Recoil nuclear size corrections in hydrogenic systems

Krzysztof Pachucki
Faculty of Physics, University of Warsaw, Pasteura 5, 02-093 Warsaw, Poland

Vojtěch Patkóš
Faculty of Mathematics and Physics, Charles University, Ke Karlovu 3, 121 16 Prague 2, Czech Republic

Vladimir A. Yerokhin
Max–Planck–Institut für Kernphysik, Saupfercheckweg 1, 69117 Heidelberg, Germany

Formulas for the combined nuclear-recoil and finite-nuclear-size effects of order $(Z\alpha)^5$ and $(Z\alpha)^6$ are derived without any expansion in the nuclear charge radius r_C, making them applicable to both electronic and muonic atoms. The obtained results are particularly relevant for high-precision determinations of root-mean-square charge radii from muonic atom spectroscopy. We demonstrate that calculations of the atomic isotope shift based on the widely used Breit approximation give rise to an unphysical nuclear-size contribution that is linear in the nuclear charge radius r_C at order $(Z\alpha)^5$. This spurious term vanishes in a full QED treatment, leaving the correct contribution quadratic in r_C. For electronic atoms, this quadratic term is significantly smaller than the spurious linear contribution.

I. INTRODUCTION

The finite nuclear size modifies the Coulomb potential in the vicinity of the nucleus. Although this effect occurs in the range of just a few femtometers — much smaller than the typical localization region of the wave function $\sim 10^5$ fm's — the resulting shift of energy levels is significant. For example, the $1S$-$2S$ transition in hydrogen is affected by as much as 1 MHz, which should be compared to the experimental accuracy of 10 Hz [1, 2] and the theoretical uncertainty of 1 kHz [3]. It is possible to determine the proton charge radius (and, simultaneously, the Rydberg constant) from observed hydrogen transition energies. A comparison of the extracted radius with an independent determination from the muonic hydrogen [4] resulted in a long-standing discrepancy, known as the "proton radius puzzle". This discrepancy has now been largely resolved in favor of the muonic-hydrogen radius [3].

For atoms with more than one electron, absolute charge radius determinations are not yet feasible, as theoretical precision has not reached the required level. However, it is possible to determine *differences* of nuclear charge radii between two isotopes of the same element. Of particular interest is the comparison of the nuclear radius differences obtained from electronic and muonic atoms. This comparison is highly sensitive to nuclear polarizability effects and provides an opportunity to test fundamental interaction theories.

This field has been developing rapidly in recent years. For instance, the difference in squared charge radii between the deuteron and proton, $r_C^2(d) - r_C^2(p)$, was found to be in perfect agreement between H-D and μH-μD determinations, after a meticulous evaluation of deuteron polarizability effects [5]. Another example is the squared charge radius difference of helium isotopes, $r_C^2(^3\mathrm{He}) - r_C^2(^4\mathrm{He})$, which was initially reported to disagree between electronic and muonic isotope shift measurements [6, 7]. However, it was recently shown that inclusion of the second-order hyperfine-interaction correction [8, 9] resolves this discrepancy. For heavier elements, multiple isotope shift measurements have been conducted for electronic Li, Be, and heavier atoms, while the corresponding muonic-atom measurements are currently being pursued by the QUARTET collaboration [10].

The influence of the finite nuclear size (fns) on atomic energy levels has been extensively studied, both within the expansion over the parameter $Z\alpha$ [11] (where Z is the nuclear charge number and α is the fine-structure constant) and to all orders in $Z\alpha$ [12]. In particularly, Friar [11] derived the fns corrections up to order $(Z\,\alpha)^6$ for the infinitely heavy nucleus. His derivation and final formulas has recently been verified and simplified in Ref. [13].

Theoretical treatment of the fns effect in the presence of a finite-mass nucleus, however, has proven to be significantly more challenging. Addressing this effect, Friar [11] obtained a contribution linear in the nuclear radius r_C at $(Z\,\alpha)^5\,m^3/M$ order, where m is the electron mass and M is the nuclear mass. If correct, this would represent a substantial contribution, as its magnitude is comparable to that of the leading fns recoil effect, which is of order $(Z\alpha)^4(m^4/M)r_C^2$. A similar approach to the fns recoil effect was later employed by Borie and Rinker in their seminal work on muonic atoms [14] and subsequently by Borie in Ref. [15]. It was, however, shown by Shabaev [16] that the linear in r_C fns recoil term disappears in the rigorous QED treatment.

In this work we derive the complete formulas for the recoil fns effects at the $(Z\,\alpha)^5$ and $(Z\,\alpha)^6$ orders. The derivation is carried out without any expansion in the nuclear radius r_C. While an expansion in mr_C is justified and commonly used for electronic atoms, it becomes entirely inadequate for muonic atoms, where $m_\mu r_C \approx 1$ (with m_μ being the muon mass). We explicitly demonstrate that the term linear in r_C is an artifact of the approximate treatment of nuclear recoil. In this approach, the nonrelativistic nuclear kinetic energy and Breit (magnetic) interaction are added to the Dirac equation, a method that is inconsistent with QED. Using the Heavy Particle formulation of QED [17, 18], we apply the exact formula for nuclear recoil effects with finite nuclear size and demonstrate limitations of the approximate treatment.

II. FINITE NUCLEAR SIZE

The finite nuclear size (fns) leads to a shift of binding energies of atomic systems, $E_{\rm fns}$. For a light atom we can perform the expansion of $E_{\rm fns}$ in the parameter $Z\alpha$, where Z is the nuclear charge number and $\alpha = e^2/(4\,\pi)$ is the fine-structure constant,

$$E_{\rm fns} = E^{(4)}_{\rm fns} + E^{(5)}_{\rm fns} + E^{(6)}_{\rm fns} + \ldots\,, \tag{1}$$

where the superscript denotes the order in $Z\alpha$. Each term of this expansion can be further expanded in the mass ratio m/M, where m is the mass of the orbiting particle (electron, muon) and M is the nuclear mass,

$$E^{(n)}_{\rm fns} = E^{(n,0)}_{\rm fns} + E^{(n,1)}_{\rm fns} + \ldots\,, \tag{2}$$

where the second superscript denotes the order in the mass ratio m/M.

The leading-order nuclear contribution is of order $(Z\alpha)^4$ and given by a simple formula

$$E^{(4)}_{\rm fns} = \frac{2\,\pi}{3}\,Z\alpha\,\phi^2(0)\,r_C^2\,, \tag{3}$$

where $\phi(0)$ is the nonrelativistic electron (muon) wave function at the position of nucleus, r_C is the root-mean-square charge radius of the nucleus,

$$r_C^2 = \int d^3r\,r^2\,\rho(\vec r)\,, \tag{4}$$

and $\rho(\vec r)$ is the nuclear charge distribution. Eq. (3) includes the exact dependence on the finite nuclear mass M through

$$\phi^2(0) = \mu^3\,\frac{(Z\alpha)^3}{\pi n^3}\,, \tag{5}$$

where the reduced mass $\mu = mM/(m+M)$.

The next-to-leading fns correction is of order $(Z\alpha)^5$. In the nonrecoil limit it was obtained by Friar [11], with the result

$$E^{(5,0)}_{\rm fns} = -\frac{\pi}{3}\,\phi^2(0)\,(Z\alpha)^2\,m\,r_F^3\,, \tag{6}$$

where

$$r_F^3 = \int d^3r_1 \int d^3r_2\,\rho(r_1)\,\rho(r_2)\,|\vec r_1 - \vec r_2|^3\,. \tag{7}$$

The finite nuclear mass (or, nuclear recoil) effects in Eq. (6) can be partially included in $\phi^2(0)$ through the reduced mass μ. However, there are further nuclear recoil corrections of order $(Z\alpha)^5$ [17], which will be addressed in Sec. V.

III. $(Z\,\alpha)^6$ NONRECOIL CORRECTION FOR nS STATES

In this section we recalculate the fns correction of order $(Z\alpha)^6$ in the nonrecoil limit, $E^{(6,0)}$, for the dipole (exponential) parametrization of the nuclear charge form factor

$$\rho(\vec q^{\,2}) = \frac{\Lambda^4}{(\Lambda^2 + \vec q^{\,2})^2}\,. \tag{8}$$

The charge radii are related to derivatives of $\rho(\vec q^{\,2})$ at $\vec q^{\,2} = 0$, namely

$$\rho'(0) = -\frac{r_C^2}{6}\,,\quad \rho''(0) = \frac{r_{CC}^4}{60}\,, \tag{9}$$

where

$$r_{CC}^4 = \int d^3r\,r^4\rho(\vec r)\,. \tag{10}$$

In the exponential parametrization, the charge radii r_C and r_{CC} are evaluated analytically as

$$r_C = \frac{2\,\sqrt{3}}{\Lambda}\,,\quad r_{CC} = \left(\frac{5}{2}\right)^{1/4} r_C\,. \tag{11}$$

$E^{(6,0)}$ was originally derived by Friar [11] and the much simplified derivation was presented in Ref. [13]. Following this simplified derivation, we split the fns correction for an nS state into the high and low-energy parts,

$$E^{(6,0)}_{\rm fns}(nS) = E_H + E_L\,. \tag{12}$$

The high-energy part E_H is given by the three-photon scattering amplitude with momenta $p_i = (m, \vec q_i)$

$$E_H = -(4\,\pi\,Z\,\alpha)^3\phi^2(0)\int\frac{d^dq_1}{(2\,\pi)^d}\int\frac{d^dq_2}{(2\,\pi)^d}\,\frac{\rho(q_1^2)}{q_1^4}\,\frac{\rho(q_2^2)}{q_2^4}\,\frac{\rho(q_3^2)}{q_3^2}\,{\rm Tr}\left[(\not p_1 + m)\,\gamma_0\,(\not p_2 + m)\,\frac{(\gamma_0 + I)}{4}\right], \tag{13}$$

where we use the dimensional regularization with $d = 3 - 2\,\epsilon$, $\vec q_3 = \vec q_1 - \vec q_2$, and $\phi^2(0) = \langle\phi|\delta^d(r)|\phi\rangle$. The above trace equals to $4\,m^2 + \vec q_1\cdot\vec q_2$, so we split E_H

$$E_H = E_{H1} + E_{H2}\,, \tag{14}$$

into the nonrelativistic E_{H1} and relativistic E_{H2} parts. Using integration formulas from Appendix A we obtain

$$E_{H1} = 4\,\pi\,(Z\,\alpha)^3\,\phi^2(0)\,4\,m^2\,\frac{r_C^4}{36}\left[\frac{1}{4\,\epsilon} + 3 + \frac{7}{128} + \frac{10}{27} + 2\,\ln(2) - \frac{3}{2}\,\ln(3) + \ln(r_C)\right], \tag{15}$$

$$E_{H2} = -4\,\pi\,(Z\,\alpha)^3\,\phi^2(0)\,\frac{r_C^2}{6}\,\biggl[\frac{1}{4\,\epsilon}+\frac{16}{27}-\frac{3}{16}+2\,\ln(2)-\frac{3}{2}\,\ln(3)+\ln(r_C)\biggr]\,. \tag{16}$$

The elimination of $1/\epsilon$ singularities will be performed in atomic units, which in d-dimensions become a little more complicated. The nonrelativistic Hamiltonian in natural units is

$$H = \frac{\vec p^{\,2}}{2\,m} - Z\,\alpha\,\biggl[\frac{1}{r}\biggr]_\epsilon\,, \tag{17}$$

where

$$\biggl[\frac{1}{r}\biggr]_\epsilon = \int\frac{d^dq}{(2\,\pi)^d}\,\frac{4\,\pi}{q^2}\,e^{i\,\vec k\cdot\vec r} = \frac{C_1}{r^{1-2\,\epsilon}}\,, \tag{18}$$

and

$$C_1 = \pi^{\epsilon-1/2}\,\Gamma(1/2-\epsilon)\,. \tag{19}$$

Using coordinates in atomic units

$$\vec r = (m\,Z\,\alpha)^{-1/(1+2\,\epsilon)}\,\vec r_{\rm au}, \tag{20}$$

the Hamiltonian can be written as

$$H = m^{(1-2\,\epsilon)/(1+2\epsilon)}\,(Z\,\alpha)^{2/(1+2\,\epsilon)}\,\biggl[\frac{\vec p_{\rm au}^{\,2}}{2}-\frac{C_1}{r_{\rm au}^{1-2\,\epsilon}}\biggr]. \tag{21}$$

If one pulls out the factor $m^{(1-2\,\epsilon)/(1+2\epsilon)}\,(Z\,\alpha)^{2/(1+2\,\epsilon)} \approx m\,(Z\,\alpha)^2\,(Z\,\alpha\,m)^{-4\,\epsilon}$ from H, then one obtains the nonrelativistic Hamiltonian in atomic units. For the leading relativistic correction, one needs to pull out the factor $m\,(Z\,\alpha)^4\,(Z\,\alpha\,m)^{-8\,\epsilon}$. Similarly for $H^{(6)}$, the common factor $m\,(Z\,\alpha)^6\,(Z\,\alpha\,m)^{-12\,\epsilon}$ is pulled out from all the terms, which corresponds to the replacement $m\to 1, Z\,\alpha\to 1$ in atomic units. This factor is also pulled out from E_H, which is denoted by using the calligraphic symbols,

$$\mathcal{E}_{H1} = 4\,\pi\,\phi^2(0)_{\rm au}\,\frac{m^4\,r_C^4}{36}\,\biggl[\frac{1}{4\,\epsilon}+3+\frac{7}{128}+\frac{10}{27}+2\,\ln(2)-\frac{3}{2}\,\ln(3)+\ln(Z\,\alpha\,m\,r_C)\biggr]\,, \tag{22}$$

$$\mathcal{E}_{H2} = -4\,\pi\,\phi^2(0)_{\rm au}\,\frac{m^2\,r_C^2}{6}\,\biggl[\frac{1}{4\,\epsilon}+\frac{16}{27}-\frac{3}{16}+2\,\ln(2)-\frac{3}{2}\,\ln(3)+\ln(Z\,\alpha\,m\,r_C)\biggr]\,, \tag{23}$$

where

$$\phi^2(0) = (m\,Z\,\alpha)^{d\,(1-2\,\epsilon)}\,\phi^2(0)_{\rm au}\,. \tag{24}$$

The low-energy part $\mathcal{E}_L$ is obtained from the nonrelativistic expansion of the Dirac-Coulomb Hamiltonian in atomic units

$$H_D = \frac{\vec p^{\,2}}{2} - \biggl[\frac{1}{r}\biggr]_\epsilon - \frac{p^4}{8} + \frac{\pi}{2}\,\delta^d(r) + \delta V + \delta^{(2)}V + \frac{1}{8}\,\nabla^2(\delta V)\,, \tag{25}$$

where δV and $\delta^{(2)}V$ are the fns corrections to the Coulomb potential, given by

$$\delta V = -m^2\,\rho'(0)\,4\,\pi\,\delta^d(r) = \frac{2\,\pi}{3}\,m^2\,r_C^2\,\delta^d(r)\,, \tag{26}$$

$$\delta^{(2)}V = \frac{1}{2}\,m^4\,\rho''(0)\,4\,\pi\,\nabla^2\delta^d(r) = \frac{\pi}{30}\,m^4\,r_{CC}^4\,\nabla^2\delta^d(r)\,. \tag{27}$$

$\mathcal{E}_L$ is split into two parts $\mathcal{E}_L = \mathcal{E}_{L1}+\mathcal{E}_{L2}$, where

$$\begin{aligned}\mathcal{E}_{L1} &= \langle\delta V\,\frac{1}{(E-H)'}\,\delta V\rangle + \langle\delta^{(2)}V\rangle \\ &= m^4\,r_C^4\,\frac{4}{9\,n^3}\biggl[-\frac{1}{n}-\frac{1}{2}+\gamma-\ln\frac{n}{2}+\Psi(n)\biggr] - m^4\,r_C^4\,\frac{\pi}{9\,\epsilon}\,\phi^2(0) + m^4\,r_{CC}^4\,\frac{1}{15\,n^5}\,, \qquad (28)\\ \mathcal{E}_{L2} &= 2\,\biggl\langle\delta V\,\frac{1}{(E-H)'}\,\biggl[-\frac{p^4}{8}+\frac{\pi}{2}\,\delta^d(r)\biggr]\biggr\rangle + \biggl\langle\frac{1}{8}\,\nabla^2(\delta V)\biggr\rangle\end{aligned}$$

$$= -m^2\, r_C^2\, \frac{2}{3\, n^3} \left[\frac{9}{4\, n^2} - \frac{1}{n} - \frac{5}{2} + \gamma - \ln\frac{n}{2} + \Psi(n)\right] + m^2\, r_C^2\, \frac{\pi}{6\,\epsilon}\, \phi^2(0)_{\rm au}\,. \tag{29}$$

The complete $O(\alpha^2)$ finite nuclear size correction for an arbitrary nucleus is given by the sum $E^{(6,0)}_{\rm fns} = E_L + E_H$. The diverging $1/\epsilon$ terms in Eqs. (22), (23), (28), and (29) cancel out in the sum and the result is

$$\begin{aligned} E^{(6,0)}_{\rm fns}(nS) = &-(Z\,\alpha)^6\, m^3\, r_C^2\, \frac{2}{3\,n^3} \left[-\frac{5}{4} + \frac{9}{4\,n^2} - \frac{1}{n} - \ln n + \gamma + \Psi(n) + \kappa_1 + \ln(m\, r_C\, Z\,\alpha)\right] \\ &+ (Z\,\alpha)^6\, m^5\, r_C^4\, \frac{4}{9\,n^3} \left[1 - \frac{1}{n} - \ln n + \gamma + \Psi(n) + \kappa_2 + \ln(m\, r_C\, Z\,\alpha)\right] + (Z\,\alpha)^6\, m^5\, r_{CC}^4\, \frac{1}{15\,n^5}\,, \end{aligned} \tag{30}$$

where

$$\kappa_1 = \frac{16}{27} - \frac{23}{16} + \frac{3}{2}\,\ln\frac{4}{3} \approx -0.413\,384\,, \tag{31}$$

$$\kappa_2 = \frac{10}{27} + \frac{199}{128} + \frac{3}{2}\,\ln\frac{4}{3} \approx 2.356\,581\,. \tag{32}$$

This is the complete result of order $(Z\alpha)^6$ in the non-recoil limit. Recoil corrections can partially be accounted for by the replacement $m \to \mu$. However, there are further nuclear recoil effect, which are studied in the remaining part of the paper.

IV. RECOIL FNS CORRECTION

The nuclear recoil effect to the first order in the mass ratio was described theoretically to all orders in $Z\alpha$ for the point-like nucleus [19–21]. The nuclear recoil with the finite-size effect has been derived in the heavy-particle QED (HPQED) approach [18]. The derived formula is

$$E_{\rm rec} = \frac{i}{M} \int_s \frac{d\omega}{2\,\pi}\, \langle\phi| D^j_T(\omega)\, G(E_D+\omega)\, D^j_T(\omega)|\phi\rangle\,, \tag{33}$$

where $G(E) = {}^1/_{(E-H_D)}$ is the Dirac-Coulomb Green function, H_D and E_D are the Dirac Hamiltonian and the Dirac energy, respectively, and

$$D^j_T(\omega,\vec r) = -4\pi Z\alpha\, \alpha^i\, G^{ij}_T(\omega,\vec r)\,, \tag{34}$$

$$G^{ij}_T(\omega,\vec r) = \int \frac{d^3k}{(2\,\pi)^3}\, \frac{\rho(-k^2)}{k^2} \left(\delta^{ij} - \frac{k^i\, k^j}{\omega^2}\right), \tag{35}$$

where $k^2 = \omega^2 - \vec k^2$. The subscript s at the integration sign denotes a symmetric integration around the pole at $\omega = 0$ along the Feynman or Wick rotated contour, see Fig. 1. Because the terms with $1/\omega$ singularity can be separated from terms involving branch cuts starting at $\omega = 0$, this symmetric integration can safely be implemented.

The significant difference with respect to nonrecoil corrections is in the argument of the nuclear-charge form-factor ρ. It is a function of $-k^2 = \vec k^{\,2} - \omega^2$ and the dependence on ω can not be neglected. For this reason we have to assume that $\rho(-k^2)$ can be analytically continued to the whole complex plane, apart from the negative real axis. Not all the charge densities used in the literature allow for analytical continuation. The dipole parametrization is the simplest choice that has analytic continuation on the complex plane and for this reason we use this parametrization in our work.

We now transform $E_{\rm rec}$ to a form that uses the photon propagator in the Coulomb gauge, using the identity

$$D^j_C(\omega) = D^j_T(\omega) + \frac{1}{\omega^2}\left[\omega + E_D - H_D\,,\, p^j(V_C)\right], \tag{36}$$

where

$$D^j_C(\omega,\vec r) = -4\pi Z\alpha\, \alpha^i\, G^{ij}_C(\omega,\vec r)\,, \tag{37}$$

$$G^{ij}_C(\omega,\vec r) = \int \frac{d^3k}{(2\,\pi)^3} \left[\frac{\rho(-k^2)}{k^2}\left(\delta^{ij} - \frac{k^i\, k^j}{\omega^2}\right) - \frac{k^i\, k^j}{\omega^2}\, \frac{\rho(\vec k^2)}{\vec k^2}\right] e^{i\,\vec k\,\vec r}\,. \tag{38}$$

This Coulomb gauge form of the nuclear recoil correction is

$$E_{\rm rec} = -\frac{i}{M} \int_s \frac{d\omega}{2\,\pi}\, \langle\phi|\big[p^j(V_C) - \omega\, D^j_C(\omega)\big]\, G(E_D+\omega)\, \big[p^j(V_C) + \omega\, D^j_C(\omega)\big]|\phi\rangle\, \frac{1}{\omega^2}\,, \tag{39}$$

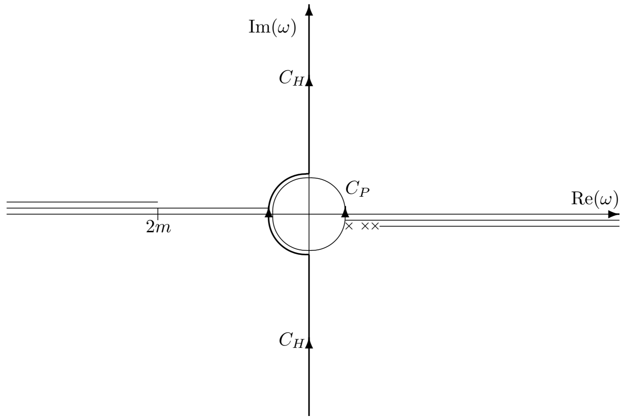

FIG. 1. Integration contours

where $p^j(V_C) = [p^j\,,\,V_C]$. This form is convenient do derive the leading recoil term, which comes from the nuclear kinetic energy and the Breit interaction. We remind at this point that subscript "s" in above equation denotes a symmetric integration around the pole at $\omega = 0$, so

$$\int_s \frac{d\omega}{2\,\pi}\,f(\omega)\,\frac{1}{\omega^2} = \int \frac{d\omega}{2\,\pi}\,f(\omega)\,\frac{1}{2}\left(\frac{1}{(\omega+\epsilon)^2} + \frac{1}{(\omega-\epsilon)^2}\right), \tag{40}$$

where the Wick rotated contour is assumed. We now split this integral in Eq. (39) into two parts

$$\int_s \frac{d\omega}{2\,\pi}\,f(\omega)\,\frac{1}{\omega^2} = \int \frac{d\omega}{2\,\pi}\,f(\omega)\,\frac{1}{2}\left(\frac{1}{(\omega+\epsilon)^2} - \frac{1}{(\omega-\epsilon)^2}\right) + \int \frac{d\omega}{2\,\pi}\,f(\omega)\,\frac{1}{(\omega-\epsilon)^2}\,. \tag{41}$$

The first term in the above yields the recoil correction in the Breit approximation; it will be referred to as the "pole" part in the following. It is calculated

$$\begin{aligned}E_{\rm pole} =&\; -\frac{i}{M}\int\frac{d\omega}{2\,\pi}\,\langle\phi|\big[p^j(V_C) - \omega\,D^j_C(\omega)\big]\,\frac{1}{E_D+\omega-H_D}\,\big[p^j(V_C)+\omega\,D^j_C(\omega)\big]|\phi\rangle\,\frac{1}{2}\left(\frac{1}{(\omega+\epsilon)^2} - \frac{1}{(\omega-\epsilon)^2}\right)\\ =&\; E_{\rm pole1} + E_{\rm pole2}\,.\end{aligned} \tag{42}$$

The first term here is evaluated as

$$\begin{aligned}E_{\rm pole1} =&\; -\frac{i}{M}\int\frac{d\omega}{2\,\pi}\,\langle\phi|p^j(V_C)\,\frac{1}{E_D+\omega-H_D}\,p^j(V_C)|\phi\rangle\,\frac{1}{2}\left(\frac{1}{(\omega+\epsilon)^2} - \frac{1}{(\omega-\epsilon)^2}\right)\\ =&\; -\frac{1}{2\,M}\,\langle\phi|p^j(V_C)\,\frac{1}{(E_D-H_D)^2}\,p^j(V_C)|\phi\rangle\\ =&\; \langle\phi|\frac{p^2}{2\,M}|\phi\rangle\,.\end{aligned} \tag{43}$$

The second term is

$$\begin{aligned}E_{\rm pole2} =&\; -\frac{i}{2\,M}\int\frac{d\omega}{2\,\pi}\,\langle\phi|p^j(V_C)\,G(E_D+\omega)\,D^j_C(\omega)|\phi\rangle\left(\frac{1}{\omega+\epsilon} - \frac{1}{\omega-\epsilon}\right) + {\rm h.c.}\\ =&\; \frac{1}{2\,M}\,\langle\phi|p^j(V_C)\,\frac{1}{E_D-H_D}\,D^j_C(0)|\phi\rangle - \frac{1}{2\,M}\,\langle\phi|D^j_C(0)\,\frac{1}{E_D-H_D}\,p^j(V_C)|\phi\rangle\\ =&\; -\frac{1}{2\,M}\,\langle\phi|\bigg\{p^j\,,\,\frac{Z\alpha}{2}\left[\frac{\delta^{ij}}{r} + \frac{r^i\,r^j}{r^3}\right]_\rho\alpha^i\bigg\}|\phi\rangle\,,\end{aligned} \tag{44}$$

where

$$\frac{1}{2}\left[\frac{\delta^{ij}}{r} + \frac{r^i\,r^j}{r^3}\right]_\rho = 4\,\pi\int\frac{d^3k}{(2\,\pi)^3}\left[\frac{\rho(\vec k^{\,2})}{\vec k^{\,2}}\left(\delta^{ij} - \frac{k^i\,k^j}{\vec k^{\,2}}\right) + \rho'(\vec k^{\,2})\,\frac{k^i\,k^j}{\vec k^{\,2}}\right]e^{i\,\vec k\,\vec r}\,. \tag{45}$$

We thus obtain

$$E_{\rm pole} = \langle\phi|H_M|\phi\rangle\,, \tag{46}$$

where H_M is the nuclear recoil operator in the Breit approximation

$$H_M = \frac{p^2}{2\,M} - \frac{1}{2\,M}\left\{p^j\,,\;\frac{Z\alpha}{2}\left[\frac{\delta^{ij}}{r}+\frac{r^i\,r^j}{r^3}\right]_\rho \alpha^i\right\}. \tag{47}$$

It should be pointed out that usage of H_M with the finite nuclear charge distribution is not fully adequate, since it leads to a numerically large spurious nuclear size correction at $(Z\,\alpha)^5$ order, which will be examined in detail in the next section.

V. $(Z\,\alpha)^5$ RECOIL FNS CORRECTION

The $(Z\,\alpha)^5$ recoil fns correction consists of two parts. The first one is the reduced-mass scalling of $\phi^2(0)$ in Eq. (5), whereas the second part is given by the two-photon exchange amplitude. The sum is

$$\begin{aligned} E^{(5,1)}_{\rm fns} =&\; -3\,\frac{m}{M}\,E^{(5,0)}_{\rm fns} + \frac{i}{M}\,\phi^2(0)\,(4\,\pi\,Z\,\alpha)^2\int_s \frac{d^4k}{(2\,\pi)^4}\,G_T^{ij}(\omega,\vec k)\,G_T^{ik}(\omega,\vec k)\,{\rm Tr}\biggl[\gamma^j\,\frac{1}{\not\psi+\not k-m}\,\gamma^k\,\frac{(\gamma_0+I)}{4}\biggr] \\ =&\; -3\,\frac{m}{M}\,E^{(5,0)}_{\rm fns} + \frac{i}{M}\,\phi^2(0)\,(4\,\pi\,Z\,\alpha)^2\int_s \frac{d^4k}{(2\,\pi)^4}\,[\rho^2(-k^2)-1]\,\frac{\omega}{k^2+2\,m\,\omega}\left(\frac{1}{\omega^4}+\frac{2}{k^4}\right). \end{aligned} \tag{48}$$

We perform the Wick rotation of the integration contour $\omega\to i\,\omega$, integrate first over the 3-dimensional sphere and then over k, obtaining

$$\begin{aligned} E^{(5,1)}_{\rm fns} =&\; -3\,\frac{m}{M}\,E^{(5,0)}_{\rm fns} - \frac{\phi^2(0)}{m\,M}\,(Z\,\alpha)^2 \\ &\times\left[\frac{3\,(1-y^2)\,(1+4\,y^2-35\,y^4)}{8\,y^4} - \frac{3+8\,y^2+40\,y^4-140\,y^6+105\,y^8}{16\,y^5}\,\ln\frac{1+y}{1-y} - \ln\frac{1-y^2}{4}\right], \end{aligned} \tag{49}$$

where $y=\sqrt{1-4\,m^2/\Lambda^2}$. The expansion of the above formula in small $m\,r_C$ reproduces the result obtained in Ref. [17],

$$E^{(5,1)}_{\rm fns} = -\frac{m}{M}\,\phi^2(0)\,(Z\,\alpha)^2\left(-\frac{43}{12}+\ln 12 - 2\,\ln m\,r_C\right)r_C^2 - 3\,\frac{m}{M}\,E^{(5,0)}_{\rm fns} + \frac{m^2}{M}\,O\bigl(m\,r_C\bigr)^4\,. \tag{50}$$

We note that $E^{(5,1)}_{\rm fns}$ for electronic atoms depends on the nuclear radius as r_C^2. If we were using the Breit approximation to derive the recoil fns correction of this order, we would obtain a very different result, which is linear in the nuclear radius $\propto r_C$ and numerically dominating. This fact was first pointed out by Friar in Ref. [11]. The disappearance of the spurious $\propto r_C$ term in a full-QED calculation was demonstrated by Shabaev [16]. Indeed, calculating the $\omega=0$ pole contribution in Eq. (48), which corresponds to the Breit approximation, we obtain

$$\begin{aligned} E^{(5,1)}_{\rm rec,pole} =&\; -3\,\frac{m}{M}\,E^{(5,0)}_{\rm fns} + \frac{i}{M}\,\phi^2(0)\,(4\,\pi\,Z\,\alpha)^2\int \frac{d^4k}{(2\,\pi)^4}\,\frac{(\rho^2(-k^2)-1)}{k^2+2\,m\,\omega}\,\frac{1}{2}\left(\frac{1}{(\omega+\epsilon)^3}-\frac{1}{(\omega-\epsilon)^3}\right) \\ =&\; -3\,\frac{m}{M}\,E^{(5,0)}_{\rm fns} - \frac{m^2}{M}\,\frac{(Z\,\alpha)^5}{n^3}\,\frac{35}{32\,\sqrt{3}}\bigl(m\,r_C - 2\,m^3\,r_C^3\bigr)\,. \end{aligned} \tag{51}$$

$E^{(5,1)}_{\rm rec,pole}$ contains a spurious term $\sim r_C$, which is much larger than the correct one $\sim r_C^2\,\ln m\,r_C$. The spurious term is only an artefact of an approximate treatment of the nuclear recoil correction; it disappears in the correct QED treatment.

We conclude that if one uses the relativistic recoil operator H_M given by Eq. (47) (as it is routinely done in many-body calculations of atomic systems, see, e.g., Ref. [22]), one obtains unphysical results for the recoil fns correction. In principle, the spurious term can be removed by an additional correction to H_M. However, the coefficient of this additional term depends on the form of the exact forms of the Breit interaction for the extended size nucleus and of the projector to the positive-energy subspace (used in the RMBPT or MCDF approaches). So, the additional correction to H_M has to be carefully adjusted to the particular approximate calculations, in order to remove this spurious linear in r_C term. A better way is to account for the QED recoil effects, e.g., by means of the model recoil operator [23].

TABLE I. Table of numerical values of function $\delta f(x)$ defined by Eq. (55).

x	$\delta f(x)$	x	$\delta f(x)$	x	$\delta f(x)$	x	$\delta f(x)$	x	$\delta f(x)$
0.45	−3.378 26	0.85	−2.41382	1.25	−1.90976	1.65	−1.59053	2.05	−1.36749
0.50	−3.208 65	0.90	−2.33488	1.30	1.86238	1.70	−1.55846	2.10	−1.34418
0.55	−3.058 29	0.95	−2.26153	1.35	−1.81749	1.75	−1.52775	2.15	−1.32169
0.60	−2.923 74	1.00	−2.19315	1.40	−1.77489	1.80	−1.49831	2.20	−1.29998
0.65	−2.802 38	1.05	−2.12921	1.45	−1.73440	1.85	−1.47005	2.25	−1.27901
0.70	−2.692 16	1.10	−2.06926	1.50	−1.69585	1.90	−1.44290	2.30	−1.25874
0.75	−2.591 49	1.15	−2.01292	1.55	−1.65911	1.95	−1.41680	2.35	−1.23914
0.80	−2.499 06	1.20	−1.95985	1.60	−1.62404	2.00	−1.39168	2.40	−1.22017

VI. $(Z\,\alpha)^6$ RECOIL FNS CORRECTION

We now will derive the fns contribution of order $(Z\alpha)^6$ coming from the recoil correction $E_{\rm rec}$ given by Eq. (33). Let us split the ω integration contour in Eq. (33) into the "pole-contribution" part C_P and the high-energy part C_H. C_P encircles the pole at $\omega = 0$, whereas C_H is the Wick-rotated integration contour along the negative real axis, which goes around the $\omega = 0$ pole from the left, see Fig. 1. Accordingly, we split $E^{(6,1)}_{\rm fns}$ into three parts, assuming dimensional regularization

$$E^{(6,1)}_{\rm fns} = E^{(1)}_H + E^{(1)}_P + E^{(1)}_L\,. \tag{52}$$

$E^{(1)}_H$ is the hard three-photon exchange with the ω integration carried out along the C_H contour. After subtracting the point-nucleus limit, the limit $\varepsilon \to 0$ can safely be approached. $E^{(1)}_P$ is the high-energy "pole" contribution, that is similar to the nonrecoil E_H in Eq. (13), while $E^{(1)}_L$ is the low-energy "pole" contribution that is similar to the nonrecoil E_L in Eqs. (28), (29).

The fns recoil high-energy part $E^{(1)}_H$ is obtained from Eq. (33) using the high-momentum three-photon exchange amplitude, which yield

$$\begin{aligned}
E^{(1)}_H = {} & \frac{i}{M}\,(-4\pi Z\alpha)^3\,\phi^2(0)\int_{C_H}\frac{d\omega}{2\,\pi}\int\frac{d^dk_1}{(2\,\pi)^d}\int\frac{d^dk_2}{(2\,\pi)^d}\,\frac{\rho(-k_1^2)\,\rho(-k_2^2)\,\rho(\vec k_3^{\,2})-1}{k_1^2\,k_2^2\,\vec k_3^{\,2}}\\
& \times\left(\delta^{ik}-\frac{k_2^i\,k_2^k}{\omega^2}\right)\left(\delta^{jk}-\frac{k_1^j\,k_1^k}{\omega^2}\right)\mathrm{Tr}\bigg[\bigg(\gamma^i\,\frac{1}{\not k_2+\not t-m}\,\gamma^0\,\frac{1}{\not k_1+\not t-m}\,\gamma^j\\
& +\gamma^0\,\frac{1}{\not k_1-\not k_2+\not t-m}\,\gamma^i\,\frac{1}{\not k_1+\not t-m}\,\gamma^j+\gamma^i\,\frac{1}{\not k_2+\not t-m}\,\gamma^j\,\frac{1}{\not k_2-\not k_1+\not t-m}\,\gamma^0\bigg)\,\frac{\gamma^0+I}{4}\bigg]\,,
\end{aligned} \tag{53}$$

where $\vec k_3 = \vec k_1 - \vec k_2$ and $k_i^2 = \omega^2 - \vec k_i^{\,2}$. We perform at first $\int d^dk_1\,d^dk_2$ integration analytically using formulas from Appendix A, and next integration over ω along C_H contour with $\varepsilon \to 0$ limit. The result is

$$E^{(1)}_H = -\,\frac{m^2}{M}\,\frac{(Z\,\alpha)^6}{n^3}\,f(m\,r_C)\,, \tag{54}$$

where

$$f(m\,r_C) = \frac{m\,r_C}{2\sqrt3}\left(\frac{13}{6}-\frac{64}{9\sqrt3}-\frac{350}{9\,\pi}+\frac{80\,\ln 2}{\pi}\right)+\frac{m^2\,r_C^2}{12}\left(\frac{1895}{216}+64\,\ln 2\right)+(m\,r_C)^3\,\delta f(m\,r_C)\,. \tag{55}$$

The function $\delta f(m\,r_C)$ was computed numerically with help of Wolfram Mathematica. The contribution of δf is negligible for electronic atoms but significant for the muonic atoms. Table I lists numerical values of $\delta f(m\,r_C)$ for the range of argument $0.45 \le m_\mu\,r_C \le 2.40$ relevant for muonic atoms.

Before considering the recoil fns "pole" high-energy part $E^{(1)}_P$, let us calculate the reduced-mass correction to $\phi^2(0)$ in the dimensional regularization. The nonrelativistic Hamiltonian in atomic units is

$$H_\mu = \frac{\vec p^{\,2}}{2}+\frac{\vec p^{\,2}}{2}\,\frac{m}{M}-\frac{C_1}{r^{1-2\,\epsilon}}\,. \tag{56}$$

Variable change $\vec r \to \vec r\,\mu^{-1/(1+2\,\epsilon)}$ leads to $H_\mu \to \mu^{\frac{1-2\,\epsilon}{1+2\,\epsilon}}\,H \approx (1-\frac{m}{M}\,(1-4\,\epsilon))\,H$, thus

$$\phi^2(0) = \langle\phi|\delta^d(r)|\phi\rangle \to \mu^{\frac{3-2\,\epsilon}{1+2\,\epsilon}}\,\phi^2(0) \approx \mu^{3-8\,\epsilon}\,\phi^2(0) \approx \left(1-(3-8\,\epsilon)\,\frac{m}{M}\right)\phi^2(0)\,. \tag{57}$$

We now examine the "pole" contribution, which is split into two parts:

$$E_P^{(1)} = E_{P1} + E_{P2}\,. \tag{58}$$

The first part E_{P1} is induced by $p^2/(2\,M)$ and evaluated as

$$\begin{aligned} E_{P1} =& -(3-8\,\epsilon)\,\frac{m}{M}\,E_H - (4\,\pi\,Z\,\alpha)^3\,\phi^2(0)\int\frac{d^dq_1}{(2\,\pi)^d}\int\frac{d^dq_2}{(2\,\pi)^d}\,\frac{\rho(q_1^2)}{q_1^2}\,\frac{\rho(q_2^2)}{q_2^2}\,\frac{\rho(q_3^2)}{q_3^2}\,\frac{1}{2\,M} \\ &\times\biggl\{\vec{q}_1^{\,2}\,\mathrm{Tr}\biggl[\frac{1}{(\not p_1 - m)}\,\gamma_0\,\frac{1}{(\not p_1 - m)}\,\gamma_0\,\frac{1}{(\not p_2 - m)}\,\frac{(\gamma_0+I)}{4}\biggr] + (1\leftrightarrow 2)\biggr\} \\ =& -(5-8\,\epsilon)\,\frac{m}{M}\,E_{H1} - (3-8\,\epsilon)\,\frac{m}{M}\,E_{H2} \\ &+ (4\,\pi\,Z\,\alpha)^3\,\phi^2(0)\int\frac{d^dq_1}{(2\,\pi)^d}\int\frac{d^dq_2}{(2\,\pi)^d}\,\frac{\rho(q_1^2)}{q_1^4}\,\frac{\rho(q_2^2)}{q_2^4}\,\frac{\rho(q_3^2)}{q_3^2}\,\frac{m}{M}\,(\vec{q}_1+\vec{q}_2)^2\,, \end{aligned} \tag{59}$$

where E_H, E_{H1}, and E_{H2} are defined in Eqs. (14), (15), and (16) correspondingly. The second term E_{P2} is due to the electron-nucleus Breit interaction. It is expressed as

$$\begin{aligned} E_{P2} =& (4\,\pi\,Z\,\alpha)^3\,\phi^2(0)\int\frac{d^dq_1}{(2\,\pi)^d}\int\frac{d^dq_2}{(2\,\pi)^d}\,\frac{\rho(q_1^2)}{q_1^2}\,\frac{\rho(q_2^2)}{q_2^2}\,\frac{\rho(q_3^2)}{q_3^2}\,\frac{1}{2\,M} \\ &\times\biggl\{\mathrm{Tr}\biggl[\gamma^i\,\frac{1}{(\not p_1 - m)}\,\gamma_0\,\frac{1}{(\not p_2 - m)}\,\gamma_0\,\frac{(\gamma_0+I)}{4}\biggr]\,q_1^j\,G_C^{ij}(0,-\vec{q}_1)\,\frac{q_1^2}{\rho(q_1^2)} \\ &+\mathrm{Tr}\biggl[\gamma_0\,\frac{1}{(\not p_1 - m)}\,\gamma^i\,\frac{1}{(\not p_2 - m)}\,\gamma_0\,\frac{(\gamma_0+I)}{4}\biggr]\,(q_1^j+q_2^j)\,G_C^{ij}(0,\vec{q}_3)\,\frac{q_3^2}{\rho(q_3^2)} \\ &+\mathrm{Tr}\biggl[\gamma_0\,\frac{1}{(\not p_1 - m)}\,\gamma_0\,\frac{1}{(\not p_2 - m)}\,\gamma^i\,\frac{(\gamma_0+I)}{4}\biggr]\,q_2^j\,G_C^{ij}(0,\vec{q}_2)\,\frac{q_2^2}{\rho(q_2^2)}\biggr\}\,. \end{aligned} \tag{60}$$

where $\vec{q}_3 = \vec{q}_1 - \vec{q}_2$. After performing traces one obtains

$$\begin{aligned} E_{P2} =& -(4\,\pi\,Z\,\alpha)^3\,\phi^2(0)\int\frac{d^dq_1}{(2\,\pi)^d}\int\frac{d^dq_2}{(2\,\pi)^d}\,\frac{\rho(q_1^2)}{q_1^4}\,\frac{\rho(q_2^2)}{q_2^4}\,\frac{\rho(q_3^2)}{q_3^4}\,\frac{1}{M} \\ &\times\biggl\{4\,q_1^2\,q_2^2 - 4\,(\vec{q}_1\cdot\vec{q}_2)^2 + \frac{\rho'(q_3^2)}{\rho(q_3^2)}\,q_3^2\,\bigl[(q_1^2-q_2^2)^2 + q_2^2\,q_3^2 + q_1^2\,q_3^2\bigr]\biggr\}\,. \end{aligned} \tag{61}$$

The complete fns recoil "pole" high-energy part $E_P^{(1)} = E_{P1} + E_{P2}$ is

$$E_P^{(1)} = -(5-8\,\epsilon)\,\frac{m}{M}\,E_{H1} - (3-8\,\epsilon)\,\frac{m}{M}\,E_{H2} + \delta E_P\,, \tag{62}$$

where

$$\begin{aligned} \delta E_P =& -(4\,\pi\,Z\,\alpha)^3\,\phi^2(0)\,\frac{m}{M}\int\frac{d^dq_1}{(2\,\pi)^d}\int\frac{d^dq_2}{(2\,\pi)^d}\,\frac{\partial}{\partial q_3^2}\frac{\rho(q_1^2)}{q_1^4}\,\frac{\rho(q_2^2)}{q_2^4}\,\rho(q_3^2)\,\biggl[\frac{(q_1^2-q_2^2)^2}{q_3^2} + q_2^2 + q_1^2\biggr] \\ =& \frac{(Z\,\alpha)^6}{n^3}\,\frac{m^2}{M}\,\frac{2471}{2592}\,m^2\,r_C^2\,. \end{aligned} \tag{63}$$

The low-energy part $E_L^{(1)}$, with $|\vec{k}| \sim m\,\alpha$, is obtained by using the nonrelativistic expansion of H_M in Eq. (47). Using

$$-\frac{1}{8\,\pi}\biggl[\frac{\delta^{ij}}{r} + \frac{r^i\,r^j}{r^3}\biggr]_\rho = -\frac{1}{8\,\pi}\biggl[\frac{\delta^{ij}}{r} + \frac{r^i\,r^j}{r^3}\biggr]_\epsilon - \rho'(0)\,\delta^d(r)\,, \tag{64}$$

we obtain

$$H_M = \frac{m}{M}\biggl[\frac{p^2}{2} - \frac{1}{2}\,p^i\left(\frac{\delta^{ij}}{r} + \frac{r^ir^j}{r^3}\right)_\epsilon p^j + \frac{1}{4}\,\{p^i,\{p^i,\delta V\}\}\biggr]\,. \tag{65}$$

This expression should be combined with the nonrelativistic expansion of the Dirac-Coulomb Hamiltonian in Eq. (25) to obtain

$$H_D + H_M = H_\mu - \frac{p^4}{8} + \frac{\pi}{2}\,\delta^d(r) + \delta V + \delta^{(2)}V + \frac{1}{8}\,\nabla^2(\delta V) + \frac{m}{M}\left[-\frac{1}{2}\,p^i\left(\frac{\delta^{ij}}{r} + \frac{r^i r^j}{r^3}\right)_\epsilon p^j + \frac{1}{4}\,\{p^i,\{p^i,\delta V\}\}\right]. \tag{66}$$

After rescaling the reduced mass, the above expression becomes

$$\begin{aligned} H_D + H_M = {}& \left(1 - \frac{m}{M}\,(1-4\,\epsilon)\right) H - \left(1 - \frac{m}{M}\,(4-8\,\epsilon)\right)\frac{p^4}{8} + \left(1 - \frac{m}{M}\,(3-8\,\epsilon)\right)\left(\frac{\pi}{2}\,\delta^d(r) + \delta V\right) \\ & + \left(1 - \frac{m}{M}\,5\right)\left(\delta^{(2)}V + \frac{1}{8}\,\nabla^2(\delta V)\right) + \frac{m}{M}\left[-\frac{1}{2}\,p^i\left(\frac{\delta^{ij}}{r} + \frac{r^i r^j}{r^3}\right)_\epsilon p^j + \frac{1}{4}\,\{p^i,\{p^i,\delta V\}\}\right]. \end{aligned} \tag{67}$$

Similarly to the derivation of the nonrecoil fns correction, the low-energy part $\mathcal{E}_L^{(1)}$ is split into two parts,

$$\mathcal{E}_L^{(1)} = \mathcal{E}_{L1}^{(1)} + \mathcal{E}_{L2}^{(1)}\,, \tag{68}$$

where $\mathcal{E}_{L1}^{(1)}$ is the nonrelativistic contribution proportional to r_C^4,

$$\mathcal{E}_{L1}^{(1)} = \langle \delta V\,\frac{1}{(E-H)'}\,\delta V\rangle + \langle \delta^{(2)}V\rangle = -(5-12\,\epsilon)\,\frac{m}{M}\,\mathcal{E}_{L1}\,, \tag{69}$$

and $\mathcal{E}_{L2}^{(1)}$ is the relativistic part proportional to r_C^2

$$\begin{aligned} \mathcal{E}_{L2}^{(1)} = {}& \frac{m}{M}\biggl\{ -\frac{5}{8}\,\langle\nabla^2(\delta V)\rangle + 2\,(6-12\,\epsilon)\left\langle \delta V\,\frac{1}{(E-H)'}\,\frac{p^4}{8}\right\rangle - 2\,(5-12\,\epsilon)\left\langle \delta V\,\frac{1}{(E-H)'}\,\frac{\pi}{2}\,\delta^d(r)\right\rangle \\ & + \frac{1}{4}\,\langle\{p^i,\{p^i,\delta V\}\}\rangle - 2\left\langle \delta V\,\frac{1}{(E-H)'}\,\frac{1}{2}\,p^i\left[\frac{\delta^{ij}}{r} + \frac{r^i r^j}{r^3}\right]_\epsilon p^j\right\rangle\biggr\} \\ = {}& -(3-12\,\epsilon)\,\frac{m}{M}\,\mathcal{E}_{L2} + \frac{m^3}{M}\,r_C^2\,\frac{1}{n^3}\left(\frac{1}{n^2} + \frac{2}{3}\right). \end{aligned} \tag{70}$$

We observe here an additional state dependence, beyond this in $\mathcal{E}_{L2}$. The sum of all calculated recoil terms is

$$E_{\rm fns}^{(6,1)} = E_H^{(1)} + E_P^{(1)} + E_L^{(1)} = -\frac{m^2}{M}\,\frac{\partial}{\partial m}E_{\rm fns}^{(6,0)} + \frac{m^2}{M}\,\frac{(Z\,\alpha)^6}{n^3}\left[m^2\,r_C^2\left(\frac{1}{n^2} + \frac{4199}{2592}\right) - f(m\,r_C)\right], \tag{71}$$

where the function f is defined in Eq. (54). In the above, the first term corresponds to the reduced-mass rescaling of the corresponding nonrecoil correction and the second one is a remainder. We note that the function f contains a contribution linear in r_C (see Eq. (55)), which is numerically large for electronic atoms. As a result, the $(Z\alpha)^6$ recoil fns contribution numerically dominates over the $(Z\alpha)^5$ contribution for electronic atoms - a surprising fact, first found in Ref. [17] basing on numerical calculations.

VII. TOTAL FNS CORRECTION WITH RECOIL

We now summarize all known contributions to the fns effect of light hydrogen-like atoms for a finite-mass nucleus, $E_{\rm fns} = E_{\rm fns}^{(4)} + E_{\rm fns}^{(5)} + E_{\rm fns}^{(6)}$. The leading-order nuclear contribution is

$$E_{\rm fns}^{(4)} = \frac{2\,\pi}{3}\,\frac{(Z\alpha)^4}{\pi n^3}\,\mu^3\,r_C^2\,\delta_{l,0}\,, \tag{72}$$

where $\mu = mM/(m+M)$ is the reduced mass. The above formula is model-independent and includes the nuclear recoil effect to all orders in m/M.

The finite nuclear size contribution of order $(Z\alpha)^5$, calculated to first order in m/M but to all orders in mr_C, is given by

$$\begin{aligned} E_{\rm fns}^{(5)} = {}& -m\,\frac{(Z\,\alpha)^5}{\pi n^3}\,\mu^3\,\delta_{l,0}\biggl\{\frac{\pi\,r_F^3}{3} + \frac{1}{M\,m^2}\biggl[\frac{3\,(1-y^2)\,(1+4\,y^2-35\,y^4)}{8\,y^4} \\ & - \frac{3+8\,y^2+40\,y^4-140\,y^6+105\,y^8}{16\,y^5}\,\ln\frac{1+y}{1-y} - \ln\frac{1-y^2}{4}\biggr]\biggr\}\,, \end{aligned} \tag{73}$$

where $y = \sqrt{1-(mr_C)^2/3}$. This contribution is model-dependent. The model dependence of the nonrecoil part can be estimated by comparing results obtained in the exponential and Gaussian models, with corresponding results for r_F summarized in Table II. The recoil part of $E^{(5)}_{\rm fns}$ is calculated within the exponential nuclear model only. In the case of an arbitrary nuclear model, the above formulas are not valid and one has to return to Eq. (48). For the integral over k in Eq. (48) to exist, the nuclear form factor $\rho(-k^2)$ should be not only an analytical function in the complex plane (with a branch cut on the negative axis), but should also vanish at complex infinity. We note that many of popular nuclear models (Gaussian, Fermi) do not satisfy this condition and are thus not suitable for describing the recoil fns effect.

For the electronic atoms, Eq. (73) can be simplified by using the fact that the parameter mr_C is small. Expanding in mr_C, we obtain

$$E^{(5)}_{\rm fns} = -\,m\,\frac{(Z\,\alpha)^5}{n^3}\,\mu^3\,\delta_{l,0}\biggl[\frac{r_F^3}{3} - \frac{1}{\pi}\biggl(\frac{43}{12} - \ln 12 + 2\,\ln m\,r_C\biggr)\frac{r_C^2}{M} + \frac{1}{m^2 M}\,O\bigl(m\,r_C\bigr)^4\biggr]\,. \tag{74}$$

The dependence on r_C is the same for all the models and only the coefficient $43/12 - \ln 12$ is a subject of a model dependence.

The finite size effect at order $(Z\alpha)^6$, calculated for nS states to first order in m/M but to all orders in mr_C is given by

$$\begin{aligned} E^{(6)}_{\rm fns}(nS) = &-(Z\,\alpha)^6\,\mu^3\,r_C^2\,\frac{2}{3\,n^3}\biggl[-\frac{5}{4} + \frac{9}{4\,n^2} - \frac{1}{n} - \ln n + \gamma + \Psi(n) + \kappa_1 + \ln(\mu\,r_C\,Z\,\alpha)\biggr] \\ &+ (Z\,\alpha)^6\,\mu^5\,r_C^4\,\frac{4}{9\,n^3}\biggl[1 - \frac{1}{n} - \ln n + \gamma + \Psi(n) + \kappa_2 + \ln(\mu\,r_C\,Z\,\alpha)\biggr] \\ &+ (Z\,\alpha)^6\,\mu^5\,r_{CC}^4\,\frac{1}{15\,n^5} + \frac{m^2}{M}\,\frac{(Z\,\alpha)^6}{n^3}\biggl[m^2\,r_C^2\biggl(\frac{1}{n^2} + \frac{4199}{2592}\biggr) - f(m\,r_C)\biggr]\,, \end{aligned} \tag{75}$$

where r_{CC} is defined by Eq. (10), κ_1 and κ_2 are defined in Eqs. (31), (32) and $f(m\,r_C)$ is defined in Eq. (55), with numerical values summarized in Table I. The contribution $E^{(6)}_{\rm fns}$ is model-dependent; the model dependence coming through r_{CC}, κ_1, κ_2, and $f(mr_C)$. The model dependence of the nonrecoil part can be estimated by comparing results obtained in the exponential and Gaussian models, with help of results summarized in Table II. The recoil part of $E^{(6)}_{\rm fns}$ is calculated for the exponential nuclear model only. For electronic atoms, $E^{(6)}_{\rm fns}$ can be expanded in mr_C, with the result

$$\begin{aligned} E^{(6)}_{\rm fns}(nS) = &-(Z\,\alpha)^6\,\mu^3\,r_C^2\,\frac{2}{3\,n^3}\biggl[-\frac{5}{4} + \frac{9}{4\,n^2} - \frac{1}{n} - \ln n + \gamma + \Psi(n) + \kappa_1 + \ln(\mu\,r_C\,Z\,\alpha)\biggr] \\ &+ \frac{m^2}{M}\,\frac{(Z\,\alpha)^6}{n^3}\biggl[-\frac{m\,r_C}{2\sqrt{3}}\biggl(\frac{13}{6} - \frac{64}{9\sqrt{3}} - \frac{350}{9\,\pi} + \frac{80\,\ln 2}{\pi}\biggr) + m^2\,r_C^2\biggl(\frac{1}{n^2} + \frac{8}{9} - \frac{16}{3}\,\ln 2\biggr) + O\bigl(m\,r_C\bigr)^3\biggr]\,, \end{aligned} \tag{76}$$

where the second line includes all terms beyond the reduced-mass scaling of the nonrecoil relativistic correction. Regarding model dependence we expect the same functional form, while the constant κ_1 and value of coefficients of r_C, r_C^2 in the second line of Eq. (76) are model dependent.

We would like to point out that for electronic atoms, the $(Z\alpha)^5$ fns correction is very small numerically (since it is suppressed both by $Z\alpha$ and a small parameter mr_C as compared to the leading fns effect). On the contrary, the $(Z\alpha)^6$ fns contribution, being enhanced by $\ln(mr_C Z\alpha)$, is numerically significant and gives the dominant correction to the leading fns correction (72).

For the P states, the finite size corrections $E^{(4)}_{\rm fns}$ and $E^{(5)}_{\rm fns}$ vanish, while at the $(Z\,\alpha)^6$ order they take the form [24]

$$E^{(6)}_{\rm fns}(nP_J) = (Z\,\alpha)^6\,\frac{1}{9}\biggl(\frac{1}{n^3} - \frac{1}{n^5}\biggr)\biggl[\biggl(\frac{1}{2} - \langle\vec{L}\cdot\vec{s}\rangle\biggr)\mu^3\,r_C^2 + \frac{1}{5}\,\mu^5\,r_{CC}^4\biggr]\,, \tag{77}$$

where $\langle\vec{L}\cdot\vec{s}\rangle = -1, 1/2$ for $J = \frac{1}{2}, \frac{3}{2}$, correspondingly. This simple formula is valid up to the first order in m/M mass ratio; the general result valid to all orders in mass ratio was obtained in Ref. [24]. $E^{(6)}_{\rm fns}$ vanishes for states with $L > 1$.

Formulas summarized in this section demonstrate that the dependence of the fns effect on the nuclear charge radius r_C is generally quite complicated. It contains odd powers of r_C, logarithms, as well as model-dependent parameters. This makes it abundantly clear that the use of the so-called Seltzer's moments [25], which assumes expansion of the fns correction to energies in even multipoles of r_C, is incorrect. It is truly astonishing that the expansion in terms of Seltzer's moments, despite lacking any physical justification, continues to appear in the literature up to this day [22, 26].

VIII. RESULTS AND DISCUSSION

In this paper we extended our previous studies of the fns effect for electronic and muonic hydrogen-like atoms [13], by calculating the nuclear recoil fns corrections of order $(Z\alpha)^5$ and $(Z\alpha)^6$. Calculations were performed without any expan-

TABLE II. Various results for the exponential and the Gaussian models of the nuclear charge distributions.

	Exponential	Gaussian
$\rho(q^2)$	$\Lambda^4/(\Lambda^2+q^2)^2$	$\exp\left(\frac{a\,q^2}{2}\right)$
$\rho(r)$	$\Lambda^3/(8\,\pi)\,e^{-\Lambda\,r}$	$(2\pi a)^{-3/2}\exp\left(-\frac{r^2}{2\,a}\right)$
$V(r)$	$(1/r)\left(1-e^{-\Lambda\,r}\right)-(\Lambda/2)\,e^{-\Lambda\,r}$	$(1/r)\,\mathrm{erf}\left(\frac{r}{\sqrt{2\,a}}\right)$
r_C	$2\sqrt{3}/\Lambda$	$\sqrt{3\,a}$
r_{CC}/r_C	1.257 433	1.136 219
r_F/r_C	1.558 965	1.514 599
κ_1	−0.413 384	−0.465 457
κ_2	2.356 581	1.688 528

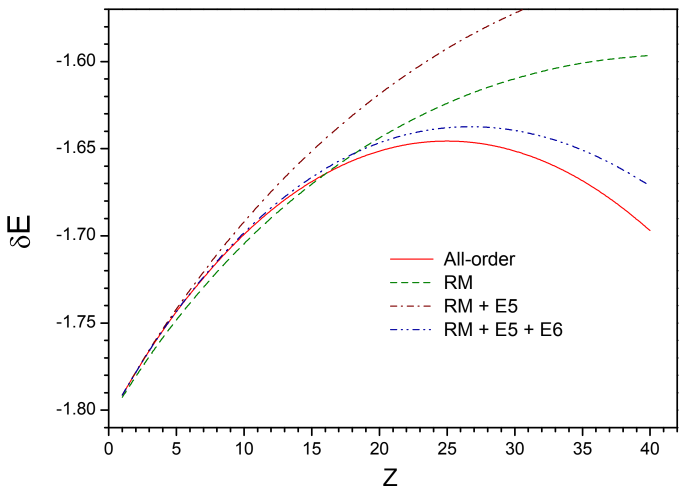

FIG. 2. Finite size recoil correction, calculated to all orders in $Z\alpha$ (red solid line) and within the $Z\alpha$ expansion, for the $1s$ state of muonic atoms with the nuclear charge radius fixed by $r_C = 1$ fm. Units are $\delta E/[(m^2/M)(Z\alpha)^4/\pi]$. The dashed green line corresponds to the reduced-mass (RM) contribution $-3(m/M)E_{\rm fns}$ coming from $\phi^2(0)$. The dashed-dot brown line shows results with inclusion of the $(Z\alpha)^5$ correction (E5), whereas the dashed-dot-dot blue line shows results with additional inclusion of the $(Z\alpha)^6$ correction (E6).

sion in the nuclear charge radius r_C, ensuring that the obtained results are applicable for muonic atoms.

The derived formulas were checked by comparing with numerical calculations performed to all order in $Z\alpha$ by method described in Ref. [27]. The comparison of the all-order and the $Z\alpha$-expansion results is in Fig. 2 shown for the $1S$ state of muonic atoms. In order to obtain smooth curves, we artificially fixed the nuclear charge radius at $r_C = 1$ fm for all nuclear charges. We observe that the $Z\alpha$-expansion results converge to the all-order values in the limit of $Z \to 0$. It is remarkable that the inclusion of the $(Z\alpha)^6$ correction is essential in order to achieve good agreement with all-order results already for small values of Z.

Now we examine the magnitude of the obtained corrections for several interesting from the experimental point of view cases. The first case is the $2S$-$1S$ transition in hydrogen, which is the basis of the determination of the Rydberg constant and has been measured with a 10 Hz accuracy [1, 2]. We obtain the following results for the $(Z\alpha)^5$ and $(Z\alpha)^6$ fns corrections:

$$
\begin{aligned}
E^{(5,0)}_{\rm fns}(\mathrm{H}, 2S{-}1S) &= 29\ \mathrm{Hz}\,,\\
E^{(5,1)}_{\rm fns}(\mathrm{H}, 2S{-}1S) &= 20\ \mathrm{Hz}\,,\\
E^{(6,0)}_{\rm fns}(\mathrm{H}, 2S{-}1S) &= -585\,(5)\ \mathrm{Hz}\,,\\
E^{(6,1)}_{\rm fns}(\mathrm{H}, 2S{-}1S) &= 20\ \mathrm{Hz}\,.
\end{aligned}
\tag{78}
$$

We see that the $E^{(5,0)}_{\rm fns}$ correction is abnormally small, being suppressed by an additional power of r_C. It is interesting that the recoil $(Z\alpha)^5$ correction has nearly the same magnitude as the nonrecoil contribution to this order. We note that for hydrogen the $(Z\alpha)^5$ corrections are already included in the nuclear-structure calculations, performed for example in Ref. [28]. The uncertainty of $E^{(6,0)}_{\rm fns}$ is the estimated model dependence, evaluated as twice the difference between the exponential and the Gaussian models. This model-dependence uncertainty is comparable with the theoretical uncertainty due to α^5 nuclear polarizability of 11 Hz [28]. The corrections in Eq. (78) are larger than experimental uncertainty but smaller than the other theoretical uncertainties (of about 1 kHz) and the proton-radius uncertainty (about 1 kHz) [3].

Next we analyze the $2P$-$2S$ transition in light muonic atoms. Our numerical results for the recoil fns correction for muonic atoms with $Z = 1$ and $Z = 2$ are presented in Table III. Recoil fns results for μH and μD are smaller than experimental uncertainty (of 2.3 and 3.4 μeV, correspondingly) and thus negligible at present. For the helium isotopes, they are close to the experimental uncertainty (48 μeV) but still smaller than the uncertainty from the unknown nuclear-polarizability effects in the three-photon exchange. One may

TABLE III. $E^{(6,1)}_{\rm fns}$ for the $2P$-$2S$ transition in light muonic atoms, in μeV.

	r_C[fm]	$m_\mu\,r_C$	$f(m_\mu\,r_C)$	$E^{(6,1)}_{\rm fns}(2P-2S)$
μH	0.840 60(39)	0.450	1.022	0.69
μD	2.127 58(78)	1.139	3.849	1.18
μ^3He	1.970 07(94)	1.055	3.450	48.7
μ^4He	1.678 6(12)	0.899	2.745	29.2

expect that the recoil fns corrections become more significant for heavier elements, such as μLi or μBe, due to enhancement by Z^2 with respect to the leading finite size.

It should be stressed that the fns corrections are only the elastic part of the total nuclear-structure effect. The remaining, inelastic part includes the nuclear polarizability effect. In principle, it is advantageous to account for the elastic and inelastic nuclear-structure parts on the same footing, but this is not always possible. The nuclear structure effects has been accurately calculated at the order $(Z\,\alpha)^5$ for H and He isotopes, both for electronic and muonic atoms, see Ref. [5] and references therein, and estimated for heavier muonic atoms [29]. However, the inelastic $(Z\,\alpha)^6$ correction is not known yet and is the source of the main theoretical uncertainty in light muonic atoms.

IX. SUMMARY

We derived formulas for the nuclear recoil fns corrections of order $(Z\alpha)^5$ and $(Z\alpha)^6$. Our calculations were performed without any expansion in the nuclear charge radius r_C, which makes the obtained results applicable both for electronic and muonic atoms. The obtained results are relevant for high-precision determinations of the root-mean-square charge radii from spectroscopy of muonic atoms [10].

We demonstrated that the application of the widely-used Breit approximation to the nuclear recoil effect with an extended nuclear charge distribution leads to appearance of an unphysical fns contribution at the $(Z\,\alpha)^5$ order, which is linear in the nuclear charge radius r_C. This spurious term disappears in the full-QED treatment, leaving the the correct contribution $\propto r_C^2 \ln r_C$, which is for the electronic atoms much smaller than this spurious term.

The recoil fns correction contributes to the nonlinearity of the so-called King plots in the isotope-shift measurements of many-electron atoms [26, 30], which are used for searches of new-physics scalar boson fields coupling to electrons and neutrons. This effect should be included into the theoretical analysis of the observed nonlinearities. It is interesting that the leading recoil fns effect $\sim (Z\alpha)^4$ does not contribute to the King's plot nonlinearities (since the reduced-mass prefactor can be effectively absorbed into the nuclear radius). Therefore, it is essential that the full QED approach is used for description of the recoil fns effect when studying these nonlinearities.

A possible future application of the method developed in this work would be a calculation of the analogous correction to the hyperfine splitting in μH, which could provide a sensitive low-energy test of the Standard Model [31, 32] by comparing the splitting intervals in electronic and muonic atoms. Further application could be a calculation of the radiative recoil fns correction, which can be as large as that obtained in this work. Yet another application could be a calculation of $(Z\,\alpha)^7$ and $\alpha(Z\,\alpha)^6$ recoil corrections to the Lamb shift and hyperfine splitting in hydrogenic systems, which are not known and limit the accuracy of the current theoretical predictions [3].

[1] C. G. Parthey, A. Matveev, J. Alnis, B. Bernhardt, A. Beyer, R. Holzwarth, A. Maistrou, R. Pohl, K. Predehl, T. Udem, T. Wilken, N. Kolachevsky, M. Abgrall, D. Rovera, C. Salomon, P. Laurent, and T. W. Hänsch, Improved measurement of the hydrogen $1S-2S$ transition frequency, Phys. Rev. Lett. **107**, 203001 (2011).

[2] A. Matveev, C. G. Parthey, K. Predehl, J. Alnis, A. Beyer, R. Holzwarth, T. Udem, T. Wilken, N. Kolachevsky, M. Abgrall, D. Rovera, C. Salomon, P. Laurent, G. Grosche, O. Terra, T. Legero, H. Schnatz, S. Weyers, B. Altschul, and T. W. Hänsch, Precision measurement of the hydrogen $1S-2S$ frequency via a 920-km fiber link, Phys. Rev. Lett. **110**, 230801 (2013).

[3] P. Mohr, D. Newell, B. Taylor, and E. Tiesinga, CODATA recommended values of the fundamental physical constants: 2022 (2024), arXiv:2409.03787 [hep-ph].

[4] R. Pohl, A. Antognini, F. Nez, F. D. Amaro, F. Biraben, J. a. M. R. Cardoso, D. S. Covita, A. Dax, S. Dhawan, L. M. P. Fernandes, A. Giesen, T. Graf, T. W. Hänsch, P. Indelicato, L. Julien, C.-Y. Kao, P. Knowles, E.-O. Le Bigot, Y.-W. Liu, J. A. M. Lopes, L. Ludhova, C. M. B. Monteiro, F. Mulhauser, T. Nebel, P. Rabinowitz, J. M. F. dos Santos, L. A. Schaller, K. Schuhmann, C. Schwob, D. Taqqu, J. a. F. C. A. Veloso, and F. Kottmann, The size of the proton, Nature (London) **466**, 213 (2010).

[5] K. Pachucki, V. Lensky, F. Hagelstein, S. S. Li Muli, S. Bacca, and R. Pohl, Comprehensive theory of the lamb shift in light muonic atoms, Rev. Mod. Phys. **96**, 015001 (2024).

[6] K. Schuhmann, L. M. Fernandes, F. Nez, M. A. Ahmed, F. D. Amaro, P. Amaro, F. Biraben, T.-L. Chen, D. S. Covita, A. J. Dax, *et al.*, The helion charge radius from laser spectroscopy of muonic helium-3 ions, arXiv preprint arXiv:2305.11679 (2023).

[7] Y. van der Werf, K. Steinebach, R. Jannin, H. Bethlem, and K. Eikema, The alpha and helion particle charge radius difference from spectroscopy of quantum-degenerate helium, arXiv preprint arXiv:2306.02333 (2023).

[8] X.-Q. Qi, P.-P. Zhang, Z.-C. Yan, L.-Y. Tang, A.-X. Chen, T.-Y. Shi, and Z.-X. Zhong, Revised ^{3}He nuclear charge radius due to electronic hyperfine mixing, arXiv preprint arXiv:2409.09279 (2024).

[9] K. Pachucki, Patkóš, and V. A. Yerokhin, Second-order hyperfine correction to H, D, and ^{3}He energy levels, Phys. Rev. A **110**, 062806 (2024).

[10] B. Ohayon, A. Abeln, S. Bara, T. E. Cocolios, O. Eizenberg, A. Fleischmann, L. Gastaldo, C. Godinho, M. Heines, D. Hengstler, G. Hupin, P. Indelicato, K. Kirch, A. Knecht, D. Kreuzberger, J. Machado, P. Navratil, N. Paul, R. Pohl, D. Unger, S. M. Vogiatzi, K. v. Schoeler, and F. Wauters, Towards precision muonic X-ray measurements of charge radii of light nuclei, Physics **6**, 206 (2024).

[11] J. L. Friar, Nuclear finite size effects in light muonic atoms, Ann. Phys. (NY) **122**, 151 (1979).

[12] V. M. Shabaev, Finite nuclear size corrections to the energy levels of the multicharged ions, J. Phys. B **26**, 1103 (1993).

[13] K. Pachucki, V. Patkóš, and V. A. Yerokhin, Three-photon-

exchange nuclear structure correction in hydrogenic systems, Phys. Rev. A **97**, 062511 (2018).
[14] E. Borie and G. A. Rinker, The energy levels of muonic atoms, Rev. Mod. Phys. **54**, 67 (1982).
[15] E. Borie, Lamb shift in light muonic atoms — revisited, Ann. Phys. **327**, 733 (2012).
[16] V. M. Shabaev, A. N. Artemyev, T. Beier, G. Plunien, V. A. Yerokhin, and G. Soff, Recoil correction to the ground-state energy of hydrogenlike ions, Phys. Rev. A **57**, 4235 (1998).
[17] K. Pachucki and V. A. Yerokhin, QED theory of the nuclear recoil with finite size, Phys. Rev. Lett. **130**, 053002 (2023).
[18] K. Pachucki and V. A. Yerokhin, Heavy-particle quantum electrodynamics, Phys. Rev. A **110**, 032804 (2024).
[19] V. M. Shabaev, Mass corrections in a strong nuclear field, Teor. Mat. Fiz. **63**, 394 (1985), [Theor. Math. Phys. **63**, 588 – 596 (1985)].
[20] V. M. Shabaev, Nuclear recoil effect in the relativistic theory of multiply charged ions, Sov. J. Nucl. Phys. **47**, 69 – 72 (1988).
[21] K. Pachucki and H. Grotch, Pure recoil corrections to hydrogen energy levels, Phys. Rev. A **51**, 1854 (1995).
[22] B. K. Sahoo, S. Blundell, A. V. Oleynichenko, R. F. G. Ruiz, L. V. Skripnikov, and B. Ohayon, Recent advancements in atomic many-body methods for high-precision studies of isotope shifts (2024), arXiv:2408.09959 [physics.atom-ph].
[23] I. S. Anisimova, A. V. Malyshev, D. A. Glazov, M. Y. Kaygorodov, Y. S. Kozhedub, G. Plunien, and V. M. Shabaev, Model-QED-operator approach to relativistic calculations of the nuclear recoil effect in many-electron atoms and ions, Phys. Rev. A **106**, 062823 (2022).
[24] Patkóš, V. A. Yerokhin, and K. Pachucki, Two-body p-state energies at order α^6, Phys. Rev. A **109**, 022819 (2024).
[25] E. C. Seltzer, k x-ray isotope shifts, Phys. Rev. **188**, 1916 (1969).
[26] J. Hur, D. P. L. Aude Craik, I. Counts, E. Knyazev, L. Caldwell, C. Leung, S. Pandey, J. C. Berengut, A. Geddes, W. Nazarewicz, P.-G. Reinhard, A. Kawasaki, H. Jeon, W. Jhe, and V. Vuletić, Evidence of two-source King plot nonlinearity in spectroscopic search for new boson, Phys. Rev. Lett. **128**, 163201 (2022).
[27] V. A. Yerokhin and N. S. Oreshkina, QED calculations of the nuclear recoil effect in muonic atoms, Phys. Rev. A **108**, 052824 (2023).
[28] O. Tomalak, Two-photon exchange correction to the Lamb shift and hyperfine splitting of s levels, Eur. Phys. J. A **55**, 1 (2019).
[29] M. Gorchtein, A hitchhiker's guide to nuclear polarization in muonic atoms (2025), arXiv:2501.15274 [nucl-th].
[30] A. Wilzewski, L. I. Huber, M. Door, J. Richter, A. Mariotti, L. J. Spieß, M. Wehrheim, S. Chen, S. A. King, P. Micke, M. Filzinger, M. R. Steinel, N. Huntemann, E. Benkler, P. O. Schmidt, J. Flannery, R. Matt, M. Stadler, R. Oswald, F. Schmid, D. Kienzler, J. Home, D. P. L. A. Craik, S. Eliseev, P. Filianin, J. Herkenhoff, K. Kromer, K. Blaum, V. A. Yerokhin, I. A. Valuev, N. S. Oreshkina, C. Lyu, S. Banerjee, C. H. Keitel, Z. Harman, J. C. Berengut, A. Viatkina, J. Gilles, A. Surzhykov, M. K. Rosner, J. R. C. López-Urrutia, and E. Fuchs, Nonlinear calcium King plot constrains new bosons and nuclear properties (2024), arXiv:2412.10277 [physics.atom-ph].
[31] J. Nuber, A. Adamczak, M. A. Ahmed, L. Affolter, F. D. Amaro, P. Amaro, P. Carvalho, Y. H. Chang, T. L. Chen, W. L. Chen, L. M. P. Fernandes, M. Ferro, D. Goeldi, T. Graf, M. Guerra, T. W. Hänsch, C. A. O. Henriques, M. Hildebrandt, P. Indelicato, O. Kara, K. Kirch, A. Knecht, F. Kottmann, Y. W. Liu, J. Machado, M. Marszalek, R. D. P. Mano, C. M. B. Monteiro, F. Nez, A. Ouf, N. Paul, R. Pohl, E. Rapisarda, J. M. F. dos Santos, J. P. Santos, P. A. O. C. Silva, L. Sinkunaite, J. T. Shy, K. Schuhmann, S. Rajamohanan, A. Soter, L. Sustelo, D. Taqqu, L. B. Wang, F. Wauters, P. Yzombard, M. Zeyen, J. Zhang, and A. Antognini, Diffusion of muonic hydrogen in hydrogen gas and the measurement of the $1s$ hyperfine splitting of muonic hydrogen (2023), arXiv:2211.08297 [physics.atom-ph].
[32] A. Vacchi, E. Mocchiutti, A. Adamczak, D. Bakalov, G. Baldazzi, M. Baruzzo, R. Benocci, R. Bertoni, M. Bonesini, H. Cabrera, *et al.*, Investigating the proton structure: The FAMU experiment, Nuclear Physics News **33**, 9 (2023).

Appendix A: $d^d k$ integration

We aim to perform the following integration in $d = 3 - 2\,\epsilon$ dimensions, assuming ϵ to be small,

$$f(m_1, m_2, m_3; n_1, n_2, n_3) = \int \frac{d^d k_1}{(2\,\pi)^d} \int \frac{d^d k_2}{(2\,\pi)^d} \times \frac{4\,\pi}{(k_1^2 + m_1^2)^{n_1}}\, \frac{4\,\pi}{(k_2^2 + m_2^2)^{n_2}}\, \frac{4\,\pi}{(k_3^2 + m_3^2)^{n_3}}\,, \tag{A1}$$

where $\vec{k}_3 = \vec{k}_1 - \vec{k}_2$, n_1, n_2 and n_3 are arbitrary integers, m_1, m_2 and m_3 are arbitrary nonnegative real numbers. If any of n_i is negative or equal to 0, then we can assume that the corresponding $m_i = 0$.

In several cases f vanishes. Namely, for arbitrary n_1, n_2 and n_3,

$$f(0,0,0; n_1, n_2, n_3) = 0\,. \tag{A2}$$

If two parameters are equal to 0, e.g., $m_1 = m_2 = 0$, then

$$f(0,0,m_3; n_1, n_2, n_3) = 0, \text{ if } n_1 \le 0 \text{ or } n_2 \le 0\,. \tag{A3}$$

In order to solve the general case, we assume at first that $n_1 = n_2 = n_3 = 1$, then the master integral f is

$$f(m_1, m_2, m_3) \equiv f(m_1, m_2, m_3; 1,1,1) = 4\,\pi\left(\frac{1}{4\,\epsilon} + \frac{1 - \gamma_E + \ln(4\,\pi)}{2} - \ln(m_1 + m_2 + m_3)\right). \tag{A4}$$

If all m_i are not equal to 0, then for positive n_1, n_2, n_3

$$f(m_1, m_2, m_3, n_1+1, n_2+1, n_3+1) = \frac{(-1)^{n_1+n_2+n_3}}{n_1!\,n_2!\,n_3!} \times \frac{\partial^{n_1}}{\partial(m_1^2)^{n_1}}\,\frac{\partial^{n_2}}{\partial(m_2^2)^{n_2}}\,\frac{\partial^{n_3}}{\partial(m_3^2)^{n_3}}\,f(m_1, m_2, m_3)\,. \tag{A5}$$

If $m_1 = 0$, then we use a general formula valid for arbitrary n_i,

$$f(0,m_2,m_3;n_1,n_2,n_3) = \frac{m_3^{2\,(d-n_1-n_2-n_3)}}{(4\,\pi)^{d-3}}\,\frac{\Gamma(d/2-n_1)\,\Gamma(n_1+n_2-d/2)\,\Gamma(n_1+n_3-d/2)\,\Gamma(n_1+n_2+n_3-d)}{\Gamma(2\,n_1+n_2+n_3-d)\,\Gamma(n_2)\,\Gamma(n_3)\,\Gamma(d/2)}$$
$$\times{}_2F_1(n_1+n_2+n_3-d,n_1+n_2-d/2,2\,n_1+n_2+n_3-d,1-m_2^2/m_3^2)\,. \tag{A6}$$

In fact, when $m_1 = 0$, one can still use differentiation as in Eq. (A5), but later one has to separate out $1/m_1^i$ terms and the remainder coincides with the general formula in Eq. (A6). A few non obvious examples are:

$$f(0,m_2,m_3,-1,1,1) = -\,4\,\pi\,m_2\,m_3\,(m_2^2+m_3^2)\,, \tag{A7}$$
$$f(0,m_2,m_3,-2,1,1) = \frac{4\,\pi}{3}\,m_2\,m_3\,(3\,m_2^2+m_3^2)\,(m_2^2+3\,m_3^2)\,. \tag{A8}$$

Appendix B: Matrix elements for S states

The following matrix elements contain $1/\epsilon$ singularity

$$\left\langle\left[\frac{1}{r^4}\right]_\epsilon\right\rangle \equiv \left\langle\left(\vec\nabla\left[\frac{1}{r}\right]_\epsilon\right)^2\right\rangle = \left\langle\frac{1}{r^4}\right\rangle + \langle\pi\,\delta^d(r)\rangle\left(-\frac{2}{\epsilon}+8\right), \tag{B1}$$
$$\left\langle\left[\frac{1}{r^3}\right]_\epsilon\right\rangle \equiv \left\langle\left[\frac{1}{r}\right]^3_\epsilon\right\rangle = \left\langle\frac{1}{r^3}\right\rangle + \langle\pi\,\delta^d(r)\rangle\left(\frac{1}{\epsilon}+2\right), \tag{B2}$$

where

$$\left\langle\frac{1}{r^3}\right\rangle = \lim_{a\to 0}\int_a^\infty\frac{dr}{r}\,f(r) + f(0)\,(\gamma+\ln a) = \frac{4}{n^3}\left(\frac{1}{2}-\frac{1}{2\,n}-\gamma-\Psi(n)+\ln\frac{n}{2}\right), \tag{B3}$$
$$\left\langle\frac{1}{r^4}\right\rangle = \lim_{a\to 0}\int_a^\infty\frac{dr}{r^2}\,f(r) - \frac{f(0)}{a} + f'(0)\,(\gamma+\ln a) = \frac{8}{n^3}\left(-\frac{5}{3}+\frac{1}{2\,n}+\frac{1}{6\,n^2}+\gamma+\Psi(n)-\ln\frac{n}{2}\right), \tag{B4}$$
$$f(r) = \int d\Omega\,\phi^*(\vec r)\,\phi(\vec r)\,, \tag{B5}$$

and

$$\left\langle\pi\,\delta^d(r)\frac{1}{(E-H)'}\frac{p^4}{8}\right\rangle = \frac{1}{n^3}\left(-\frac{3}{2}-\frac{1}{n}+\frac{5}{4\,n^2}+\gamma+\Psi(n)-\ln\frac{n}{2}\right) - \frac{1}{4\,\epsilon}\langle\pi\,\delta^d(r)\rangle\,, \tag{B6}$$
$$\left\langle\pi\,\delta^d(r)\frac{1}{(E-H)'}\pi\,\delta^d(r)\right\rangle = \frac{1}{n^3}\left(-\frac{1}{2}-\frac{1}{n}+\gamma+\Psi(n)-\ln\frac{n}{2}\right) - \frac{1}{4\,\epsilon}\langle\pi\,\delta^d(r)\rangle\,, \tag{B7}$$
$$\left\langle\pi\,\delta^d(r)\frac{1}{(E-H)'}\frac{1}{2}\,p^i\left[\frac{\delta^{ij}}{r}+\frac{r^ir^j}{r^3}\right]_\epsilon p^j\right\rangle = \frac{2}{n^3}\left(-\frac{9}{4}-\frac{1}{n}+\frac{5}{4\,n^2}+\gamma+\Psi(n)-\ln\frac{n}{2}\right) - \frac{1}{2\,\epsilon}\langle\pi\,\delta^d(r)\rangle\,. \tag{B8}$$

The regular matrix elements in a.u. are evaluated as

$$E = -\frac{1}{2\,n^2}\,, \tag{B9}$$
$$\left\langle\frac{1}{r}\right\rangle = \frac{1}{n^2}, \tag{B10}$$
$$\left\langle\frac{1}{r^2}\right\rangle = \frac{2}{n^3}, \tag{B11}$$
$$\langle\pi\,\delta^3(r)\rangle = \frac{1}{n^3}, \tag{B12}$$
$$\langle\pi\,\nabla^2\delta^d(r)\rangle = \frac{2}{n^5}\,, \tag{B13}$$
$$\langle\{p^i,\{p^i,\pi\,\delta^d(r)\}\}\rangle = -\frac{2}{n^5}\,, \tag{B14}$$
$$\left\langle p^i\left(\frac{\delta^{ij}}{r}+\frac{r^ir^j}{r^3}\right)p^j\right\rangle = \frac{1}{n^3}\left(-\frac{2}{n}+4\right), \tag{B15}$$
$$\left\langle p^i\left(\frac{\delta^{ij}}{r^2}+\frac{r^ir^j}{r^4}\right)p^j\right\rangle = \frac{1}{n^3}\left(-\frac{4}{3\,n^2}+\frac{16}{3}\right). \tag{B16}$$