Finite nuclear size corrections to the recoil effect in hydrogenlike ions

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Abstract

The finite nuclear size corrections to the relativistic recoil effect in H-like ions are calculated within the Breit approximation. The calculations are performed for the 1s, 2s, and 2p¹/₂ states in the range \(Z = 1 - 110\). The obtained results are compared with previous evaluations of this effect. It is found that for heavy ions the previously neglected corrections amount to about 20% of the total nuclear size contribution to the recoil effect calculated within the Breit approximation.

Keywords: highly-charged ions, nuclear recoil effect, finite nuclear size corrections

1. Introduction

In the last decade, great progress was achieved in experiments aimed at investigations of the finite nuclear size and nuclear recoil effects in highly charged ions. These effects led to the isotope shifts of the binding energies, which were measured in [1, 2]. In [1], the measurement was carried out at the electron beam ion trap using a high-resolution grating spectrometer. This experiment provided the first test of the relativistic theory of the nuclear recoil effect with highly charged ions (namely, B-like argon) [3]. In [2], the measurements of the isotope shifts in dielectronic recombination spectra for Li-like neodymium ions were used to determine the nuclear charge radii difference. The values obtained in this experiment were also sensitive to the relativistic nuclear recoil contribution (see [4] and references therein). It is expected that the accuracy of the isotope shift measurements will be significantly increased with the new Facility for Antiproton and Ion Research (FAIR) facilities in Darmstadt [5], so that it is required to perform high-precision calculations, including the nuclear size corrections to the recoil effect.

It is well known that in nonrelativistic theory the nuclear recoil effect for a hydrogenlike atom can be easily taken into account to all orders in \(m/M\) by using the reduced mass \(\mu = mM/(m + M)\) instead of the electron mass \(m\) (\(M\) is the nuclear mass). The full relativistic theory of the nuclear recoil effect can be formulated only in the framework of QED [6–11]. For the point-nucleus case, the total recoil correction of the first order in \(m/M\) to the energy of a state \(|a\rangle\) of a hydrogenlike ion can be written as a sum of a low-order term \(\Delta E_\text{L}\) and a higher-order term \(\Delta E_\text{H}\) [6, 7] (in units \(\hbar = c = 1\)):

\[
\Delta E = \Delta E_\text{L} + \Delta E_\text{H},
\]

\[
\Delta E_\text{L} = \frac{1}{2M} \langle a | \left( p^2 - [D(0) \cdot p + p \cdot D(0)] \right) | a \rangle,
\]

\[
\Delta E_\text{H} = \frac{i}{2\pi M} \int_{-\infty}^{\infty} d\omega \langle a | \left( D(\omega) - \frac{[p, V]}{\omega + i0} \right) \times G(\omega + E_a) \left( D(\omega) + \frac{[p, V]}{\omega + i0} \right) | a \rangle,
\]

where \(V(r) = -aZ/r\) is the Coulomb potential of the nucleus, \(G(\omega) = \left[ \omega - H(1 - i0) \right]^{-1}\) is the relativistic Coulomb Green function, \(H = a \cdot p + \beta m + V\), \(D_j(\omega, r) = -4\pi aZ^2 D_j(\omega, r)\), and \(D_j(\omega, r)\) is the transverse part of the photon propagator in the Coulomb gauge, which in coordinate space has the following form:

\[
D_j(\omega, r) = -\frac{i}{4\pi} \left\{ \frac{\exp(i |\omega| r)\delta_{ij}}{r} + \frac{V_i V_j \exp(i |\omega| r) - 1}{a^2r} \right\}.
\]
the \((aZ)^2 m^2/M\) approximation (the so-called Breit approximation). Its calculation, based on the virial relations for the Dirac equation \([16, 17]\), leads to \([6]\)

\[
\Delta E_L = \frac{m^2 - E_{\alpha 0}^2}{2M}, \tag{4}
\]

where \(E_{\alpha 0}\) is the Dirac electron energy for the point-nucleus case. The second term \(\Delta E_{\text{FI}}\) contains the contribution of order \((aZ)^2 m^2/M\) and all contributions of higher orders in \(aZ\), which are not included in \(\Delta E_L\). Its evaluation to all orders in \(aZ\) was performed in \([11–13]\).

According to \([10]\), the nuclear size corrections to the recoil effect can be partly taken into account by employing the potential of an extended nucleus in formulas (1) and (2), including the values of \(E_a, |a|\), and \(G(\omega)\). The corresponding calculations were carried out in \([14, 15]\). This approach allows one to evaluate the nuclear size corrections completely for the Coulomb part of the recoil effect:

\[
\Delta E_C = \left\langle a \left| \frac{p^2}{2M} \alpha \right. \right\rangle + \frac{2\pi i}{M} \int_{-\infty}^\infty d\omega \delta_2^2(\omega) \langle a | [p, V] \right\rangle G(\omega + E_a) [p, V] |a\rangle, \tag{5}
\]

and only partly for the one-transverse-photon and two-transverse-photon parts:

\[
\Delta E_{\text{FI(1)}} = -\frac{1}{2M} \langle a | (D(0)p + pD(0)) | a\rangle - \frac{1}{M} \int_{-\infty}^\infty d\omega \delta_2^2(\omega) \left\langle a \left| \left( [p, V] G(\omega + E_a) D(\omega) - D(\omega) G(\omega + E_a) [p, V] \right) |a\rangle \right\rangle, \tag{6}
\]

\[
\Delta E_{\text{FI(2)}} = \frac{i}{2M} \int_{-\infty}^\infty d\omega \langle a | D(\omega) G(\omega + E_a) D(\omega) |a\rangle. \tag{7}
\]

In this paper we present the complete evaluation of the nuclear size correction to the low-order nuclear recoil contribution \(\Delta E_L\) which corresponds to the Breit approximation. The calculations are performed for the 1s, 2s, and 2p_{1/2} states in the range \(Z = 1–110\).

### 2. Nuclear recoil operator within the Breit approximation

To derive the nuclear recoil operator for a hydrogenlike ion within the Breit approximation, one should account for the one-photon exchange between the electron and the nucleus in the Coulomb gauge (see figure 1) and consider the nucleus as a nonrelativistic particle. Discarding the nucleus spin-dependent terms, one gets the following electron–nucleus interaction potential in momentum space \([18, 19]\):

\[
V_{\text{eff}}(q) = -aZ \left\{ \frac{F(q)}{q^2} + \frac{1}{2M} \left\{ \frac{F(q)}{q^2} \alpha \cdot p \right\} \right. \]
\[
- \frac{1}{2M} \left\{ \alpha \cdot p \left[ p^2 \cdot \frac{F(q)}{q^2} \right] \right\}, \tag{8}
\]

where \(F(q)\) is the nuclear form factor. In coordinate space, equation (8) reads:

\[
V_{\text{eff}}(r) = -V(r) + \frac{1}{2M} \left\{ V(r) \alpha \cdot p \right\} + \frac{1}{4M} \left\{ \alpha \cdot p \left[ p^2 \cdot W(r) \right] \right\}. \tag{9}
\]

where

\[
V(r) = -aZ \int d\rho \rho(r') \frac{r-r'}{|r-r'|}, \tag{10}
\]

\[
W(r) = -aZ \int d\rho \rho(r)|r-r'|, \tag{11}
\]

and \(\rho(r)\) is the density of the nuclear charge distribution \(\int d\rho \rho(r) = 1\). We note that the function \(W(r)\) is normalized as in \([18]\), while in \([19]\) a different definition was used. Taking into account the nonrelativistic kinetic energy of the nucleus in the centre-of-mass frame, one obtains the low-order nuclear recoil operator accounting for the nuclear size effect:

\[
H_M = \frac{p^2}{2M} + \frac{1}{2M} \left\{ V(r) \alpha \cdot p \right\} + \frac{1}{4M} \left\{ \alpha \cdot p \left[ p^2 \cdot W(r) \right] \right\}. \tag{12}
\]

To first order in \(m/M\), the nuclear recoil contribution is given by the expected value of \(H_M [19]\):

\[
\Delta E = \langle a | H_M |a\rangle = \frac{1}{2M} \langle E_a^2 - m^2 \rangle - \frac{m}{M} \langle a | \beta V(r) |a\rangle - \frac{1}{2M} \langle a | (W'(r) V'(r) + V^2(r)) |a\rangle. \tag{13}
\]

For the case of a point nucleus \(W'(r) V'(r) + V^2(r) = 0\) and using the virial relations \([16, 17]\), we get equation (4). To evaluate the finite nuclear size corrections to the recoil effect expressed by equation (13) (it corresponds to the low-order term \(\Delta E_L\)), one should use the values of \(E_a, |a|, V(r),\)
Table 1. Finite nuclear size corrections to the low-order recoil contribution for the 1s state expressed in terms of the function $\Delta F_L(aZ),$ which is defined by equation (18). The values of the nuclear radii used were taken from [20] (for $Z \leq 92$) and [21] (for $Z = 100, 110$). The last column refers to the higher-order recoil term, which was evaluated in [14] using slightly different values of the nuclear radii.

| $Z$ | $(r^2)^{1/2}$ (fm) | $\Delta F_L^{\text{(point)}}(aZ)$ | $\Delta F_L^{\text{(finite)}}(aZ)$ | $\delta \Delta F_L(aZ)$ | $\Delta F_L^{\text{(point)}}(aZ)$ [14] |
|-----|-------------------|-----------------------------|-----------------------------|----------------------|-----------------------------|
| 1   | 0.878             | $-0.345 \times 10^{-8}$    | $-0.345 \times 10^{-8}$    | 0.23 $\times 10^{-8}$ |                             |
| 2   | 1.676             | $-0.520 \times 10^{-7}$    | $-0.519 \times 10^{-7}$    | 0.35 $\times 10^{-7}$ |                             |
| 5   | 2.406             | $-0.102 \times 10^{-5}$    | $-0.102 \times 10^{-5}$    | 0.76 $\times 10^{-6}$ |                             |
| 10  | 3.006             | $-0.969 \times 10^{-3}$    | $-0.964 \times 10^{-3}$    | 0.5 $\times 10^{-3}$  | 0.77 $\times 10^{-3}$ |
| 20  | 3.478             | $-0.934 \times 10^{-4}$    | $-0.920 \times 10^{-4}$    | 0.14 $\times 10^{-4}$ | 0.71 $\times 10^{-4}$ |
| 30  | 3.949             | $-0.108 \times 10^{-3}$    | $-0.396 \times 10^{-3}$    | 0.12 $\times 10^{-4}$ | 0.29 $\times 10^{-3}$ |
| 40  | 4.285             | $-0.127 \times 10^{-2}$    | $-0.121 \times 10^{-2}$    | 0.6 $\times 10^{-4}$  | 0.79 $\times 10^{-3}$ |
| 50  | 4.644             | $-0.339 \times 10^{-2}$    | $-0.316 \times 10^{-2}$    | 0.23 $\times 10^{-3}$ | 0.19 $\times 10^{-2}$ |
| 60  | 4.942             | $-0.826 \times 10^{-2}$    | $-0.752 \times 10^{-2}$    | 0.74 $\times 10^{-3}$ | 0.35 $\times 10^{-2}$ |
| 70  | 5.305             | $-0.0194$                   | $-0.0172$                   | 0.22 $\times 10^{-2}$ | 0.52 $\times 10^{-2}$ |
| 80  | 5.458             | $-0.0436$                   | $-0.0376$                   | 0.60 $\times 10^{-2}$ | 0.17 $\times 10^{-2}$ |
| 90  | 5.785             | $-0.0992$                   | $-0.0830$                   | 0.0162                | $-0.034$                  |
| 92  | 5.857             | $-0.117$                    | $-0.097$                    | 0.020                 | $-0.053$                  |
| 100 | 5.986             | $-0.224$                    | $-0.182$                    | 0.042                 | $-0.25$                   |
| 110 | 5.961             | $-0.517$                    | $-0.407$                    | 0.110                 | $-1.7$                    |

and $W(r)$ for an extended nucleus. For a spherically symmetric $\rho(r) = \rho(r),$ we have

$$V(r) = -4\pi a Z \left[ \frac{1}{r} \int_0^r d r' r'^2 \rho(r') + \int_r^\infty d r' \rho(r') \right], \quad (14)$$

$$W(r) = -4\pi a Z \left[ \frac{1}{r} \int_0^r d r' r'^2 \left( r'^2 + \frac{r'^2}{3} \right) \rho(r') + \int_r^\infty d r' \left( r'^2 + \frac{r'^2}{3} \right) \rho(r') \right]. \quad (15)$$

Assuming the nucleus to be a homogeneously charged sphere with radius $R = \sqrt{3/5} (r^2)^{1/2}$ one can obtain

$$V(r) = \begin{cases} -\frac{a Z}{r} & r \geq R, \\ -\frac{a Z}{R} \left( \frac{3}{2} - \frac{r^2}{2R^2} \right) & r < R, \end{cases} \quad (16)$$

$$W(r) = \begin{cases} -a Z \left( 1 + \frac{R^2}{5r^2} \right) & r \geq R, \\ -a Z \left( \frac{3}{4} + \frac{r^2}{2R^2} - \frac{r^4}{20R^4} \right) & r < R. \end{cases} \quad (17)$$

The nuclear size corrections to the low-order recoil term were calculated numerically, and the corresponding results are presented in the next section.

3. Numerical results and discussion

The nuclear size corrections to the low-order recoil effect for the 1s, 2s, and 2p_{1/2} states are summarized in tables 1, 2, and 3, respectively. They are expressed in terms of the function $\Delta F_L(aZ),$ which is defined by

$$\Delta F_L = \frac{m^2 - E_0^2}{2M} \left[ 1 + \Delta F_L(aZ) \right]. \quad (18)$$

The homogeneously charged-sphere model was used to describe the nuclear charge distribution. The function $\Delta F_L^{\text{(point)}}(aZ)$ corresponds to the approximate evaluation of [14, 15] that employs the point-nucleus recoil operator and the extended-nucleus Dirac wave functions. Our calculations within this approximation are in perfect agreement with those from [14, 15]. The function $\Delta F_L^{\text{(finite)}}(aZ)$ represents the values obtained by using equation (13) and includes all finite nuclear size corrections to the Breit term $\Delta F_L.$ The difference between $\Delta F_L^{\text{(finite)}}(aZ)$ and $\Delta F_L^{\text{(point)}}(aZ)$ is displayed in the fifth column.

The finite nuclear size corrections to the higher-order recoil term $\Delta F_L^{\text{(point)}}(aZ),$ calculated using the point-nucleus recoil operator [14, 15], are also presented. As was shown in [14], the leading nuclear size corrections to the low-order and higher-order terms cancel each other for $aZ \ll 1.$ The difference between $\Delta F_L^{\text{(finite)}}(aZ)$ and $\Delta F_L^{\text{(point)}}(aZ),$ being negligible for low-$Z$ ions, grows when $Z$ increases and reaches about 20% of $\Delta F_L^{\text{(point)}}(aZ)$ at $Z = 110.$ It is also worth noting that the values of $\Delta F_L^{\text{(point)}}(aZ)$ change the sign at $Z \approx 80,$ leading to a strong enhancement of the total nuclear size correction for heavy ions.

To conclude, in the present paper we have performed the complete evaluation of the nuclear size correction to the low-order (Breit) recoil contribution. We have found that the corrections, which are beyond the previously used approximation [14, 15], can contribute on the level of 20% of the total nuclear size contribution to the low-order recoil effect. To calculate the nuclear size corrections to the higher-order recoil term, which are beyond the approximation used in...
Table 2. Finite nuclear size corrections to the low-order recoil contribution for the 2s state expressed in terms of the function \( \Delta F(t, \alpha_z) \), which is defined by equation (18). The values of the nuclear radii used were taken from [20] (for \( Z \leq 92 \)) and [21] (for \( Z = 100, 110 \)). The last column refers to the higher-order recoil term which was evaluated in [15] using slightly different values of the nuclear radii.

| \( Z \) | \( \langle r^2 \rangle / 2 \) (fm) | \( \Delta F(t, 0Z) \) (aZ) | \( \Delta F(t, 0Z) \) (aZ) | \( \Delta \delta \) (aZ) |
|-------|----------------|----------------|----------------|----------------|
| 1     | 0.878          | -0.172 \times 10^{-8} | -0.172 \times 10^{-8} |                  |
| 2     | 1.676          | -0.260 \times 10^{-7} | -0.260 \times 10^{-7} |                  |
| 5     | 2.406          | -0.513 \times 10^{-6} | -0.513 \times 10^{-6} |                  |
| 10    | 3.006          | -0.487 \times 10^{-5} | -0.484 \times 10^{-5} | 0.3 \times 10^{-7} | 0.4 \times 10^{-5} |
| 20    | 3.478          | -0.474 \times 10^{-4} | -0.466 \times 10^{-4} | 0.8 \times 10^{-6} | 0.4 \times 10^{-4} |
| 30    | 3.949          | -0.211 \times 10^{-3} | -0.204 \times 10^{-3} | 0.7 \times 10^{-5} | 0.1 \times 10^{-3} |
| 40    | 4.285          | -0.669 \times 10^{-3} | -0.637 \times 10^{-3} | 0.32 \times 10^{-4} | 0.4 \times 10^{-3} |
| 50    | 4.644          | -0.185 \times 10^{-2} | -0.172 \times 10^{-2} | 0.13 \times 10^{-3} | 0.1 \times 10^{-2} |
| 60    | 4.942          | -0.468 \times 10^{-2} | -0.426 \times 10^{-2} | 0.42 \times 10^{-3} | 0.2 \times 10^{-2} |
| 70    | 5.305          | -0.0115          | -0.0102          | 0.13 \times 10^{-2} | 0.3 \times 10^{-2} |
| 80    | 5.458          | -0.0271          | -0.0233          | 0.0038          | 0.0066          |
| 90    | 5.785          | -0.0653          | -0.0545          | 0.0108          |                  |
| 92    | 5.857          | -0.0779          | -0.0646          | 0.0133          | -0.03           |
| 100   | 5.886          | -0.156           | -0.127           | 0.029           |                  |
| 110   | 5.961          | -0.382           | -0.300           | 0.082           |                  |

Table 3. Finite nuclear size corrections to the low-order recoil contribution for the 2p_{1/2} state expressed in terms of the function \( \Delta F(t, \alpha_z) \), which is defined by equation (18). The values of the nuclear radii used were taken from [20] (for \( Z \leq 92 \)) and [21] (for \( Z = 100, 110 \)).

| \( Z \) | \( \langle r^2 \rangle / 2 \) (fm) | \( \Delta F(t, 0Z) \) (aZ) | \( \Delta F(t, 0Z) \) (aZ) | \( \Delta \delta \) (aZ) |
|-------|----------------|----------------|----------------|----------------|
| 10    | 3.006          | -0.942 \times 10^{-8} | -0.905 \times 10^{-8} | 0.37 \times 10^{-9} |
| 20    | 3.478          | -0.207 \times 10^{-6} | -0.196 \times 10^{-6} | 0.11 \times 10^{-7} |
| 30    | 3.949          | -0.204 \times 10^{-5} | -0.192 \times 10^{-5} | 0.12 \times 10^{-6} |
| 40    | 4.285          | -0.117 \times 10^{-4} | -0.109 \times 10^{-4} | 0.8 \times 10^{-6}  |
| 50    | 4.644          | -0.518 \times 10^{-4} | -0.474 \times 10^{-4} | 0.44 \times 10^{-5} |
| 60    | 4.942          | -0.196 \times 10^{-3} | -0.175 \times 10^{-3} | 0.21 \times 10^{-4} |
| 70    | 5.305          | -0.688 \times 10^{-3} | -0.600 \times 10^{-3} | 0.88 \times 10^{-4} |
| 80    | 5.458          | -0.225 \times 10^{-2} | -0.191 \times 10^{-2} | 0.34 \times 10^{-3} |
| 90    | 5.785          | -0.741 \times 10^{-2} | -0.613 \times 10^{-2} | 0.128 \times 10^{-2} |
| 92    | 5.857          | -0.942 \times 10^{-2} | -0.774 \times 10^{-2} | 0.168 \times 10^{-2} |
| 100   | 5.886          | -0.0242          | -0.0195          | 0.0047          |                  |
| 110   | 5.961          | -0.0825          | -0.0643          | 0.0182          |                  |

[14, 15], one should first derive the corresponding corrections to formulas equations (6)–(7). Such a derivation, which seems rather problematic, requires further theoretical investigations that are beyond the scope of this paper.

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