Nuclear Size Correction to the Electron Self-Energy

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The nuclear size correction to the self-energy of an electron in the $1S_{1/2}$, $2S_{1/2}$, or $2P_{1/2}$ state in hydrogenlike ions is calculated. The results modify theoretical predictions required for experimental tests of quantum electrodynamics in strong fields, and they resolve differences among previous calculations for the Lamb shift in hydrogenlike uranium. Results are presented for a number of elements ranging from iron ($Z = 26$) to fermium ($Z = 100$). An estimate of the nuclear model dependence of the effect is made, and, based on the numerical results, a simple formula for the correction as a function of the nuclear radius is provided.

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The distribution of charge in the nucleus influences the quantum electrodynamic (QED) corrections to the structure of atoms. Theoretical consequences of the nuclear size for the Dirac energy eigenvalue and for the vacuum polarization correction are understood [1–5], but the effect on the self-energy correction has been more difficult to quantify. For example, in hydrogen, there has been dispute over the order of magnitude of the effect [6, 7], and in lithiumlike uranium, theoretical estimates span a range that is four times the experimental uncertainty [2, 8, 9].

We address this issue here, and describe a precise calculation of the nuclear size effect on the self-energy in high-Z hydrogenlike atoms. Besides providing results for a broad range of special cases, we study the nuclear model dependence, and the charge radius dependence of the effect. The hydrogenic value is not only important for tests of QED in high-Z hydrogenlike atoms, it also gives a first approximation to the correction in high-Z few-electron atoms and in inner shells of heavy neutral atoms.

Despite the fact that the nuclear size correction is small compared to the point nucleus QED effects, standard perturbation theory is not valid for this type of correction at the higher-Z range [5]. Therefore, we carry out a complete calculation of the self-energy in the field of a finite-size nucleus, and subtract the known Coulomb contribution in order to identify the nuclear size effect. This procedure entails a loss of numerical precision, particularly at low Z, so that a precise numerical treatment is required to obtain reliable results.

Previous calculations of this correction have been confined to high nuclear charge number Z, and have numerical uncertainties that are of order 25% of the effect, or higher [2, 8, 10–12]. The calculation reported here extends from $Z = 26$ to $Z = 100$, with an estimated numerical precision of about 0.003% of the size correction in the best case. As a consequence, the uncertainty in the predictions for this effect is dominated by the nuclear model dependence, which is of order 0.2% at $Z = 90$ for the charge distribution employed here, or by uncertainty in the measured charge radius of the nucleus which is relatively large in some cases.

To model the nucleus, we note the fact that the Dirac eigenvalue depends only weakly on the details of the nuclear model, provided the root-mean-square (rms) radius is fixed to a particular value [4]. We assume that the self-energy behaves similarly. In particular, for convenience in the calculation, we employ a model where the nuclear charge distribution ρ is spherically symmetric, uniform, and has a surface radius R_u:

$$\rho_u(x) = \frac{Ze}{\frac{4}{3}\pi R_u^3}\,\theta(R_u - x). \tag{1}$$

An indication of the model dependence of the nuclear size correction to the self-energy is obtained by also calculating the correction for a hollow shell charge distribution with radius R_s

$$\rho_s(x) = \frac{Ze}{4\pi R_s^2}\,\delta(x - R_s) \tag{2}$$

in a number of cases. The radii in (1) and (2) are related to the rms radius

$$R = \left[\frac{1}{Ze}\int d\mathbf{x}\; x^2\rho(x)\right]^{\frac{1}{2}} \tag{3}$$

by $R_u = \sqrt{\frac{5}{3}}R$ and $R_s = R$, respectively.

The self-energy in the field of the nucleus is given by (in units in which $\hbar = c = m_e = 1$)

$$E = -\frac{i\alpha}{2\pi}\int_{C_F} dz \int d\mathbf{x}_2 \int d\mathbf{x}_1\, \phi_n^\dagger(\mathbf{x}_2)\alpha_\mu G(\mathbf{x}_2, \mathbf{x}_1, z)\alpha^\mu \phi_n(\mathbf{x}_1)\frac{e^{-bx_{21}}}{x_{21}} - \delta m \int d\mathbf{x}\; \phi_n^\dagger(\mathbf{x})\beta\phi_n(\mathbf{x}), \tag{4}$$

where $b = -i[(E_n - z)^2 + i\delta]^{1/2}$, $\mathrm{Re}(b) > 0$, C_F denotes the Feynman contour, ϕ_n and E_n are the eigenfunction and eigenvalue of the Dirac equation for the bound state n, G is the Green's function for the Dirac equation corresponding to the operator $G = (H - z)^{-1}$, where $H = \boldsymbol{\alpha}\cdot\mathbf{p} + V + \beta$ is the Dirac Hamiltonian, $\mathbf{x}_{21} = \mathbf{x}_2 - \mathbf{x}_1$, and δm is the mass renormalization constant. We employ the values $\alpha = 1/137.036$ and $\lambda\!\!\!^{-}_e = 386.1593$ fm. For the nuclear models considered here, the external potential is given by

$$V(x) = \begin{cases} V_0 + V_2 x^2 & \text{for} \quad x < R_0, \\ -Z\alpha/x & \text{for} \quad x \geq R_0, \end{cases} \tag{5}$$

with $V_0 = -\frac{3}{2}Z\alpha/R_0$, $V_2 = \frac{1}{2}Z\alpha/R_0^3$, and $R_0 = R_u$ for the uniform model, or $V_0 = -Z\alpha/R_0$, $V_2 = 0$, and $R_0 = R_s$ for the shell model.

The evaluation of (4) is carried out entirely in coordinate space, with a method of extracting the infinite mass renormalization that is described in detail elsewhere [13]. The numerical calculation is based on expansion of the Green's function in angular momentum eigenfunctions. Construction of the Green's functions for the case of a finite nucleus potential is discussed in Refs. [3, 14]. In the exterior region ($x \geq R_0$), the Green's functions consist of Coulomb functions that are evaluated as described in Ref. [15]. In the interior region ($x < R_0$), for the spherical shell charge distribution, the solutions are linear combinations of spherical Bessel functions. In the case of the uniform sphere charge distribution, we numerically evaluate the solution of the radial Dirac equation by calculating power series in the radial coordinate x. The well-known solution, regular at the origin, has a lowest power $x^{|\kappa|-1}$, where κ is the Dirac angular momentum quantum number, and the power series converges well for the range of x required for this calculation. Linearly independent solutions, irregular at the origin, have a lowest power of $x^{-|\kappa|-1}$. We factor out a dominant exponential term, and in most cases it is sufficient to employ a simple power-series expansion for the numerical evaluation of the remaining factor. However, when the intermediate-state energy parameter $|z|$ is large, e.g., of order 10^3 to 10^5, and $|\kappa|$ is small, the numerical evaluation is carried out with the aid of an asymptotic expansion in $1/|z|$ of the coefficients in the power series in x. This method provides numerically stable results in the cases where the simple power series does not. The rate of convergence of the summation over $|\kappa|$ is improved by subtracting the dominant terms with the method described in [16]. This is a departure from the basic method described in [13]. The modification is compensated by including the difference between the renormalization subtractions in [16] and [13], which can be calculated as a three-dimensional integral to high accuracy. Summation over $|\kappa|$ is carried out before integration over the coordinates or z, so the convergence is geometric in the ratio of the smaller to the larger coordinate, in the worst case. The error in terminating the sum is determined by calculating the remainder in the approximation that the subsequent terms in the sum are replaced by the leading term in their asymptotic expansion in $1/|\kappa|$. The summation is carried out to an absolute precision of order 10^{-7}, compared to a maximum term of order 1. Numerical evaluation of the integrals over the radial coordinates and z is carried out as described in Ref. [17]. A more detailed account of the numerical methods will be published separately.

Results of the evaluation of Eq. (4) are expressed as a function $F(Z\alpha, R)$ defined by

$$E = \frac{\alpha}{\pi}\frac{(Z\alpha)^4}{n^3} F(Z\alpha, R)\, m_e c^2. \tag{6}$$

This gives the complete self-energy in the field of a finite-size nucleus. The finite-size correction ΔE to the Coulomb self-energy is obtained by taking the difference between E defined by (6), and the precisely known Coulomb value corresponding to $R = 0$ [18], i.e.,

$$\Delta E = \frac{\alpha}{\pi}\frac{(Z\alpha)^4}{n^3} \Delta F(Z\alpha, R)\, m_e c^2, \tag{7}$$

where

$$\Delta F(Z\alpha, R) = F(Z\alpha, R) - F(Z\alpha, 0). \tag{8}$$

Table I gives the numerical results of this calculation for the $1S_{1/2}$ state at $Z = 80$ for both the uniform sphere and spherical shell models, and the correction obtained by subtracting the Coulomb contribution. Results for the uniform sphere model for a number of elements ranging from $Z = 26$ to $Z = 100$ are listed in Table II. Values for the $1S_{1/2}$, $2S_{1/2}$, and $2P_{1/2}$ states are expressed there in terms of $\Delta F(Z\alpha, R)$. The numbers in parentheses are uncertainties that are expected to be larger

TABLE I. The function $F(Z\alpha, R)$ and the correction $\Delta F(Z\alpha, R)$ for $Z = 80$ and $R = 5.475$ fm for the $1S_{1/2}$ state.

Contribution		Value
Total (uniform sphere model)	$F(Z\alpha, R)$	1.495447(1)
Total (spherical shell model)	$F(Z\alpha, R)$	1.495413(1)
Coulomb [18]	$F(Z\alpha, 0)$	1.5027775(4)
Correction (uniform sphere model)	$\Delta F(Z\alpha, R)$	−0.007330(1)
Correction (spherical shell model)	$\Delta F(Z\alpha, R)$	−0.007365(1)

TABLE II. Special cases of the function $\Delta F(Z\alpha, R)$.

Z	R (fm)	$1S_{1/2}$	$2S_{1/2}$	$2P_{1/2}$
26	3.730	−0.000172(1)	−0.00018(1)	−0.00000(1)
36	4.230	−0.000383(1)	−0.000401(2)	−0.000001(2)
54	4.826	−0.001275(1)	−0.001462(1)	−0.000021(1)
60	4.915	−0.001836(1)	−0.002191(1)	−0.000047(1)
70	5.273	−0.003695(1)	−0.004746(1)	−0.000170(1)
80	5.475	−0.007330(1)	−0.010256(1)	−0.000558(1)
82	5.505	−0.008432(1)	−0.012018(1)	−0.000707(1)
90	5.707	−0.015429(1)	−0.023776(1)	−0.001887(1)
92	5.863	−0.018492(1)	−0.029090(2)	−0.002483(1)
100	5.976	−0.034961(1)	−0.059986(2)	−0.006873(1)

than the actual numerical error in most cases. We have also calculated the corresponding results for the spherical shell model. The fractional difference between the size correction for the spherical shell model and the uniform sphere model is slowly varying over the entire range considered here. In particular, the fractional difference is 0.55% for all three states at $Z = 100$, and 0.3% for the $S_{1/2}$ states at $Z = 54$. The difference is less than the numerical uncertainty when $Z < 54$ for the $S_{1/2}$ states or when $Z < 70$ for the $2P_{1/2}$ state. We expect that the model dependence of the uniform sphere model is somewhat less than this difference in each case.

For comparison, the previous calculation by Johnson and Soff [2] for the $1S_{1/2}$ state at $Z = 80$ leads to $\Delta E = -1.6$ eV, while this work yields $\Delta E = -1.0105$ eV for the uniform sphere model and $\Delta E = -1.0154$ eV for the spherical shell model. A similar comparison to the work of Johnson and Soff [2] and to Cheng, Johnson, and Sapirstein [8] for the Lamb shift in hydrogenlike uranium is given in Table III. Blundell has done a calculation that is in agreement with but less accurate than our calculation for this splitting [20]. Cheng, Johnson, and Sapirstein have recently obtained results that agree with our work [21].

Since the nuclear size correction depends on the experimentally determined charge radius of the nucleus, and this quantity changes as measurements improve, it is useful to fit the correction by a simple function of R in order to accommodate changes in the value and to estimate the error in the nuclear size correction due to uncertainty in the measured radius. To study the dependence of the correction on R, we consider the functional form

$$\Delta F(Z\alpha, R) = aR^p(1 + bR + cR^2 + \cdots), \tag{9}$$

as suggested by the analytic form of the nuclear size correction to the Dirac energy eigenvalue [1]. In order to determine the parameters in (9), we calculated the nuclear size correction in the $1S_{1/2}$ state for $Z = 30$, 60, and 90 over the range $R = 1.0$ fm to 5.0 fm, in steps of 0.5 fm, and $R = 6.0$ fm. An estimate for p was made by extrapolating to $R = 0$ the function $\ln[F(Z\alpha, 2R)/F(Z\alpha, R)] = p\ln 2 + bR + \cdots$. The coefficients a, b, and c were evaluated by a least squares fit to (9), for fixed p. The results are displayed in Table IV, where the parameters a, b, and c are normalized for an rms nuclear radius expressed in fermis. Equation (9) with the parameters in Table IV reproduces the calculated values of the size correction to better than 0.07% over the range $R = 1$ fm to 6 fm. A simpler function, suggested by (9), is

$$\Delta F(Z\alpha, R) \approx a' R^{p'}, \tag{10}$$

where a' and p' are effective constants for fixed Z and a limited range of R. For example, for $Z = 90$, $R = 5.2$ fm to 6.2 fm, and $p' = 1.353$, (10) agrees with (9) to within 1 part in 10^4, which is nearly an order of magnitude better than a linear best fit. Although Eq. (9) is likely to be a better representation of the functional form of ΔF, Eq. (10) is clearly preferable for an extensive tabulation. In accord with Eq. (10) the fractional uncertainty u in the nuclear size correction to the self-

TABLE III. Calculations of the finite nuclear size correction to the self-energy of the $2P_{1/2}$-$2S_{1/2}$ splitting (Lamb shift) in hydrogenlike uranium ($R = 5.863$ fm).

Reference	Correction (eV)
Johnson and Soff [2]	−1.0(1)
Cheng, Johnson, and Sapirstein [8, 19][a]	−0.6
This work (uniform sphere model)	−0.8020(1)
This work (spherical shell model)	−0.8062(1)

[a]Includes electron screening effects.

TABLE IV. Fitted parameters in Eq. (9) for the nuclear size correction.

Z	a (fm^{-p})	b (fm^{-1})	c (fm^{-2})	p
30	−0.00001770	−0.0027	0.0	1.911
60	−0.0001207	−0.0060	0.00004	1.728
90	−0.001410	−0.0144	0.00036	1.416

energy due to uncertainty in the measured charge radius ΔR is approximately

$$u = p' \frac{\Delta R}{R}. \tag{11}$$

It is of interest to note that the exponent p in Table IV does not exactly match the corresponding power $2[1-(Z\alpha)^2]^{1/2}$ in the nuclear size correction to the eigenvalue. However, it appears that the fitted values are consistent with a low-Z limit $p \to 2$. This is in agreement with the perturbative order-of-magnitude estimate given by Lepage, Yennie, and Erickson of the nuclear size correction to the self-energy in hydrogen [7]. It is also consistent with the analytic expression for the low-Z limit of the nuclear size correction to the vacuum polarization calculated by Hylton [5].

In summary, we have calculated the nuclear size correction to the self-energy over a wide range of Z. There are significant differences between these results and the work of Johnson and Soff [2]. The sources of error in the present calculation are the numerical uncertainties, which appear to be small, the model dependence, which is somewhat less than 0.3% to 0.55%, depending on Z, of the nuclear size correction, and the uncertainty in the measured values of the nuclear radius that can be taken into account according to Eq. (11). A more extensive calculation of the nuclear size correction is in progress.

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