

0 0 - 0 4 3 3 4 3 1 0

Presented at the 4th International Conference  
on Beam-Foil Spectroscopy and Heavy-Ion  
Atomic Physics Symposium, Gatlinburg, TN,  
September 15 - 19, 1975

LBL-3876  
c1

LAMB SHIFT IN HYDROGENLIKE IONS

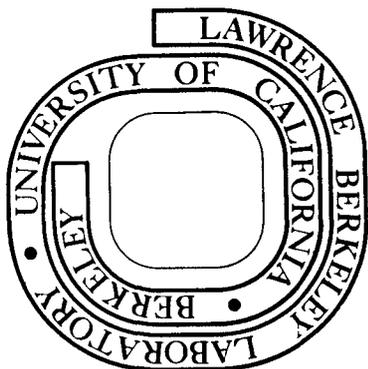
Peter J. Mohr

November 11, 1975

Prepared for the U. S. Energy Research and  
Development Administration under Contract W-7405-ENG-48

**For Reference**

Not to be taken from this room



LBL-3876  
c1

## **DISCLAIMER**

This document was prepared as an account of work sponsored by the United States Government. While this document is believed to contain correct information, neither the United States Government nor any agency thereof, nor the Regents of the University of California, nor any of their employees, makes any warranty, express or implied, or assumes any legal responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by its trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof, or the Regents of the University of California. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof or the Regents of the University of California.

## LAMB SHIFT IN HYDROGENLIKE IONS\*

Peter J. Mohr

Department of Physics and Lawrence Berkeley Laboratory

University of California, Berkeley, California 94720

## I. INTRODUCTION

Recent progress in the measurement of the Lamb shift  $S = E(2S_{1/2}) - E(2P_{1/2})$  in hydrogenic atoms and ions has been made in two directions. An experimental value with a substantial increase in precision over previous values has been obtained for atomic hydrogen,<sup>1</sup> and experimental values have been obtained for many higher-Z hydrogenic ions.<sup>2,3</sup> Quantum electrodynamics makes unambiguous predictions for the Lamb shift in these systems, so that a comparison between the theoretical and experimental values provides an important test of the theory. To aid in such a comparison, we compile here theoretical values for the various contributions to the Lamb shift for Z in the range 1 - 30. Compilations for small Z are given elsewhere,<sup>4-7</sup> but we include here some additional corrections which are significant at higher Z.

## II. SELF ENERGY

Recently, the self-energy radiative correction of order  $\alpha$  has been evaluated numerically to all orders in  $Z\alpha$  for the  $2S_{1/2}$  and  $2P_{1/2}$  states for  $Z = 10, 20, 30, \dots, 110$ .<sup>7</sup> The method of evaluation is based on the expansion of the bound electron propagation function in terms of the known Coulomb radial Green's functions.<sup>8</sup> In order to display the results for the self-energy contribution to the Lamb shift  $S_{SE} = \Delta E(2S_{1/2}) - \Delta E(2P_{1/2})$ , it is convenient to isolate the known low-order terms by writing<sup>6,7</sup>

TABLE I. Calculated Values of  $G_{SE}(Z\alpha)$ 

Z	$G_{SE}(Z\alpha)$
10	- 20.13(34)
20	- 17.674(28)
30	- 15.776(11)
40	- 14.1376(62)
50	- 12.6650(28)

$$S_{SE} = \frac{\alpha}{\pi} \frac{(Z\alpha)^4}{6} mc^2 \left[ \ln(Z\alpha)^{-2} - \ln \frac{K_0(2,0)}{K_0(2,1)} + \frac{11}{24} + \frac{1}{2} \right. \\ \left. + 3\pi \left( 1 + \frac{11}{128} - \frac{1}{2} \ln 2 \right) (Z\alpha) - \frac{3}{4} (Z\alpha)^2 \ln^2(Z\alpha)^{-2} \right. \\ \left. + \left( \frac{299}{240} + 4 \ln 2 \right) (Z\alpha)^2 \ln(Z\alpha)^{-2} + (Z\alpha)^2 G_{SE}(Z\alpha) \right]. \quad (1)$$

Values of the remainder  $G_{SE}(Z\alpha)$ , corresponding to the calculated values of  $S_{SE}$ , for  $Z$  in the range 10 - 50 appear in Table I. To obtain values for  $G_{SE}(Z\alpha)$  for all  $Z$  in the range 1 - 30, we fit the interpolation function

$$a + b (Z\alpha) \ln(Z\alpha)^{-2} + c (Z\alpha) \quad (2)$$

to the calculated values of  $G_{SE}(Z\alpha)$  at  $Z = 10, 20, \text{ and } 30$ .<sup>7</sup> The corresponding interpolated values of  $G_{SE}(Z\alpha)$  appear in Table II. The numbers in parentheses with each entry in the table are error estimates which take into account the uncertainty in the calculated values of  $G_{SE}(Z\alpha)$  and the uncertainty associated with the interpolation procedure.

### III. VACUUM POLARIZATION

Evaluation of the energy level shift associated with the vacuum polarization of order  $\alpha$  is facilitated by considering the expansion of the vacuum polarization potential in powers of the external Coulomb potential. Only odd powers of the external potential contribute as a consequence of Furry's theorem.<sup>9</sup>

The first term in the expansion gives rise to the modification of the external potential known as the Uehling potential<sup>10,11</sup>

$$U(r) = - \frac{\alpha}{\pi} \frac{Z\alpha}{r} \hbar c \int_1^\infty dt (t^2 - 1)^{1/2} \left( \frac{2}{3t^2} + \frac{1}{3t^4} \right) \exp(-2tr/\lambda). \quad (3)$$

The corresponding contribution to the Lamb shift is

$$\langle U \rangle_{2S_{1/2}} - \langle U \rangle_{2P_{1/2}} = \frac{\alpha}{\pi} \frac{(Z\alpha)^4}{6} mc^2 \left[ -\frac{1}{5} + \frac{5}{64} \pi(Z\alpha) - \frac{1}{10} (Z\alpha)^2 \ln(Z\alpha)^{-2} + (Z\alpha)^2 G_U(Z\alpha) \right]. \quad (4)$$

The first three terms in the square brackets in (4) give the known contribution of the Uehling potential for small  $Z\alpha$ .<sup>6</sup> We have numerically evaluated the expectation values of  $U(r)$  which appear in (4). The results are given in Table II in terms of the function  $G_U(Z\alpha)$  which is defined by (4).

The second non-vanishing term in the expansion is third order in the external potential. Wichmann and Kroll have examined the vacuum polarization in detail and have obtained results from which one readily finds that the third order term contributes<sup>12</sup>

$$\frac{\alpha}{\pi} \frac{(Z\alpha)^6}{6} mc^2 \left[ \frac{19}{60} - \frac{\pi^2}{36} + \left( \frac{3}{64} - \frac{31\pi^2}{3840} \right) \pi(Z\alpha) + \dots \right] \quad (5)$$

to the Lamb shift. The terms omitted from (5) are higher order in  $Z\alpha$ .

The total vacuum polarization contribution to the Lamb shift is thus given by

$$S_{VP} = \frac{\alpha}{\pi} \frac{(Z\alpha)^4}{6} mc^2 \left[ -\frac{1}{5} + \frac{5}{64} \pi(Z\alpha) - \frac{1}{10} (Z\alpha)^2 \ln(Z\alpha)^{-2} + (Z\alpha)^2 G_{VP}(Z\alpha) \right] \quad (6)$$

where

$$G_{VP}(Z\alpha) = G_U(Z\alpha) + .0425 - .1030(Z\alpha) \pm .1(Z\alpha). \quad (7)$$

The last term in (7) is an approximation for the uncertainty due to higher order omitted terms.

#### IV. FOURTH ORDER

The contribution to the Lamb shift from the fourth order radiative corrections is known exactly to lowest order in  $Z\alpha$ . It is given by

$$S_{FO} = \left( \frac{\alpha}{\pi} \right)^2 \frac{(Z\alpha)^4}{6} mc^2 \left[ \pi^2 \ln 2 - \frac{37\pi^2}{144} - \frac{3767}{1728} - \frac{3}{2} \zeta(3) \pm \pi(Z\alpha) \right]. \quad (8)$$

Recent work on the evaluation of this term is discussed in Ref. 6. The last term in (8) is an approximation for the uncertainty due to higher order uncalculated terms.

## V. REDUCED MASS AND RELATIVISTIC RECOIL

The lowest order reduced mass and relativistic recoil contributions to the Lamb shift are given by<sup>6</sup>

$$S_{RM} = \frac{\alpha}{\pi} \frac{(Z\alpha)^4}{6} mc^2 \left( -\frac{3m}{M} \right) \left[ \ln(Z\alpha)^{-2} - \ln \frac{K_0(2,0)}{K_0(2,1)} + \frac{23}{60} \right] \quad (9)$$

and

$$S_{RR} = \frac{\alpha}{\pi} \frac{(Z\alpha)^4}{6} mc^2 \left( \frac{Zm}{M} \right) \left[ \frac{1}{4} \ln(Z\alpha)^{-2} - 2 \ln \frac{K_0(2,0)}{K_0(2,1)} + \frac{97}{12} \right] \quad (10)$$

where  $M$  is the nuclear mass. We employ the uncertainty estimate of Erickson<sup>5</sup> for these terms for  $Z = 1$  and the  $Z$ -dependent estimate of Erickson and Yennie<sup>13</sup>

$$\Delta S = \frac{m}{M} (Z\alpha)^6 mc^2 \quad (11)$$

for  $Z > 1$ . We also include Salpeter's estimate of  $0.1 \times S_{RR}$  for the uncertainty due to uncalculated nuclear structure effects in deuterium.<sup>14</sup>

## VI. NUCLEAR SIZE

The potential for an electron in a hydrogenlike ion is not a pure Coulomb potential due, in part, to the fact that the nuclear charge is distributed over a finite radius. We evaluate the energy shift due to the difference between the finite size potential and the Coulomb potential  $\delta V(r)$  in first order perturbation theory with Dirac wavefunctions. Assuming that the nuclear charge is distributed uniformly inside a sphere, we obtain

$$S_{NS} = \left[ 1 + 1.70(Z\alpha)^2 \right] \frac{(Z\alpha)^2}{12} mc^2 \left( \frac{Z\alpha R}{\chi} \right)^{2s} \quad (12)$$

for the nuclear size contribution to the Lamb shift. In Eq. (12)  $s = \sqrt{1 - (Z\alpha)^2}$  and  $R$  is the r.m.s. charge radius of the nucleus. The expression in (12) neglects terms of relative order  $(Z\alpha)^4$  or  $Z\alpha R/\chi$ . This nuclear size correction  $S_{NS}$  agrees to lowest order in  $(Z\alpha)^2$  with the nonrelativistic expression in Ref. 13.

It is known that first order perturbation theory gives inaccurate results for the finite size correction when  $Z$  is large.<sup>15,16</sup> We find that the fractional difference between the perturbation result and the result obtained by numerically solving the Dirac equation for a finite nucleus is approximately 3% at  $Z = 30$ . We therefore assign an uncertainty  $\Delta S_{NS}$  to Eq. (12), where

$$\Delta S_{NS} = \left( 0.7(Z\alpha)^2 + 2 \frac{\Delta R}{R} \right) S_{NS} \quad (13)$$

TABLE II. Values for the functions  $G_{SE}(Z\alpha)$ ,  $G_U(Z\alpha)$ , assumed values for the nuclear charge radii, and Lamb shift values

Z	A	$G_{SE}(Z\alpha)$	$G_U(Z\alpha)$	R[fm]	LAMB SHIFT[GHz]
1	1	-23.4(1.2)	-0.5587	.81(2)	1.057867(13)
1	2	"	"	2.10(2)	1.059241(27)
2	4	-22.9(1.0)	-0.5493	1.644(5)	14.04205(55)
3	6	-22.49(88)	-0.5411	2.56(5)	62.7375(66)
4	9	-22.10(77)	-0.5339	2.52(2)	179.791(25)
5	11	-21.72(68)	-0.5273	2.4(1)	404.57(10)
6	12	-21.37(60)	-0.5213	2.45(1)	781.99(21)
7	14	-21.04(52)	-0.5157	2.54(2)	1361.37(47)
8	16	-20.72(45)	-0.5106	2.72(3)	2196.21(92)
9	19	-20.42(39)	-0.5059	2.90(2)	3343.1(1.6)
10	20	-20.13(34)	-0.5015	3.02(4)	4861.1(2.7)
11	23	-19.85(29)	-0.4974	2.94(4)	6809.0(4.0)
12	24	-19.58(24)	-0.4936	3.01(3)	9256.0(5.8)
13	27	-19.31(20)	-0.4900	3.03(3)	12,264.7(8.0)
14	28	-19.06(17)	-0.4867	3.09(2)	15,907(11)
15	31	-18.81(14)	-0.4836	3.19(2)	20,254(13)
16	32	-18.57(11)	-0.4807	3.24(2)	25,373(17)
17	35	-18.338(84)	-0.4781	3.34(3)	31,347(20)
18	40	-18.111(63)	-0.4756	3.45(5)	38,250(25)
19	39	-17.890(44)	-0.4733	3.41(3)	46,133(29)
20	40	-17.674(38)	-0.4711	3.48(3)	55,116(37)
21	45	-17.464(34)	-0.4691	3.54(8) <sup>a</sup>	65,259(55)
22	48	-17.259(31)	-0.4673	3.60(1)	76,651(56)
23	51	-17.059(28)	-0.4656	3.60(5)	89,345(78)
24	52	-16.863(26)	-0.4641	3.66(5)	103,482(98)
25	55	-16.672(24)	-0.4627	3.72(7)	$1.1912(13) \times 10^5$
26	56	-16.485(22)	-0.4614	3.73(6)	$1.3632(15) \times 10^5$
27	59	-16.302(21)	-0.4603	3.80(5)	$1.5525(18) \times 10^5$
28	58	-16.123(19)	-0.4593	3.78(3)	$1.7585(21) \times 10^5$
29	63	-15.948(18)	-0.4584	3.93(3)	$1.9854(26) \times 10^5$
30	64	-15.776(17)	-0.4576	3.95(4)	$2.2303(32) \times 10^5$

<sup>a</sup>Interpolated value

to allow for this error, for model dependence error, and for the measured charge radius uncertainty  $\Delta R$ .

Values we assume for the nuclear r.m.s. charge radii are given in Table II. Those numbers are representative values based on values in the compilations of nuclear charge radii deduced from electron scattering data,<sup>17</sup> and from muonic atom transition energies.<sup>18</sup>

### VII. LAMB SHIFT VALUES

The sum of the contributions listed in the preceding sections gives the total Lamb shift  $S$ . The values are listed in Table II. We employ the recently recommended values<sup>19</sup>  $R_{\infty}c = 3.28984200(25) \times 10^{15}$  Hz and  $\alpha^{-1} = 137.03604(11)$ . The uncertainty in  $\alpha$  produces a relative uncertainty of  $3\Delta\alpha/\alpha = 2.4 \times 10^{-6}$  in the total Lamb shift. The uncertainty listed with each Lamb shift value is the quadrature sum of the contributing uncertainties and is meant to be considered on a par with a one standard deviation uncertainty in the experimental value. The theoretical values listed here differ somewhat from the values compiled by Erickson.<sup>5,6</sup> The difference is due mainly to differences between the values used for the self-energy contribution.

Measured values for the  $n=2$  hydrogenic Lamb shifts are listed

TABLE III. Comparison between theory and direct measurement of the Lamb shift  $E(2S_{1/2}) - E(2P_{1/2})$

	THEORY ( $1\sigma$ )	EXPERIMENT ( $1\sigma$ )	REF.
H	1057.867(13) MHz	1057.893(20) MHz 1057.90(6) " 1057.77(6) "	1 20a 21a
D	1059.241(27) MHz	1059.24(6) MHz 1059.00(6) "	22a 21a
${}^4\text{He}^+$	14,042.05(55) MHz	14,046.2(1.2) MHz 14,040.2(1.8) "	23 24a
${}^6\text{Li}^{2+}$	62,737.5(6.6) MHz	62,765(21) MHz 62,880(190) " 63,031(327) "	25 26 27
${}^{12}\text{C}^{5+}$	781.99(21) GHz	780.1(8.0) GHz	28
${}^{16}\text{O}^{7+}$	2196.21(92) GHz	2215.6(7.5) GHz 2202.7(11.0) "	29 30

<sup>a</sup>See Reference 31 for a discussion of the experimental value.

in Table III. In addition to the measurements listed there, we note the recent work of Kugel et al. who have measured the separation  $E(2P_{3/2}) - E(2S_{1/2})$  in hydrogenlike fluorine.<sup>32</sup> They combine their result with the theoretical value of the fine structure splitting to obtain the Lamb shift value  $S = 3339(35)$  GHz.

## ACKNOWLEDGMENT

I wish to thank Professor Glen Erickson for a helpful discussion of the nuclear recoil uncertainty estimate.

## REFERENCES

\* Work supported by the Energy Research and Development Administration.

1. S. R. Lundeen and F. M. Pipkin, Phys. Rev. Letters 34, 1368 (1975).
2. M. Leventhal, Nucl. Instr. and Meth. 110, 343 (1973).
3. See Table III.
4. S. J. Brodsky and S. D. Drell, Ann. Rev. Nuc. Sci., 20, 147 (1970).
5. G. W. Erickson, Phys. Rev. Letters 27, 780 (1971).
6. B. E. Lautrup, A. Peterman, and E. de Rafael, Phys. Reports 3, 193 (1972). This paper gives complete references to the original work.
7. P. J. Mohr, Phys. Rev. Letters 34, 1050 (1975).
8. P. J. Mohr, Ann. Phys. (N.Y.) 88, 26,52 (1974).
9. W. H. Furry, Phys. Rev. 51, 125 (1937).
10. R. Serber, Phys. Rev. 48, 49 (1935).
11. E. A. Uehling, Phys. Rev. 48, 55 (1935).
12. E. H. Wichmann and N. M. Kroll, Phys. Rev. 101, 843 (1956).
13. G. W. Erickson and D. R. Yennie, Ann. Phys. (N.Y.) 35, 271, 447 (1965).
14. E. E. Salpeter, Phys. Rev. 87, 328 (1952).
15. E. K. Broch, Arch. Math. Naturvidenskab 48, 25 (1945).
16. K. W. Ford and D. L. Hill, Phys. Rev. 94, 1630 (1954).
17. R. Hofstadter and H. R. Collard in Nuclear Radii, Group I, Vol. 2 of the Landolt-Börnstein new series, H. Schopper, ed., (Springer-Verlag, Berlin, 1967), p. 21, and C. W. de Jager, H. de Vries, and C. de Vries, At. Data and Nuc. Data Tables, 14, 479 (1974).
18. R. Engfer, H. Schneuwly, J. L. Vuilleumier, H. K. Walter, and A. Zehnder, At. Data and Nuc. Data Tables, 14, 509 (1974). For He, see A. Bertin et al., Phys. Letters 55B, 411 (1975).
19. E. R. Cohen and B. N. Taylor, J. Phys. Chem. Ref. Data, 2, 663 (1973).

20. R. Robiscoe and T. Shyn, Phys. Rev. Letters 24, 559 (1970).
21. S. Triebwasser, E. S. Dayhoff and W. E. Lamb, Jr., Phys. Rev. 89, 98 (1953).
22. B. Cosens, Phys. Rev. 173, 49 (1968).
23. M. A. Narasimham and R. L. Strombotne, Phys. Rev. A 4, 14 (1971).
24. E. Lipworth and R. Novick, Phys. Rev. 108, 1434 (1957).
25. M. Leventhal, Phys. Rev. A 11, 427 (1975).
26. D. Dietrich, B. Dacosta, R. DeZafra, and H. Metcalf, Abstract submitted to the Fourth Int. Conf. on Atomic Phys. [Heidelberg] (1974).
27. C. Y. Fan, M. Garcia-Munoz, and I. A. Sellin, Phys. Rev. 161, 6 (1967).
28. H. W. Kugel, M. Leventhal, and D. E. Murnick, Phys. Rev. A 6, 1306 (1972).
29. G. P. Lawrence, C. Y. Fan, and S. Bashkin, Phys. Rev. Letters 28, 1612 (1972).
30. M. Leventhal, D. E. Murnick, and H. W. Kugel, Phys. Rev. Letters 28, 1609 (1972).
31. B. N. Taylor, W. H. Parker, D. N. Langenberg, Rev. Mod. Phys. 41, 375 (1969).
32. H. W. Kugel, M. Leventhal, D. E. Murnick, C. K. N. Patel, and O. R. Wood, II, Phys. Rev. Letters 35, 647 (1975).

**LEGAL NOTICE**

*This report was prepared as an account of work sponsored by the United States Government. Neither the United States nor the United States Energy Research and Development Administration, nor any of their employees, nor any of their contractors, subcontractors, or their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness or usefulness of any information, apparatus, product or process disclosed, or represents that its use would not infringe privately owned rights.*

TECHNICAL INFORMATION DIVISION  
LAWRENCE BERKELEY LABORATORY  
UNIVERSITY OF CALIFORNIA  
BERKELEY, CALIFORNIA 94720