Improved Lamb-Shift Calculation for All Values of Z†

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A previous covariant evaluation of the Lamb shift for small atomic numbers Z is extended to be valid for large Z and agrees with independent numerical evaluations for Z near 80. The results improve the precision tests of quantum electrodynamics and could be used for one-electron atoms with any Z, x rays at large Z, and superheavy elements with $Z\alpha > 1$. A substantially new value (due to deuteron size) is found for the deuterium Lamb shift: 1059.27 ± 0.03 MHz.

The usual calculations[1] of the $Z\alpha$ dependence of the Lamb shift are concerned with the reduction of the operators and wave functions to forms which yield successive coefficients in the expansion

$$\Delta E_n = \frac{4\alpha(Z\alpha)^4 mc^2}{3\pi n^3}[C_{41}\ln(Z\alpha)^{-2} + C_{40} + H(Z\alpha)], \tag{1}$$

where

$$(Z\alpha)^4 H(Z\alpha) = C_5(Z\alpha)^5 + C_{62}(Z\alpha)^6\ln^2(Z\alpha)^{-2} + C_{61}(Z\alpha)^6\ln(Z\alpha)^{-2} + C_{60}(Z\alpha)^6 + \cdots. \tag{1a}$$

However, the expansion seems to converge only for $Z\alpha < 1$ and is useful only for small Z since the uncalculated terms become of the order of magnitude of the calculated terms when $Z \gtrsim 10$. The approach used here avoids this truncation of an infinite expansion and yields a higher-order sum $H(Z\alpha)$ which is valid (approximately) for all $Z\alpha$ and agrees, by construction, with the small-$Z\alpha$ expansion (1a).

The calculation follows a covariant formulation and evaluation[1] of the one-photon self-energy expression corresponding to Fig. 1 which contains all the $Z\alpha$ dependence (but no other α or nuclear dependence). That formulation reduces the expression to obtain the lowest-order contributions (i.e., the coefficients C_{41} and C_{40}) plus higher-order remainders which were then further reduced[2] so as to obtain all terms contributing to the coefficients C_5, C_{62}, and C_{61}. The present calculation also considers all those terms, but no longer reduces them so far as to yield only successive coefficients. The total [in square brackets in Eq. (1)] is found to be a slowly decreasing function of $Z\alpha$ which vanishes for infinite $Z\alpha$ when nonrelativistic forms are used. Relativistic corrections yield only small contributions at small Z which are found to remain finite for $Z \leq 1$ (even for point nuclei) and to be smooth functions[3] for larger Z if finite nuclear size is included. We approximate these and the other smallest terms (including non-S-state contributions) by convenient functional forms which are correct for small $Z\alpha$, are finite for all $Z\alpha$, and vanish for infinite $Z\alpha$. The larger terms are treated exactly,[4] and the result is expected to be a good approximation for all $Z\alpha$, with an uncertainty (68% confidence level) taken to be of the order of $\pm 0.5(Z\alpha)^2$ for small $Z\alpha$ and ± 1 for large $Z\alpha$.

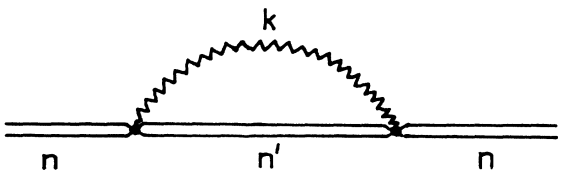

FIG. 1. Self-energy graph for an electron in the bound state $|n\rangle$. The double line for the electron denotes propagation in the Coulomb potential $V = -Z\alpha/r$.

Results.—Our calculation improves the small-$Z\alpha$ self-energy results by providing a better value for the coefficient $C_{60} = -19.3435 \pm 0.5$ (previously estimated in Ref. 2 as -19.08 ± 5) and another term in Eq. (1a), $+9.56\pi(Z\alpha)^7$, previously estimated to be $\pi^3(Z\alpha)^7$ but not included. This series is an accurate representation of the results for $Z \leq 10$, and those for $10 \leq Z \leq 100$ are shown in Fig. 2. (For $Z > 100$, the values continue smoothly through 0.88 ± 0.28 at $Z \simeq 137$ and 0.16 ± 0.88 at $Z = 1000$.) These are only for the $1S$ state, but the n dependence is only about the order of magnitude of the uncertainty for $Z > 10$. Results for all states are available and are included (with vacuum-polarization and higher-order corrections) in the values given later in Ta-

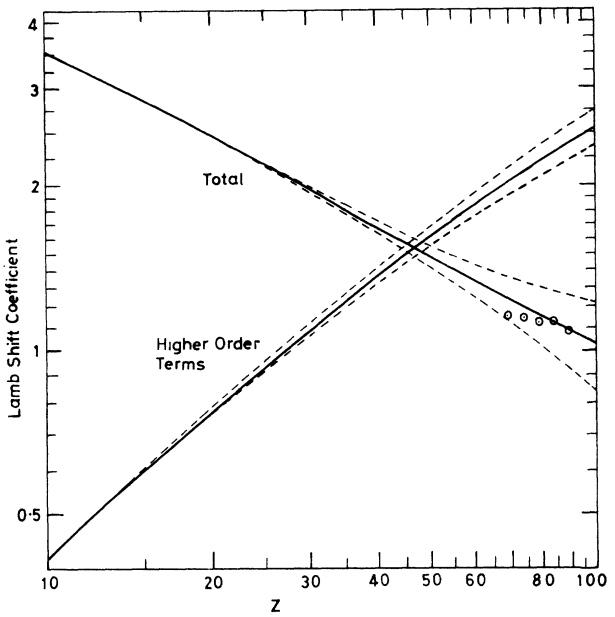

FIG. 2. S-state Lamb shift in units of $(4\alpha/3\pi)(Z\alpha)^4 \times mc^2/n^3$, neglecting terms of higher order in α, nuclear size, or recoil The dashed curves represent uncertainties at roughly the 68% confidence level. The points at $Z=70$, 75, 80, 85, and 90 are results of complete numerical calculations of Ref. 5. The higher-order coefficient is the function $H(Z\alpha)$ discussed in the text. The total coefficient is $H(Z\alpha)+\ln(Z\alpha)^{-2}$ plus the constants $B(n)+11/24$. The Bethe logarithm $B(n)$ and $H(Z\alpha)$ are slightly n dependent; the results here are for $n=1$.

ble I.

For $Z=70$, 75, 80, 85, and 90 we see that the results in Fig. 2 agree quite well with the numerical evaluation of Desiderio and Johnson[5] using a method developed for tightly bound electrons by Brown, Langer, and Schaeffer[6] (but not believed by them to be applicable to light atoms). In particular, our result of 15.6 ± 1.9 Ry for mercury ($Z=80$) confirms Desiderio and Johnson's 15.0 Ry, which disagrees with the much earlier result, 41 Ry, of Brown and Mayers.[7] The accuracy of the Brown-Langer-Schaeffer method is said to be hard to judge (although Desiderio and Johnson put a lower bound of 0.05% on the error in their numerical work), but we note that the K-electron binding energy in mercury calculated by Desiderio and Johnson agrees with experiment to within 3% of the self-energy. The reader is referred to that paper for accurate results for $70 \leq Z \leq 90$ and for a discussion of the relevant effects in many-electron atoms. We take their results as confirming the validity of our method and turn our attention to the higher-order effects and uncertainties in one-electron atoms. These effects (such as fourth-order terms adding only $0.4\alpha/\pi=0.0009$ to Fig. 2) are negligibly smaller than the $H(Z\alpha)$ uncertainties for large Z except for nuclear size effects at very large Z) and are needed for accurate results only at smaller Z.

Higher-order effects and uncertainties.—These have been changed somewhat from the forms given in I, but for brevity we will only note the important modifications and the uncertainties for the $2S_{1/2}$-$2P_{1/2}$ Lamb shift in hydrogen, for which the $H(Z\alpha)$ uncertainty yields ±0.005 MHz.

The fourth-order terms have been the cause of a discrepancy between theory and experiment only recently resolved by a detailed numerical calculation of Appelquist and Brodsky.[8] We use [for Eq. (4.5) in I] an exact coefficient which is the sum of recent results of Peterman[9] for the cross graph, of Barbieri, Mignacco, and Remiddi[10] for the corner graphs, and of Soto[11] (with an overall sign correction) for the other graphs, each of which is in agreement with the Appelquist-Brodsky calculations. The uncertainty due to the neglect of binding effects (of relative order $\pi Z\alpha$) and of sixth-order terms (of relative order α/π) is taken as ±0.006 MHz in H.

Reduced mass and other nuclear recoil effects are as in I, with an uncertainty now taken as ±0.003 MHz in H.

Nuclear size effects and uncertainties are essentially as in I, with the nuclear sizes now taken mostly from the compilation of Hofstadter and Collard,[12] yielding ±0.006 MHz due to proton size uncertainty. For deuterium, however, we use the recent measurements of Bumiller *et al.*[13] to deduce a radius of 2.08 ± 0.02 F which we note is smaller than the compiled value[12] of 2.17 ± 0.05 F but larger than that used in previous Lamb-shift calculations, 1.95 ± 0.07 F. This is found to change the calculated Lamb shift substantially, bringing it into close agreement with the latest measurement and into disagreement with the earlier measurement.

The uncertainties used here are smaller than those used in I. One reason is that we now have better knowledge of the quantities involved. In particular, $\alpha^{-1}=137.036\,02\pm0.000\,21$ (giving ±0.004 MHz in H) has been more precisely determined,[14] the fourth-order calculation in Eq. (3) has been completed, and our more complete calculation of the higher-order term $H(Z\alpha)$ and its independent verification at $Z\sim80$ have increased

TABLE I. Precision tests of Lamb-shift calculations (in MHz).

	interval	theory (±1σ)	experiment (±1σ)	$\frac{\text{theory-exp}}{\sigma}$
H	$2S_{\frac{1}{2}} - 2P_{\frac{1}{2}}$	1057.912 ± 0.011	1057.90 ± 0.06 [a]	+0.2
			1057.77 ± 0.06 [b]	+2.3
	$2P_{\frac{3}{2}} - 2S_{\frac{1}{2}}$	9911.123 ± 0.031	9911.17 ± 0.04 [c]	-0.9
			9911.25 ± 0.06 [d]	-1.9
			9911.38 ± 0.03 [e]	-6.0
D	$2S_{\frac{1}{2}} - 2P_{\frac{1}{2}}$	1059.272 ± 0.025	1059.28 ± 0.06 [f]	-0.1
			1059.00 ± 0.06 [b]	+4.2
He^+	$2S_{\frac{1}{2}} - 2P_{\frac{1}{2}}$	14,044.78 ± 0.61	14,045.4 ± 1.2 [g]	-0.5
			14,040.2 ± 1.8 [b]	+2.4
	$3S_{\frac{1}{2}} - 3P_{\frac{1}{2}}$	4184.42 ± 0.18	4183.17 ± 0.54 [h]	+2.2
	$3P_{\frac{3}{2}} - 3S_{\frac{1}{2}}$	47,843.39 ± 0.23	47,844.05 ± 0.48 [h]	-1.2

[a] R. T. Robiscoe and T. W. Shyn, Phys. Rev. Lett. 24, 559 (1970), with uncertainty as assigned in Ref. 14.

[b] Experiment done before 1958 and discussed in Ref. 14, which gives the 1-standard-deviation uncertainty used here.

[c] B. L. Cosens and T. V. Vorburger, Phys. Rev. A 2, 16 (1970).

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[f] B. L. Cosens, given in Ref. 14.

[g] M. A. Narasimham, given in Ref. 14.

[h] D. L. Mader, M. Leventhal, and W. E. Lamb, Jr., Phys. Rev. A 3, 1832 (1971).

our confidence in the precision of its results. Another reason is that the uncertainties in I represented "estimated limits of error" while those given here are an attempt to estimate uncertainties at the "68% confidence level" in order that they may be considered on the same basis as the "1 standard deviation" increasingly in use for experimental uncertainties. Our combined uncertainty (± 0.011 MHz in H) is therefore the root of the sum of squares of the individual uncertainties and should be similarly combined with "1-standard-deviation" experimental uncertainties. Such comparisons of theory and experiment are thus expected to differ by more than the combined uncertainty for 32% of the cases and should not be considered in unsatisfactory agreement unless the difference is larger than 2 or 3 times the combined uncertainty.

Table I lists results for the Lamb shifts that may be considered the most precise tests of theory since the experimental uncertainties are no more than 10 times larger than the combined uncertainties in the calculations. The experimental situation is clouded by lack of agreement between the different measurements, but in each of these cases the calculation agrees very closely with one of the experimental values (usually the more recent measurement). We thus find excellent confirmation of the calculated values within 1 standard deviation in about 68% ($\frac{4}{6}$) of the intervals tested. Because of the importance of these very basic tests of quantum electrodynamics (QED), we would encourage investigation of the discrepancies, especially since a term like (0.25 MHz)$Z^4(2/n)^3\delta_{l0}$ would shift theory back to many of the now discrepant experiments. However, we expect no such term and find the precision tests generally satisfactory. The other less precise

but more general tests at larger n and Z listed in Ref. 8 all agree with theory. We also find that the recent measurements[15] in hydrogen for $n=3$, 4, and 5 all agree with theory and the expected 32% ($\frac{5}{15}$) differ by more than 1 standard deviation. In summary, we find quite satisfactory confirmation of these predictions of QED calculated with an uncertainty often better than 100 ppm, and sometimes approaching 10 ppm.

These results may thus be used to calculate atomic energy levels to a higher degree of precision and for larger values of Z than previously attainable.[16] The entire calculation (including the usual expressions for relativistic binding energies and recoil corrections) has been computerized, and so results (with details of various terms) for any energy levels or splittings (including the associated uncertainties) may be provided on request. However, the previous tabulation[16] is still quite valid for all except very high-precision purposes.

A more complete discussion of this calculation and its results will be published in the near future.

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[1]See G. W. Erickson and D. R. Yennie, Ann. Phys. (New York) 35, 271 (1965), for references to the earlier calculations, for the covariant formulation used here, and for a summary of the higher-order terms. We will refer to this paper as I.

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Spatial Determination of the Direction of the Magnetic Field in a Tokamak Configuration

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A method is suggested by which the local magnetic field direction can be determined in Tokamaks. A numerical application is made to the Princeton ST Tokamak.

Much interest is presently being given to the spatial determination of the direction of the total magnetic field (or local current density distribution) in a Tokamak configuration. Methods have been proposed using laser scattering[1-5] or particle deflection.[6] The possibility of using coupling of the characteristic electromagnetic modes has also been suggested.[7-8]