More Nuclear Size Corrections to the Lamb Shift

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An evaluation of previously uncalculated finite size effects on the Lamb shift of normal atoms, with use of methods which are well known from muonic atoms, gives corrections which are larger than the experimental uncertainties (40 ppm for the Lamb shift in hydrogen). The additional corrections tend to restore agreement between theory and experiment.

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The precision which has been reached in experimental tests of QED in atomic systems makes it necessary to reexamine the theoretical calculations to ensure that they have been carried through to a precision comparable to that reached in the experiments. This requires not only the calculation of higher-order terms, but also the examination of approximations made in the calculation of lower-order terms. For the case of the Lamb shift in hydrogen and other light elements, such a reconsideration seems to be particularly necessary since the most recent experimental results[1,2] are not in good agreement with theory. In addition, there is an as yet unresolved discrepancy in the calculations[3,4] of the higher-order relativistic and binding corrections amounting to about 40 ppm. In the present work, I examine some corrections to the lower-order terms which are well known in muonic atoms but which have been neglected up to now for normal atoms, and find an additional contribution of 40 ppm which tends to remove the potential discrepancy between theory and experiment. After presenting a derivation of the new contributions, I shall briefly discuss the present status of the calculations and compare the results with experiment.

As is well known from work on muonic atoms,[5-7] the fact that the nucleus has a finite extension affects the electron's wave function and the operators which appear in the calculation of radiative corrections to atomic energy levels. Thus the correct expression for the self-energy or vertex correction is given to lowest order in α by

$$\Delta E_{\rm SE} = \frac{\alpha}{3\pi m^2}\langle\nabla^2 V\rangle\left[\ln\frac{m}{2K(n,l)}+\frac{11}{24}\right]+\frac{\alpha}{8\pi m^2}\left\langle\nabla^2 V+\frac{2m}{m_R}\frac{1}{r}\frac{dV}{dr}\vec{\sigma}\cdot\vec{\rm L}\right\rangle, \quad (1)$$

where $K(n,l)$ is the average excitation energy defined by the Bethe sum and m_R is the reduced mass. The effect of vacuum polarization is treated to a first approximation by adding $-\frac{1}{5}$ to the $\frac{11}{24}$ appearing in Eq. (1). Nuclear size effects enter this expression (and hence the theoretical values for the Lamb shift) in two places: in the term $\langle\nabla^2 V\rangle=\langle-4\pi\rho\rangle$ and in the Bethe logarithm. We consider first the correction to $\langle\rho\rangle$.

The modification of $\langle\rho\rangle$ due to finite nuclear size can be calculated without recourse to a model for normal atoms and for very light muonic atoms. By a calculation analogous to that of Zemach[8] for the size correction to the hyperfine structure and to that used by Friar[9] for the case of size corrections in muonic atoms, I find (keeping only the nonrelativistic contribution) for s states

$$\langle\rho\rangle_{ns}=|\varphi_{ns}(0)|^2(1-2m_R\alpha Z\langle r\rangle_{(2)}), \quad (2)$$

where

$$\langle r\rangle_{(2)}=\int r\rho(|\vec{r}-\vec{u}|)\rho(u)\,d^3u\,d^3r \equiv \int r\rho^{(2)}(r)\,d^3r. \quad (3)$$

As a check, I compared the result of this estimate with those of an exact numerical calculation of $\langle\rho\rangle$ for the case of muonic helium.[10] The agreement is excellent.

This correction will affect almost all (with the exception of the spin-orbit term) of the leading contributions to the Lamb shift. Since $2m_e\alpha = 3.7795\times10^{-5}\ \mathrm{fm}^{-1}$ and since $\langle r\rangle_{(2)}$ is of the order of 1 fm for the case of hydrogen, one can expect a correction of about -38 ppm to the theoretical value of the Lamb shift from this source. The correction will be larger for other systems.

For the case of hydrogen, I assume an exponential form for the charge distribution and obtain $\langle r\rangle_{(2)}$ in terms of the nuclear mean square radius $\langle r^2\rangle$:

$$\langle r\rangle_{(2)} = (35/16\sqrt{3})\langle r^2\rangle^{1/2} \simeq 1.08 \pm 0.03 \text{ fm}.$$

The correction to the theoretical value of the Lamb shift that comes from use of the correct value of $\langle \rho\rangle$ in Eq. (1) gives rise to a shift of -0.042 ± 0.002 MHz for the case of hydrogen. This effect is as large as the theoretical discrepancy in the higher-order corrections[3,4] and, as will be shown subsequently, is such as to improve agreement between theory and experiment.[1,2]

The corrections to the Bethe sum due to finite nuclear size turn out to be of order $(\alpha Zm)^2\langle r^2\rangle$ and hence are negligible. Following the definitions of Klarsfeld and Maquet[11] and Klarsfeld[12] we have

$$\ln K(n,l) = \frac{\sum_{n'l'} f_{nl\to n'l'}\,\omega^2(n',n)\ln|\omega(n',n)|}{\sum_{n'l'} f_{nl\to n'l'}\,\omega^2(n',n)}, \quad (4)$$

where $f_{nl\to n'l'}$ is the oscillator strength for the transition $|n,l\rangle \to |n'l'\rangle$. It is to be expected that only the Bethe sum for s states will be affected, and so it will be sufficient to estimate the correction to $\ln K(2,0)$ due to finite nuclear size. We make use of the fact that

$$f_{n0\to n'1} = \tfrac{1}{3}\,\omega(n',n)(R_{n0}{}^{n'1})^2, \quad (5)$$

where

$$R_{nl}{}^{n'l'} = \int_0^\infty dr\, r^3 \varphi_{nl}(r)\varphi_{n'l'}(r), \quad (6)$$

and consider only deviations from the point (p) values. Thus $\omega(n,n') = \omega_p(n,n') - \Delta\omega(n)$ with $\Delta\omega(n) = Z^2R_\infty[(m\alpha Z)^2/6]\langle r^2\rangle$,

$$R_{20}{}^{n1} = R_p + \Delta R_{20}{}^{n1} \simeq R_p + \int_0^\infty dr\, r^3\varphi_{n1}(r)\Delta\varphi_{20}(r). \quad (7)$$

Using the notation $S_k = \sum_n \omega_p{}^k f_p$, as in Ref. 12, we find, after some algebra

$$\Delta\ln K(2,0) \simeq -S_1\Delta\omega(2)/S_2 + S_2^{-1}\sum_n[\tfrac{2}{3}\omega_p{}^3R_p\Delta R_{20}{}^{n1} - 3\Delta\omega\omega_pf_p]\ln(|\omega_p|/K(2,0)), \quad (8)$$

where only terms of first order in the deviations from the point values were kept.

Obviously the terms proportional to $\Delta\omega$ in Eq. (8) are proportional to $(m\alpha Z)^2r^2$ and hence negligible. Thus

$$\Delta\ln K(2,0) \simeq \tfrac{2}{3}S_2^{-1}\sum_n \omega_p{}^3R_p\Delta R_{20}{}^{n1}\ln(|\omega_p|/K_p(2,0)). \quad (8a)$$

It remains to calculate $R_{20}{}^{n1}$. Friar[13] has given an expression for the correction to the radial wave function φ_{ns} which can be used for this purpose. For the present estimate it is sufficient to take the nucleus as a uniformly charged sphere. Using results of Ref. 13, we find

$$\Delta\varphi_{2s}(r) \simeq \varphi_{2s}(0)m\alpha Z(r - r^2/2R_N - \tfrac{3}{4}R_N + r^4/20R_N{}^3), \quad r \le R_N,$$
$$\simeq \varphi_{2s}(0)(m\alpha ZR_N)^2(e^{-y/2}/5)\{-y^{-1} + 3 + (2-y)[\ln y - \psi(2) - \tfrac{5}{4}]\}, \quad r \ge R_N, \quad (9)$$

with $y = m\alpha Zr$; contributions of higher order in $m\alpha ZR_N$ are neglected. I use standard expressions[14] for the $\varphi_{np}(r)$ and p-state Coulomb wave functions for the continuum contribution. For small values of r, the p-state wave functions are proportional to r, and hence the contribution to $\Delta R_{20}{}^{n1}$ from the nuclear interior is proportional to

$$\int_0^{R_N} dr\, r^4\varphi_{2s}(0)m\alpha Z(r - r^2/2R_N - \tfrac{3}{4}R_N + r^4/20R_N{}^3) \sim (m\alpha ZR_N)^6 \quad (10a)$$

and is clearly negligible. The contribution from the nuclear exterior is given by

$$\varphi_{2s}(0)[(m\alpha ZR_N)^2/5]\int_{R_N}^\infty dr\, r^3\varphi_{np}(r)e^{-y/2}|3 - y^{-1} + (2-y)[\ln y - \psi(2) - \tfrac{5}{4}]|. \quad (10b)$$

The result is a convergent, but (at least for the continuum contribution) very lengthy expression which will not be given here, but which is clearly proportional to $(m\alpha ZR_N)^2 \sim 10^{-9}$–$10^{-10}$. The correction to the Bethe sum is thus negligible in comparison to the correction arising from taking $\langle\rho\rangle \ne |\varphi_{2s}(0)|^2/4\pi$.

Another nuclear size correction which has been neglected up to now in normal atoms is a correction to the Breit correction for relativistic recoil.[15-17] Friar[9] has given a model-independent expression for the case of light muonic atoms, which is also valid for the present case:

$$\Delta B \simeq [(\alpha Z)^4m^3/n^3m_N]\langle r\rangle_{(2)}\delta_{l0}. \quad (11)$$

This correction decreases the Lamb shift in hydrogen by 0.0005 MHz.

For completeness, we remind the reader that the known shift of the $2s$ level due to nuclear size is given by

$$\Delta B = [-2(\alpha Z)^4 m^3/3n^3]\,(\langle r^2\rangle - \tfrac{1}{2}\alpha Z m\langle r^3\rangle_{(2)}). \tag{12}$$

Use of the measured[18] charge radius for hydrogen, $\langle r^2\rangle^{1/2} = 0.86 \pm 0.02$ fm, results in a correction of 0.144 ± 0.007 MHz.

In order to discuss the status of the theory of the Lamb shift, it is necessary to summarize the theoretical contributions to the $2s_{1/2} - 2p_{1/2}$ splitting in hydrogenlike atoms. Following the notation of Mohr,[3] one has

$$S = \frac{\alpha^3 Z^4 R_\infty}{3\pi}\Bigg\{\left[\frac{19}{30} + \ln\left(\frac{m}{m_R}(Z\alpha)^{-2}\right) + \ln\frac{K(2,1)}{K(2,0)}\right]\left(\frac{m_R}{m}\right)^3 \frac{\langle\rho\rangle}{|\varphi_{2s}(0)|^2} + \frac{1}{8}\left(\frac{m_R}{m}\right)^2 + 0.32\,206\frac{\alpha}{\pi}\left(\frac{m_R}{m}\right)^3 + 2.2962\pi\alpha Z + (Z\alpha)^2\left[-\frac{3}{4}\ln^2(Z\alpha)^{-2} + 3.9184\ln(Z\alpha)^{-2} + G_{\rm VP}(Z\alpha) + G_{\rm SE}(Z\alpha)\right]\Bigg\} + S_{\rm size} + S_{\rm rec}. \tag{13}$$

Here $S_{\rm size}$ is given by Eq. (12) and

$$S_{\rm rec} = \frac{\alpha^3 Z^5 R_\infty}{3\pi}\frac{m}{m_N}\left(\frac{m_R}{m}\right)^3\left(2\ln\frac{K(2,1)}{K(2,0)} + \frac{1}{4}\ln(Z\alpha)^{-2} + \frac{97}{12}\right) - \frac{\alpha^2 Z^4 R_\infty}{4mm_N} m_R{}^3\langle r\rangle_{(2)}. \tag{14}$$

The higher-order binding corrections are a major source of uncertainty in the theory of the Lamb shift. According to Mohr,[3] the value of $G_{\rm VP}$ can be calculated reliably from the Ühling contribution; terms coming from the Wichmann-Kroll correction[19] contribute only 0.0003 MHz in the case of hydrogen.

Two estimates of the higher-order binding correction to the self energy, $G_{\rm SE}$, exist in the literature, and they are in slight disagreement. Mohr's extrapolation[3] gives

$$G_{\rm SE}(Z\alpha) = -24.1 + 7.5Z\alpha\ln(Z\alpha)^{-2} + 15.3Z\alpha \pm 1.2, \quad G_{\rm SE}(\alpha) = -23.4 \pm 1.2;$$

while Erickson's expansion[4] gives

$$G_{\rm SE}(Z\alpha) = -17.2 + 17.2Z\alpha \pm 0.6, \quad G_{\rm SE}(\alpha) = -17.1 \pm 0.6.$$

The contributions to the Lamb shift in hydrogen are, respectively, -0.169 ± 0.009 and -0.124 ± 0.009 MHz. The difference of 0.045 MHz is about the same size as the finite-size contributions presented here and somewhat larger than either the experimental or theoretical uncertainties. The numerical prediction for the hydrogen Lamb shift is [with use of constants $\alpha^{-1} = 137.035\,99(3)$, $R_\infty = 109\,737.3143(10)$ cm^{-1}, and $m_e/m_p = 0.000\,5446$][20] summarized in the form (energies in MHz, radii in fm)

$$S_H = 1057.910 + 0.007\,22G_{\rm SE}(\alpha) + 0.1955\langle r^2\rangle - 0.391\langle r\rangle_{(2)} = 1058.012 + 0.007\,22G_{\rm SE}(\alpha)$$
$$= 1057.843 \pm 0.015 \text{ or } 1057.888 \pm 0.015,$$

depending on the value of $G_{\rm SE}$ used. The most recent experimental values quoted in the literature are $S_{\rm exp} = 1057.862 \pm 0.020$[2] and $S_{\rm exp} = 1057.845 \pm 0.009$.[1] Theory and experiment are in reasonable agreement if all nuclear size corrections discussed here are included.

Since it is probably worthwhile to investigate the Z dependence of the higher-order corrections by studying other systems, such as He^+ and Li^{++} as well, I give numerical predictions for these cases also:

$$S_{\rm He} = 14\,052.9 + 0.4623G_{\rm SE}(2\alpha) + 3.132\langle r^2\rangle - 1.025\langle r\rangle_{(2)} \pm 0.3 = 14\,050.6 + 0.4623G_{\rm SE}(2\alpha)$$
$$= 14\,040.0 \pm 0.7 \text{ or } 14\,043.3 \pm 0.7;$$

$S_{\rm expt} = 14\,046.2 \pm 1.2$ (Ref. 21) or $14\,040.2 \pm 1.8$ (Ref. 22) or $14\,040.2 \pm 2.9$ (Ref. 23).

$$S_{\rm Li} = 62\,750.3 + 5.266G_{\rm SE}(3\alpha) + 15.85\langle r^2\rangle - 6.78\langle r\rangle_{(2)} \pm 1.2 = 62\,833 + 5.27G_{\rm SE}(3\alpha)$$
$$= 62\,714 \pm 11 \text{ or } 62\,744 \pm 11;$$

$S_{\rm expt} = 62\,765 \pm 21$ (Ref. 24).

Here values for the charge radii were taken to be $r_{He} = 1.673 \pm 0.001$[10] and $r_{Li} = 2.57 \pm 0.10$.[25] The contribution from the new size effects are −2.2 MHz for helium and −23 MHz for lithium. The theoretical predictions are in reasonable agreement with experiment, but more work on the higher-order binding corrections remains to be done before definite conclusions are drawn.

It has been argued[26] that the finite nuclear size corrections to the nonrelativistically reduced self-energy operator [Eq. (1)] which have been presented here may be canceled by higher-order and relativistic effects. Equation (1) was derived by means of a nonrelativistic reduction of the full self-energy operator for momenta small compared to the electron mass and it may not be valid for distances of the order of a nuclear radius. In this case, it should not be used in a high-precision calculation. On the other hand, if Eq. (1), which has been in general use for many years, is applied consistently, the correction presented here must be included. A similar correction is known to be important for muonic atoms. The absence of such corrections would indicate even more difficulty associated with use of a simple formula based on the scattering approximation than had been expected. Although it might be surprising that nuclear size corrections, which involve relativistic electrons ($qR_N \sim 1$), could be significant in an essentially nonrelativistic problem, one must recall that the effect is only of the order of a part in 10^5. However, this is significant compared with experimental accuracy and with other theoretical uncertainties. The only way to settle the question of the applicability of this correction is a unified investigation of higher-order corrections and nuclear size effects which avoids perturbative expansions in the binding potential, similar to that performed by Johnson and co-workers,[27] although the numerical difficulties may turn out to be insuperable. Pending such a calculation, the additional nuclear size correction presented here should be regarded as a possible explanation for the disagreement between theory and experiment.

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