Finite nuclear size and Lamb shift of p-wave atomic states

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(Dated: December 25, 2021)

We consider corrections to the Lamb shift of p-wave atomic states due to the finite nuclear size (FNS). In other words, these are radiative corrections to the atomic isotopic shift related to FNS. It is shown that the structure of the corrections is qualitatively different from that for s-wave states. The perturbation theory expansion for the relative correction for a p1/2-state starts from \( \alpha \ln(1/Z\alpha) \)-term, while for s1/2-states it starts from \( Z\alpha^2 \) term. Here \( \alpha \) is the fine structure constant and \( Z \) is the nuclear charge. In the present work we calculate the \( \alpha \)-terms for 2p-states, the result for 2p1/2-state reads \((8\alpha/9\pi)[\ln(1/(Z\alpha)^2) + 0.710]\). Even more interesting are p3/2-states. In this case the “correction” is by several orders of magnitude larger than the “leading” FNS shift.

PACS numbers: 11.30.Er, 31.30.Jv, 32.80.Ys

Experimental and theoretical investigation of the radiative shift (Lamb shift) of energy levels in heavy atoms is an important way to test Quantum Electrodynamics in presence of a strong external electric field. One of the effects related to this problem is a dependence of the Lamb shift on the finite nuclear size (FNS). One can also look at this effect from another point of view. It is well known that there is an isotop shift of atomic levels due to the finite nuclear size (FNS). The corrections we are talking about are the radiative corrections to the isotop shift.

The corrections for 1s-, 2s-, and 2p-states have been calculated numerically, exactly in \( Z\alpha \), in Refs. [1, 2, 3]. The self-energy and the vertex corrections to the FNS effect for any s-wave state have been calculated analytically in order \( \alpha(Z\alpha) \) in Refs. [4, 5]. However, the structure of the higher order \( Z\alpha \) corrections and, in particular, their logarithmic dependence on the nuclear size has not been understood even for s-states. Our interest to FNS radiative corrections has been stimulated by our work on the radiative corrections to atomic parity non-conservation [6]. Technically the parity nonconservation effect has some common features with that of the FNS radiative correction: in both cases the effective size of the perturbation source is much smaller than the Compton wavelength \( \lambda_C \). In the paper [6] we have elucidated the structure of higher order in \( Z\alpha \) FNS radiative corrections for s-electrons, and have calculated analytically \( \alpha(Z\alpha) \) and \( \alpha(Z\alpha)^2 \ln(\lambda_C/r_o) \) self-energy and vertex FNS relative radiative corrections. Here \( r_o \) is the nuclear radius. In the present work we calculate FNS radiative corrections for p-wave electrons. We demonstrate that the structure of the corrections for p-wave states is very much different from that for the s-wave states. Physically it happens because of different infrared behavior.

Due to the finite nuclear size, the electric potential \( V(r) \) of the nucleus is different from that for a pointlike nucleus. The deviation is

\[
\delta V(r) = V(r) - \left( -\frac{Z\alpha}{r} \right)
\]

Throughout the paper we set \( \hbar = c = 1 \). The diagram that describe the FNS effect in the leading order is shown in Fig.1(a). The double line corresponds to the exact electron wave function in the Coulomb field, and the zigzag line with cross denotes the perturbation (1).

![Diagram](image.png)

**FIG. 1:** The leading contribution to the FNS effect is given by diagram (a), and one loop radiative corrections to the effect are given by diagrams (b-c). The double line denotes the exact electron Green’s function in the Coulomb field of the nucleus, the cross denotes the nucleus, the zigzag line denotes the FNS perturbation (1), and the dashed line denotes the photon.

Diagrams Fig.1(b) and Fig.1(c) correspond to the contributions of the electron self-energy operator and the vertex operator, respectively. The diagram Fig.1(d) describes a modification of \( \delta V \) (see eq. (1)) due to the vacuum polarization, and the diagram Fig.1(e) corresponds...
to a modification of the electron wave function due to the polarization of the vacuum by the Coulomb field (Uehling potential).

Technically the most complicated are the self-energy and the vertex FNS (SEVFNS) corrections given by diagrams in Fig. 1(b) and Fig. 1(c). According to our previous work [3], the SEVFNS relative correction for an s-wave state is of the form

$$\Delta_s = -\alpha \left( \frac{(Z\alpha)}{2} - \frac{23}{4} - 4 \ln 2 \right) + \frac{(Z\alpha)^2}{\pi} \left( \frac{15}{4} - \frac{\pi^2}{6} \right) \ln(b\lambda_C/r_0) \right).$$ \hspace{1cm} (2)

Here \( b = \exp\left(1/(2\gamma) - C - 5/6\right), \) \( C \approx 0.577 \) is the Euler constant, and \( r_0 \), as we already mentioned, is the nuclear radius. The total relative SEVFNS correction is the ratio of the sum of diagrams Fig. 1(b) and Fig. 1(c) divided by the diagram Fig. 1(a). Value of \( \Delta_s \) is not proportional to the nuclear radius squared because it is a relative quantity. Plot of \( \Delta_s \) versus the nuclear charge \( Z \) is shown in Fig. 2 by the dashed line. Results of computations of \( \Delta_s \) for 1s and 2s states are shown by squares and triangles, respectively. The \( \alpha(Z\alpha) \) term in (2) comes from distances \( r \sim \lambda_C \), and the \( \alpha(Z\alpha)^2 \ln(\lambda_C/r_0) \) term comes from distances \( r_0 < r < \lambda_C \). An important point is that there is no contribution that comes from distances \( r \gg \lambda_C \). Because of this reason the correction \( \Delta_s \) is exactly the same for 1s, 2s, 3s,... states. Why there is no contribution of larger distances into \( \Delta_s \)? The reason is very simple. In the leading order the correction \( \Delta_s \) can be expressed in terms of the forward electron-nucleus scattering amplitude $\Omega$. There is a rigorous QED theorem that claims that there is no an infrared divergence in the forward scattering amplitude, see e.g. Ref. [3]. Therefore, quantum fluctuations from distances \( r > \lambda_C \) cannot contribute to \( \Delta_s \) (see also Ref. [4]). Let us look now at the p-wave SEVFNS correction \( \Delta_p \). From the point of view of the scattering problem it corresponds to scattering at finite angle. The finite-angle scattering amplitude is always infrared divergent. Therefore, there must expect a contribution to \( \Delta_p \) from quantum fluctuations at distances \( r > \lambda_C \). This is the contribution we calculate in the present work.

Formally we assume that \( Z\alpha \ll 1 \). Therefore, at distances \( r \sim \lambda_C/(Z\alpha) \gg \lambda_C \) dynamics of the electron is described by usual nonrelativistic Coulomb wave functions. However, the nucleus radius is small, \( r_0 \ll Z\alpha\lambda_C \ll \lambda_C \).

At small distances, generally speaking, one must use relativistic Dirac wave function even at \( Z = 1 \). The electron Dirac wave function at \( r < Z\alpha\lambda_C \) is of the form

$$\Psi(r) = N r^{\gamma-1} \left( (\kappa - \gamma)\Omega \right)_{iZ\alpha\Omega},$$ \hspace{1cm} (3)

where \( \Omega \) and \( \hat{\Omega} = - (\sigma \cdot n)\Omega \) are spherical spinors ; \( \kappa = -1 \) for \( s_{1/2} \)-state, \( \kappa = 1 \) for \( p_{1/2} \)-state, and \( \kappa = -2 \) for \( p_{3/2} \)-state ; \( \gamma = \sqrt{\kappa^2 - (Z\alpha)^2} \); and \( N \) is a constant known for each particular state, see Ref. [3]. For \( s_{1/2} \)- and \( p_{3/2} \)-states the upper component of the Dirac spinor \( \Psi \) is much larger than the lower one. Hence, the upper component determines the FNS shift of such a state. On the other hand, for \( p_{1/2} \)-state the lower component and hence its contribution to the FNS shift is dominating. A straightforward calculation gives the following values for the FNS shifts of \( 2s \) and \( 2p \) states (diagram Fig. 1a)

$$\delta E^{(0)}(2s_{1/2}) = \frac{1}{12} (Z\alpha)^4 m^3 < r^2 >,$$

$$\delta E^{(0)}(2p_{1/2}) = \frac{1}{64} (Z\alpha)^6 m^3 < r^2 >,$$

$$\delta E^{(0)}(2p_{3/2}) = \frac{1}{480} (Z\alpha)^6 m^5 < r^4 >.$$ \hspace{1cm} (4)

Here \( < r^2 > \) and \( < r^4 > \) are values of \( r^2 \) and \( r^4 \) averaged over charge density of the nucleus. The low-momentum expansion of the nuclear electric form factor is of the form

$$F(q^2) \approx 1 - \frac{q^2}{6} < r^2 > + \frac{q^4}{120} < r^4 >.$$ \hspace{1cm} (5)

Modeling the nucleus as a uniformly charged ball one gets

$$< r^2 > = \frac{3}{5} r_0^2, \hspace{1cm} < r^4 >= \frac{3}{7} r_0^4,$$ \hspace{1cm} (6)
where \( r_0 = 1.1 A^{1/3} \text{fm} \) is the nucleus radius, and \( A \) is the nucleus mass number. As one should expect the FNS corrections obey the following inequalities
\[
\delta E^{(0)}(2s_{1/2}) \gg \delta E^{(0)}(2p_{1/2}) \gg \delta E^{(0)}(2p_{3/2}).
\]

Let us calculate now the leading in \( Z_0 \) loop SEVFNS radiative correction \( E^{(1)} \) for \( p_{1/2} \) and \( p_{3/2} \)-states. This correction is given by diagrams in Fig. 1(b) and Fig. 1(c). Since we consider the leading correction, it is sufficient to use the nonrelativistic approximation for electron wave functions (two-component wave functions).

It is sufficient also to use the effective FNS perturbation that reproduces FNS correction for s-wave states,
\[
\delta V_{\text{eff}}(r) = g \delta(r) , \quad g = \frac{2\pi Z\alpha}{3} < r^2 > . \tag{7}
\]

Rest of the calculation is very similar to the textbook calculation of the Lamb shift, see, e.g. Ref. [8]. We introduce the parameter \( \mu \) such that \( m > \mu > m(Z_0)^2 \).

Hence the correction \( E^{(1)} \) can be represented as a sum of “high frequency” and “low frequency” contributions
\[
E^{(1)} = E_h + E_l, \quad \text{where \"high\" and \"low\" correspond to frequencies above and below } \mu, \text{ respectively. In the momentum representation, the effective potential corresponding to the high frequency contribution is of the form [8]}
\]
\[
\delta \Phi(q) = \left[ -\frac{\alpha q^2}{3\pi m^2} \left( \ln \frac{m}{2\mu} + \frac{11}{24} \right) + \frac{\alpha}{4\pi m} q \cdot \gamma \right] \delta \Phi_{\text{eff}}(q) , \tag{8}
\]
where \( q = p_1 - p_2 \) is momentum transfer, and \( \gamma \) is the Dirac matrix. Taking the p-wave component of the potential and transferring it to the coordinate representation, we get the following expression for the SEVFNS high frequency correction for a p-wave state \( |\psi\rangle \)
\[
E_h = \frac{g\alpha}{\pi m^2} |\psi\rangle \left\{ \frac{2}{3} \left[ \ln \frac{m}{2\mu} + \frac{11}{24} \right] (p \delta(r) p) + \frac{1}{4} (s \rho \rho \rangle \delta(r) (s \rho \rho) |\psi\rangle \right\} . \tag{9}
\]

This gives the following values for 2p-states
\[
E_h(2p_{1/2}) = F \left( \ln \frac{m}{2\mu} + \frac{19}{12} \right) ,
\]
\[
E_h(2p_{3/2}) = F \left( \ln \frac{m}{2\mu} + \frac{11}{24} \right) ,
\]
where \( F = \frac{\alpha(Z_0)^2 gm^3}{48\pi^2} \). \tag{10}

The contribution of the vacuum polarization, diagram Fig. 1(d), can be taken into account in Eqs. [8],[10] by substitution \( \ln(m/2\mu) \rightarrow \ln(m/2\mu) - 1/5 \). The Uehling potential, diagram Fig. 1(e), does not contribute in this order.

The low frequency contribution is given by the usual nonrelativistic quantum mechanics expression
\[
E_l = \frac{2g\alpha}{3\pi m^2} \Re \int_{0}^{\mu} \omega d\omega \langle \psi|p \frac{1}{E_{2p}^{(0)} - \omega + i0} \delta(r) |\psi\rangle . \tag{11}
\]

Here \( \Re \) stays for real part, \( \omega \) is frequency of the virtual photon, \( H = p^2/2m - Z_0/r \) is the nonrelativistic Hamiltonian, and \( E_{2p}^{(0)} = -(mZ_0)^2/8 \) is the energy of 2p-state. We have also taken into account that interaction with the photon is of the form \(-e\mathbf{p} \cdot \mathbf{A}/m \), where \( \mathbf{A} \) is the vector potential of the photon. The contribution \( E_l \) is the same for \( p_{1/2} \)- and for \( p_{3/2} \)-state. Using explicit form of 2p wave function, one can represent \([11]\) as
\[
E_l = \frac{2g\alpha(Z_0)^2}{3\pi} \Re \int_{0}^{\mu} \omega d\omega |\phi\rangle \frac{1}{E_{2p}^{(0)} - \omega + i0} \delta(r) |\phi\rangle , \tag{12}
\]
where
\[
\phi(r) = \frac{1}{\sqrt{32\pi a^3/2}}(1 - r/6a) \exp(-r/2a) , \quad a = (mZ_0)^{-1}. \tag{13}
\]

Eigenvalues of \( H \) are \( \epsilon_n = -(mZ_0)^2/2n^2 \). Therefore, the first impression is that the integrand in Eq. \([12]\) is singular at \( \omega = 0 \) and \( \omega = \epsilon_2 - \epsilon_1 \). However, the function \( \phi(r) \) is orthogonal to the wave function \( \psi_{2s}(r) \), hence, there is no real singularity at \( \omega = 0 \). There is a real singularity at \( \omega = \epsilon_2 - \epsilon_1 \) that is related to the possibility of emission of real photons, and this slightly complicates integration in \([13]\). To overcome this technical problem, it is convenient to represent \( \phi(r) \) as \( \phi(r) = \varphi(r) + \beta \psi_{1s}(r) \) with \( \beta = \sqrt{2/\pi (2/3)^3} \). In this form \( \varphi(r) \) is orthogonal both to \( \psi_{2s}(r) \) and \( \psi_{1s}(r) \). Then \([12]\) is transformed to
\[
E_l = \frac{2g\alpha(Z_0)^2}{3\pi} \Re \int_{0}^{\mu} \omega d\omega \left\{ \langle 0 | \frac{1}{E_{2p}^{(0)} - \omega + i0} |\varphi\rangle^2 + \frac{\beta^2 \psi_{1s}^{(0)}}{(E_{2s} - E_{1s} - \omega + i0)^2} + \frac{2\beta \psi_{1s}^{(0)}}{(E_{2s} - E_{1s} - \omega + i0)} |0 | \frac{1}{E_{2p}^{(0)} - \omega} |\varphi\rangle \right\} \tag{14}
\]
where \( |0\rangle \) denotes the electron localized at origin. In this form the matrix element \( \langle 0 | \left( E_{2p}^{(0)} - \omega - 1\right) |\varphi\rangle \) has no singularities. Using explicit expression for the nonrelativistic Coulomb Green’s function \([10]\)
\[
G(0, r | E) = |r| \frac{1}{E - H} |0\rangle = \frac{m}{2\pi r} \Gamma(1 - \eta) W_{\eta,1/2}(2pr) , \tag{15}
\]
where $p = \sqrt{2mE}$, $\eta = mZ\alpha/p$, $\Gamma$ is the gamma-function and $W$ is the Whittaker function, and taking the integral over $r$, and then over $\omega$, we obtain

$$E_l = F \left[ \ln \frac{\mu}{m(Z\alpha)^2} + 0.0198 \right].$$  \hfill (16)

Combining (10) and (14), we finally obtain the total SEVFNS radiative corrections (diagrams Fig.1(b) and Fig.1(c)) in the leading order

$$E^{(1)}(2p_{1/2}) = F \left[ \ln \frac{1}{(Z\alpha)^2} + 0.910 \right],$$  \hfill (17)

$$E^{(1)}(2p_{3/2}) = F \left[ \ln \frac{1}{(Z\alpha)^2} - 0.215 \right].$$  \hfill (17)

As one should expect, the result is independent of the parameter $\mu$. We have already mentioned that to account for the vacuum polarization (the diagram Fig.1(d)) one has to replace $\ln(1/(Z\alpha)^2) \to \ln(1/(Z\alpha)^2) - 1/5$. Therefore the total FNS radiative corrections (diagrams Fig.1(b), Fig.1(c), and Fig.1(d)) in the leading order are

$$E_{tot}^{(1)}(2p_{1/2}) = F \left[ \ln \frac{1}{(Z\alpha)^2} + 0.710 \right],$$  \hfill (18)

$$E_{tot}^{(1)}(2p_{3/2}) = F \left[ \ln \frac{1}{(Z\alpha)^2} - 0.415 \right].$$  \hfill (18)

Let us have a look now at the relative FNS radiative correction for $2p_{1/2}$ state. According to Eqs. (1) and (15), the relative correction is

$$\frac{E_{tot}^{(1)}(2p_{3/2})}{E_{tot}^{(1)}(2p_{1/2})} = \frac{20}{3\pi} \frac{\alpha}{m^2} \frac{\lambda < r^2 > - \lambda_c < r^2 >}{\ln \frac{1}{(Z\alpha)^2} - 0.415}. \hfill (19)$$

For example, for Hydrogen atom the radiative correction is by a factor $2.6 \times 10^4$ larger than the “leading” contribution.

According to the present calculation, the leading in powers of $Z\alpha$ SEVFNS relative radiative correction (diagrams Fig.1(b) and Fig.1(c)) for $2p_{1/2}$-state is equal to (see comment [13])

$$\Delta_{p}^{(0)} = \frac{E^{(1)}(2p_{1/2})}{E^{(0)}(2p_{1/2})} = \frac{8\alpha}{9\pi} \ln \frac{1}{(Z\alpha)^2} + 0.910. \hfill (20)$$

As we have already explained, the correction comes from quantum fluctuations at distances $\lambda_c < r < \lambda_c/(Z\alpha)$. There is also a contribution

$$- \frac{\alpha(Z\alpha)^2}{\pi} \left( \frac{15}{4} - \frac{\pi^2}{6} \right) \ln(b\lambda_c/r_0)$$

that comes from distances $r_0 < r < \lambda_c$, this contribution has been calculated in our previous work [3]. The contribution $\propto \alpha(Z\alpha)$ that comes from $r \sim \lambda_C$ has not been calculated yet. Therefore, altogether one gets the following formula for the relative correction $\Delta_p$:

$$\Delta_p = -\alpha \left[ -\frac{8}{9\pi} \left( \ln \frac{1}{(Z\alpha)^2} + 0.910 \right) \right. \hfill (21)$$

$$+ a_1(Z\alpha) + \frac{(Z\alpha)^2}{\pi} \left( \frac{15}{4} - \frac{\pi^2}{6} \right) \ln(b\lambda_c/r_0) \right],$$

where $a_1$ is an unknown coefficient. To determine the coefficient $a_1$, we fit results of numerical calculation of $\Delta_p$ for $2p_{1/2}$-state [3]. As a result of the fit we find $a_1 = 2.75$. The correction $\Delta_p$ given by Eq. (21) is plotted in Fig.2 by the solid line. The results of computations [3] are shown by diamonds. Agreement is very good.

Concluding, we have shown that corrections to the Lamb shift of p-wave atomic states due to the finite nuclear size are qualitatively different from that for s-wave states. The difference is related to the infrared behavior of quantum fluctuations. As a result, the leading relative p-wave correction is proportional to $\alpha \ln(1/Z\alpha)$ while the leading s-wave correction is proportional to $\alpha(Z\alpha)$. The leading p-wave correction has been calculated analytically.

O.P.S. thanks the Institute for Nuclear Theory at the University of Washington for its hospitality and the Department of Energy for partial support during the completion of this work.

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