$
1	500.000 000 0	499.999		
2	125.000 000 0	124.997	124.996	
3	55.555 555 56	55.553	55.552	55.556
4	31.250 000 00	31.247	31.246	31.249
5	20.000 000 00	19.996	19.995	19.997
6	13.888 888 89	13.884	13.882	13.885
7	10.204 081 63	10.197	10.189	10.199
8	7.812 500 000	7.79	7.78	7.80
9	6.172 839 506	5.7	5.8	5.9

TABLE IV. Energy eigenvalues (in GeV) for the Cornell potential for $l=0$. Numerical eigenvalues (momentum space) were calculated using a set of 18 basis functions and 80 integration points as explained in the text. The basis function used was $g_i(p)=1/[(i^2/M)^2+p^4]$. Parameters were $m_1=m_2=1.5$ GeV, $k=0.18$ GeV^2, and $\lambda=-0.3$.

n	Numerical (coordinate space)	Numerical (momentum space)
1	0.4756	0.4757
2	1.0215	1.0216
3	1.4433	1.4444
4	1.8094	1.8119
5	2.1408	2.1459
6	2.4477	2.4582
7	2.7362	2.7524
8	3.0100	3.0359
9	3.2717	3.4247

$$V(r)=kr+\frac{\lambda}{r} . \tag{11}$$

The momentum-space solution of the Schrödinger equation with the linear part of this potential has been discussed in Refs. [8,10]. Using our basis-function expansion technique, we compare the momentum-space results for the energy eigenvalues to the results obtained with a coordinate space numerical solution in Table IV. One can see that the technique works well for this particular case.

IV. SUMMARY AND CONCLUSIONS

Using the Landé subtraction method for the Coulomb potential in momentum space, numerical solutions for eigenvalues and eigenfunctions were presented and compared to exact results. Many eigenvalues and eigenfunctions were able to be found very accurately. In addition, it was shown how to implement the Landé subtraction method in those cases where the momentum integrals must be evaluated explicitly. The technique used was to expand the wave function in terms of a known set of basis functions. Very good numerical results were also obtained with this method, although the results were not nearly as extensive as those obtained without basis functions.

In summary, we have very thoroughly tested the Landé subtraction method numerically and found the results to be excellent. This yields confidence that the method can be arbitrarily applied to momentum-space solutions of problems that involve the Coulomb potential and some other potential. This is true even if the other potential has singularities of higher order than the Coulomb singularity, which requires modification of the Landé technique using the basis-function expansion technique.

One of the most significant results of the present work is the demonstration that eigenvalues can be calculated with very high accuracy using the Landé method. This means that the method will be very useful in the investigation of fine-structure effects and other small corrections to the energy levels. In addition, being able to calculate as many as 50 eigenvalues means that the method should be quite suitable for the study of Rydberg atoms.

ACKNOWLEDGMENTS

We wish to thank Franz Gross for suggesting the basis-function expansion technique. We would also like to thank Peter Tandy for arranging a week-long meeting of our collaboration at Kent State University. J.W.N. would also like to thank Warren Buck for arranging a visit to Hampton University. K.M.M. was supported by NSF Grant No. HRD-9154080.

[1] R. H. Landau, *Quantum Mechanics II; A Second Course in Quantum Theory* (Wiley, New York, 1990).
[2] R. H. Landau, Phys. Rev. C **27**, 2191 (1983).
[3] R. H. Landau, Phys. Rev. C **28**, 1324 (1983).
[4] Y. R. Kwon and F. Tabakin, Phys. Rev. C **18**, 932 (1978).
[5] W. Buck and F. Gross, Phys. Rev. D **20**, 2361 (1979).
[6] F. Gross, *Relativistic Quantum Mechanics and Field Theory* (Wiley, New York, 1993).
[7] C. Stubbins, Phys. Rev. A **48**, 220 (1993).
[8] J. W. Norbury, D. E. Kahana, and K. Maung Maung, Can. J. Phys. **70**, 86 (1992).
[9] E. Eichten, K. Gottfried, T. Kinoshita, K. D. Lane, and T. M. Yan, Phys. Rev. D **17**, 3090 (1978).
[10] K. Maung Maung, D. E. Kahana, and J. W. Norbury, Phys. Rev. D **47**, 1182 (1993).
[11] H. A. Bethe and E. E. Salpeter, *Quantum Mechanics of One and Two Electron Atoms* (Plenum, New York, 1977).
[12] A. Landé, as quoted in Ref. [4] above.
[13] G. Hardekopf and J. Sucher, Phys. Rev. A **30**, 703 (1984).
[14] W. Dykshoorn, R. Koniuk, and R. Munoz-Tapia, Phys. Rev. A **41**, 60 (1990).
[15] D. Griffiths, *Introduction to Elementary Particles* (Wiley, New York, 1987).
[16] F. Gross (private communication).