Nuclear recoil effect in the Lamb shift of light hydrogen-like atoms

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We report high-precision calculations of the nuclear recoil effect to the Lamb shift of hydrogen-like atoms to the first order in the electron-nucleus mass ratio and to all orders in the nuclear binding strength parameter $Z\alpha$. The results are in excellent agreement with the known terms of the $Z\alpha$ expansion and allow an accurate identification of the nonperturbative higher-order remainder. For hydrogen, the higher-order remainder was found to be much larger than anticipated. This result resolves the long-standing disagreement between the numerical all-order and the analytical $Z\alpha$-expansion approaches to the recoil effect and completely removes the second-largest theoretical uncertainty in the hydrogen Lamb shift of the 1S and 2S states.

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The hydrogen atom is one of the simplest and the most accurately measured atomic systems in physics. The highest precision has been achieved for the 1S-2S transition, whose frequency was measured\textsuperscript{1} with the relative uncertainty of $4.2 \times 10^{-15}$ or 10 Hz. In future, it should be possible to increase the experimental accuracy even further, closely approaching the 1.3 Hz natural linewidth of the 2S level. A combination of measured transition frequencies in hydrogen with sophisticated theoretical calculations provides the method for determination of the Rydberg constant\textsuperscript{2}, which is currently the most accurately known fundamental constant. A coproduct of the determination procedure of the Rydberg constant is the proton charge radius.

The proton charge radius has recently received much attention, after the experiments on the muonic hydrogen\textsuperscript{3,4} reported a large ($7\sigma$) unexplained difference of the proton charge radius values extracted from the muonic hydrogen and the usual (electronic) hydrogen. One of the possible explanations of this puzzle might be a yet undiscovered problem in the theory of the electronic hydrogen. For this reason, investigations of possible inconsistencies in the hydrogen theory are of particular importance today. In the present Letter we report calculations that remove the second-largest theoretical uncertainty in the hydrogen theory and resolve a long-standing discrepancy between the analytical and the numerical approach to the nuclear recoil effect.

General expressions for the nuclear recoil effect to first order in the electron-nucleus mass ratio $m/M$ and to all orders in the nuclear binding strength parameter $Z\alpha$ ($Z$ is the nuclear charge number and $\alpha$ is the fine-structure constant) were obtained by one of us\textsuperscript{5,6} (see also\textsuperscript{7}) and later rederived by other authors\textsuperscript{8-10}. Numerical calculations to all orders in $Z\alpha$ were reported in Refs.\textsuperscript{11-13}. The results of these calculations agreed well with the first terms of the $Z\alpha$ expansion\textsuperscript{9,12,15}. However, a significant disagreement was later found for the higher-order $Z\alpha$ expansion terms. Specifically, the $Z\alpha$-expansion result for the $(Z\alpha)^2 m/M$ contribution for the 1s state obtained within the leading logarithmic approximation\textsuperscript{16,17} yielded $-(18/\pi) (Z\alpha)^2 m^2/M$, whereas the all-order numerical calculations\textsuperscript{13} provided the result of comparable magnitude but of the opposite sign, $(10/\pi) (Z\alpha)^2 m^2/M$. The disagreement, repeatedly mentioned in reviews of hydrogen theory, notably, in Refs.\textsuperscript{12,18,19}, remained unexplained for fifteen years. The 0.7 kHz difference between the all-order and the $Z\alpha$-expansion results for the hydrogen ground state is the second-largest theoretical uncertainty in the hydrogen Lamb shift of the 1S and 2S states.

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The nuclear recoil effect to the Lamb shift of hydrogen-like atoms, to first order in $m/M$ and to all orders in $Z\alpha$, is represented as a sum of four terms,

$$\Delta E_{\text{rec}} = \Delta E_{\text{L}} + \Delta E_{\text{C}} + \Delta E_{\text{tr}(1)} + \Delta E_{\text{tr}(2)},$$

(1)

where $\Delta E_{\text{L}}$ (the low-order part) is the recoil correction as can be derived from the Breit equation, $\Delta E_{\text{C}}$ (the Coulomb part) is the QED recoil correction induced by the exchange of an arbitrary number of virtual Coulomb photons between the electron and the nucleus, $\Delta E_{\text{tr}(1)}$ and $\Delta E_{\text{tr}(2)}$ (the one-transverse-photon and two-transverse-photons parts, respectively) are the QED recoil corrections induced by the ex-
change of one or two transverse photons and an arbitrary number of virtual Coulomb photons.

**Point nucleus.** We first consider the nucleus to be the point source of Coulomb field. In this case, the low-order part $\Delta E_L$ is given by [5]

$$\Delta E_L = \frac{1}{2M}(a | p^2 - D(0) \cdot p - p \cdot D(0)|a),$$  \hspace{1cm} (2)

where $p$ is the electron momentum operator, $D_j(\omega) = -4\pi \alpha Z \delta_{ij}(\omega, r)$, and $D_{ij}(\omega, r)$ is the transverse part of the photon propagator in the Coulomb gauge [7]. Eq. (2) can be conveniently parameterized in a very simple form [5],

$$\Delta E_L = \frac{m^2 - \epsilon_a^2}{2M},$$  \hspace{1cm} (3)

where $\epsilon_a$ is the Dirac energy of the reference state.

The corrections $\Delta E_C$, $\Delta E_{\pi,1}$, and $\Delta E_{\pi,2}$ in Eq. (1) can be calculated only within the QED theory [5–10]. The results for them are

$$\Delta E_C = \frac{2\pi i}{M} \int_{-\infty}^{\infty} d\omega \left[ G(\omega + \epsilon_a) - G(\omega) \right] |a|,$$

$$\Delta E_{\pi,1} = -\frac{1}{M} \int_{-\infty}^{\infty} d\omega \left[ G(\omega + \epsilon_a) - G(\omega) \right] \frac{1}{|a|},$$

$$\Delta E_{\pi,2} = \frac{i}{2\pi M} \int_{-\infty}^{\infty} d\omega \left[ G(\omega + \epsilon_a) - G(\omega) \right] \frac{1}{|a|},$$

where the scalar product is implicit, $\delta_+(\omega) = i/(2\pi)(\omega + i0)$, $V(r) = -Z\alpha/r$ is the nuclear Coulomb potential, $G(\omega)$ is the relativistic Coulomb Green function, and $[\cdot, \cdot]$ denotes commutator.

For low-$Z$ ions, the QED part of the recoil effect can be conveniently parameterized as

$$\Delta E_C + \Delta E_{\pi,1} + \Delta E_{\pi,2} = \frac{m^2 (Z\alpha)^5}{M \pi n^3} P(Z\alpha),$$

where $P(Z\alpha)$ is a slowly-varying dimensionless functions, whose $Z\alpha$ expansion is

$$P(Z\alpha) = \ln(Z\alpha)^{-2} D_{51} + D_{50} + (Z\alpha) D_{60} + (Z\alpha)^2 G_{\text{rec}}(Z\alpha),$$

and $G_{\text{rec}}(Z\alpha)$ is the higher-order remainder containing all higher orders in $Z\alpha$.

The coefficients of the $Z\alpha$ expansion are [5, 14, 17]

$$D_{51} = \frac{1}{3} \delta_{1,0}, \quad D_{50} = \left[ -\frac{8}{3} \ln k_0(n, l) + d_{50} \right],$$

$$D_{60} = \left( 4 \ln 2 - \frac{7}{2} \right) / \pi \delta_{1,0} + \left[ 3 - \frac{l(l+1)}{n^2} \right] / \left( 4l^2 - 1)(2l + 3) \right),$$

where $\ln k_0(n, l)$ is the Bethe logarithm, whose numerical values are [20] $\ln k_0(1s) = 2.984 128 556$, $\ln k_0(2s) = 2.811 769 893$, $\ln k_0(2p) = -0.030 016 709$. The values of the coefficients $d_{50}$ for the states of interest are

$$d_{50}(1s) = \frac{14}{3} \ln 2 + \frac{62}{9}, \quad d_{50}(2s) = \frac{187}{18}, \quad d_{50}(2p) = -\frac{7}{18}.$$  \hspace{1cm} (13)

The first numerical calculations of the QED recoil corrections [4–6] to all orders in $Z\alpha$ were performed in Refs. [11, 12]. Results with an improved precision were later reported for hydrogen in Ref. [13]. The numerical accuracy of these calculations, however, was not high enough. The general opinion [2, 18, 19] was that these results were not fully consistent with the higher-order $Z\alpha$-expansion terms derived in Refs. [16, 17]. In the present work we improve the numerical accuracy of the QED recoil corrections by 2-3 orders of magnitude as compared to the previous studies.

The general scheme of the calculation was described in detail in Ref. [11]. The Dirac-Coulomb Green function in Eqs. (4–6) was evaluated by summing over the whole spectrum of the Dirac equation with the help of the finite basis set constructed with $B$-splines [21]. In the previous calculations [11, 13], the convergence of the results in the low-$Z$ region with increase of the basis size was hampered by numerical instabilities associated with the limitations of the double-precision arithmetics. In the present work we implemented the procedure of solving the Dirac equation with the $B$-splines basis set in the quadruple-precision (32-digit) arithmetics. After that we were able to achieve a clear convergence pattern of the calculated results when the size of the basis set was increased. The largest basis size used in actual calculations was $N = 250$. The numerical uncertainty of the obtained results was estimated by changing the size of the basis set by 30-50% and by increasing the number of integration points in numerical quadratures.

The numerical results for the $n = 1$ and $n = 2$ states and $Z = 1-5$ are presented in Table 1. For the 1s and 2$p_j$ states of hydrogen, we find perfect agreement with the previous calculations [12, 13]. For the 2$s$ state there is a small deviation caused by a minor mistake in the previous calculation. At the same time, we observe a strong contrast between the all-order results for $G_{\text{rec}}(1s)$ and $G_{\text{rec}}(2s)$ and the corresponding $Z\alpha$-expansion results. We recall that the $Z\alpha$-expansion results for $G_{\text{rec}}$ include only the double-log contribution $D_{72} \ln^2(Z\alpha)^{-2}$ and neglect the higher-order terms.
For hydrogen, $\ln(\alpha)^{-2} \approx 10$ is a large parameter, and the leading logarithmic approximation is routinely used for estimating the tail of the $Z\alpha$ expansion, with typical uncertainty of 50% [18].

In order to make a detailed comparison with the $Z\alpha$-expansion results, we performed our calculations for a series of $Z$ including fractional values as low as $Z = 0.3$. The results obtained for the higher-order remainder $G_{\text{rec}}(Z\alpha)$ are plotted in Fig. 1. We discover a rapidly changing structure at very low values of $Z$. Most remarkably, the bending of the curve is practically undetectable for results with $Z \geq 2$. In order to access such a structure in an all-order calculation, one needs to achieve a very high numerical accuracy at very low (and fractional) values of $Z$.

Fitting our numerical results for the function $G_{\text{rec}}(Z\alpha)$ to the form of Eq. (9), we obtain results for the expansion coefficients. For the double-log contribution we find $D_{72}(1s) = -0.183(1)$ and $D_{72}(2s) = -0.183(1)$, in agreement with the analytical value $-11/60 \approx -0.183$. The fitted results for the next two coefficients are:

\[
D_{71}(1s) = 2.919(10), \quad D_{70}(1s) = -1.32(10), \quad (14)
\]

\[
D_{71}(2s) = 3.335(10), \quad D_{70}(2s) = -0.26(6), \quad (15)
\]

\[
D_{71}(2p_{1/2}) = 0.149(5), \quad D_{70}(2p_{1/2}) = -0.04(2), \quad (16)
\]

\[
D_{71}(2p_{3/2}) = -0.283(5), \quad D_{70}(2p_{3/2}) = 0.69(2). \quad (17)
\]

We thus conclude that our all-order results are perfectly consistent with all known coefficients of the $Z\alpha$ expansion. The deviation observed for the $S$ states in Table II comes from the higher-order terms, whose contribution turns out to be unexpectedly large. Specifically, the single-log coefficient $D_{71}$ is found to be 16 times larger than the double-log coefficient $D_{72}$. As a result, the inclusion of the single-log contribution changes drastically the $Z\alpha$ expansion result for the higher-order recoil effect.

Finite nuclear size. – We now consider the correction to the nuclear recoil effect induced by the finite nuclear size (fns), $E_{\text{ins,rec}} = E_{\text{rec}}(\text{ext}) - E_{\text{rec}}(\text{pnt})$, where $E_{\text{rec}}(\text{ext})$ and $E_{\text{rec}}(\text{pnt})$ are the recoil corrections evaluated with the extended and the point-nucleon-charge distributions, respectively. In the hydrogen theory, the leading part of the recoil fns effect is accounted for by introducing the reduced mass prefactor $[M/(m + M)]^3$ in the expression for the fns correction. To the first order in $m/M$, the reduced-mass fns correction is

\[
E_{\text{ins,rm}} = -3 \frac{m}{M} [\epsilon_a(\text{ext}) - \epsilon_a(\text{pnt})], \quad (18)
\]

where $\epsilon_a(\text{ext})$ and $\epsilon_a(\text{pnt})$ are the eigenvalues of the Dirac equation with the extended and the point nuclear distributions, respectively. In the present Letter, we are interested in the higher-order fns recoil correction $E_{\text{ins,rec}}^{\text{ho}}$ beyond the reduced-mass part. It will be parameterized in terms of the function $\delta_{\text{ins}}P$.

\[
E_{\text{ins,rec}}^{\text{ho}} \equiv E_{\text{ins,rec}} - E_{\text{ins,rm}} = \frac{m^2}{M} \frac{(Z\alpha)^3}{\pi n^3} \delta_{\text{ins}}P. \quad (19)
\]

The fns recoil correction was studied in Refs. [22–24]. The numerical accuracy of these studies, however, was not sufficient for making any conclusions about the higher-order fns recoil effect for hydrogen. In the present Letter, we perform the first high-precision evaluation of this effect.

The low-order part of the recoil correction for an extended nuclear charge is given by $E_{\text{ins,rec}}^{\text{ho}}$ (see also [24])

\[
\Delta E_L = \frac{1}{2M} \langle a | \frac{e^2}{a} m^2 - 2m\beta V(r) - W'V(r) - V^2(r) | a \rangle, \quad (20)
\]

where $\beta = (\alpha / 3) \approx 0.2$. For hydrogen, $\alpha$ is such that $\Delta E_L \approx 0.034$ at $Z = 2$.
where $V'(r) = dV(r)/dr$, $W'(r) = dW(r)/dr$,

$$
V(r) = -Z\alpha \int dr' \frac{\rho(r')}{|r - r'|},
$$

and $\rho(r)$ is the density of the nuclear charge distribution ($\int dr \rho(r) = 1$). The Coulomb part of the recoil correction $\Delta E_C$ is given by the same formula (21) with $V(r)$ being the potential of the extended nucleus (21). Exact expressions for the one-transverse-photon part $\Delta E_{tr(1)}$ and the two-transverse-photon part $\Delta E_{tr(2)}$ for the extended nucleus case are not yet known. In the present work, we will use the expressions (5) and (6) derived for the point nucleus and evaluate the matrix elements with the extended-nucleus potential $V(r)$, wave functions, energies, and propagators.

In order to estimate the uncertainty introduced by this approximation, we compare the low-order part as evaluated in two ways: first, by the exact formula (21), $\Delta E_L$, and, second, using the operators derived for a point nucleus (see Eq. (4) of Ref. [22]), $\Delta E_{\text{appr}}$. We then estimate the approximation error as the absolute value of

$$
2 \frac{\Delta E_L - \Delta E_{\text{appr}}}{E_{\text{fns,rec}}^{\text{fns}}} \left[ \Delta E_{\text{tr(1),fns}} + \Delta E_{\text{tr(2),fns}} \right],
$$

where $\Delta E_{\text{tr(1),fns}}$ and $\Delta E_{\text{tr(2),fns}}$ are the fns corrections to the one-transverse-photon and the two-transverse-photon parts, respectively. We note that one should not use $\Delta E_L$ in the denominator of Eq. (21) because of a cancellation of spurious terms between $\Delta E_L$ and $\Delta E_C$ [22]. It might be also mentioned that the full two-transverse-photon fns correction contains terms induced by virtual nuclear excitations [7,14]. These terms should be considered together with the nuclear polarization effects [27,28] and are beyond the scope of this Letter.

The numerical results for the higher-order fns recoil effect are presented in Table II. The calculations for an extended nucleus were performed by the Dual kinetic balance method [30] implemented in the quadruple-precision arithmetics. The results listed in the table have two uncertainties, the first one representing the estimated uncertainty of the approximation and the second one reflecting the dependence of the results on the nuclear model. In order to estimate the model dependence, we performed our calculations for two models of the nuclear charge distribution, the Gauss model [29] and the homogeneously charged sphere model, with the same root-mean-square radii $R$. The results obtained with the Gauss model are listed in the table, whereas the second uncertainty represents the absolute value of the difference of the results of the two models. The error due to uncertainties of the nuclear radii is not included in the table. It should be accounted for separately, e.g., by a simple estimate $(2\delta R/R)\delta_{\text{fns}}P$, where $\delta R$ is the uncertainty of the radius $R$.

In summary, we calculated the nuclear recoil effect to the Lamb shift. The calculation is performed to the first order in the electron-nucleus mass ratio $m/M$ and to all orders in the nuclear binding strength parameter $Z\alpha$, with inclusion of the finite nuclear size effect. The results were shown to be in excellent agreement with the known terms of the $Z\alpha$ expansion. The higher-order recoil contribution beyond the previously known $Z\alpha$-expansion terms was identified.

Our calculation resolves the previously reported disagreement between the numerical all-order and the analytical $Z\alpha$-expansion approaches and eliminates the second-largest theoretical uncertainty in the hydrogen Lamb shift of the 1S and 2S states. For the point nucleus, the higher-order correction beyond the previously known $Z\alpha$-expansion terms for the hydrogen 1S and 2S Lamb shift was found to be 0.05 and 0.08 kHz, respectively. In addition, we found the corresponding shifts from the finite nuclear size recoil effect beyond the reduced mass of $-0.08$ and $-0.01$ kHz. These results may be compared with the 0.01 kHz experimental uncertainty of the 1S-2S transition [11].

The higher-order recoil corrections are also important for the interpretation of experimental results for the hydrogen-deuterium isotope shift. Indeed, the higher-order recoil corrections calculated in the present Letter increase the theoretical value of the hydrogen-deuterium 1S-2S isotope shift by 0.36 kHz (including 0.28 kHz from the point nucleus and 0.08 kHz from the finite nuclear size), which may be compared with the experimental uncertainty of 0.015 kHz [31] and the theoretical uncertainty of 0.6 kHz [32]. The change of the theoretical value increases the deuterium-heavy mean-square charge radii difference as obtained in Ref. [32] by 0.00026 fm².

The results obtained in the present Letter demonstrate the importance of the non-perturbative (in $Z\alpha$) calculations as an alternative to the traditional $Z\alpha$-expansion approach. De-

### Table II: Finite nuclear size recoil correction, expressed in terms of $\delta_{\text{fns}}P$.

| $Z$ | $R$ [fm] | $1s$ | $2s$ | $2p_{1/2}$ | $2p_{3/2}$ |
|-----|----------|------|------|------------|------------|
| 1   | 0.8775   | -0.000 1840 (8)(9) | -0.000 1840 (8)(8) | -0.000 000 01 | -0.000 000 01 |
| 2   | 1.6755   | -0.000 628 (4)(4)  | -0.000 629 (4)(4)  | -0.000 000 06 (6)(0) | -0.000 000 04 (4)(0) |
| 3   | 2.4440   | -0.001 28 (1)(1)   | -0.001 29 (1)(1)   | -0.000 0002 (4)(0)   | -0.000 000 1 (1)(0)   |
| 4   | 2.5190   | -0.001 50 (2)(1)   | -0.001 50 (2)(1)   | -0.000 0003 (7)(0)   | -0.000 000 2 (2)(0)   |
| 5   | 2.4060   | -0.001 56 (2)(1)   | -0.001 56 (2)(1)   | -0.000 0004 (10)(0)  | -0.000 00002 (2)(0)   |

a Shabaev et al. 1998 [22]
spite the smallness of the parameter $Z\alpha$ for hydrogen, $\alpha \approx 0.0073$, the convergence of the (semi-analytical) $Z\alpha$ expansion is complicated by the presence of powers of logarithms. Moreover, the predictive power of the $Z\alpha$ expansion calculations is limited by the difficulty to reliably estimate contributions of the uncalculated tail of the expansion.

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