Recoil Correction to Hydrogen Energy Levels: A Revision

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Abstract

Recent calculations of the order \((Z\alpha)^4\) pure recoil correction to hydrogen energy levels are critically revised. The origins of errors made in the previous works are elucidated. In the framework of a successive approach, we obtain the new result for the correction to \(S\) levels. It amounts to \(-16.4\) kHz in the ground state and \(-1.9\) kHz in the \(2S\) state.
1 Introduction

The correction to $S$ levels of hydrogen atom, that is first-order in $m/M$ and fourth-order in $Z\alpha$, has become recently a point of controversy. Initially, this correction was calculated in Ref.[1]. Then, a different result for the same correction was obtained in Ref.[2]. While in both papers it was employed the same (exact in $Z\alpha$) starting expression for the pure recoil correction, the methods of calculation, and in particular the regularization schemes used were rather different. To resolve the discrepancy between two results, in Ref.[3] an attempt was undertaken to prove the correctness of the earlier result of Ref.[1] applying the method of calculation used by the present author in Ref.[2]. An extra contribution due to the peculiarities of the regularization procedure was found by the authors of Ref.[3], which exactly compensated the difference of the Ref.[2] result from that of Ref.[1]. This finding has led the authors of Ref.[3] to conclusion “that discrepancies between the different results for the correction of order $(Z\alpha)^6(m/M)$ to the energy levels of the hydrogenlike ions are resolved and the correction of this order is now firmly established”.

Taking criticism of the Ref.[3] as completely valid, we nevertheless cannot agree with the conclusion cited above. The point is that the authors of Ref.[3] emphasizing an importance of an explicit regularization of divergent expressions, pay no attention to an accurate matching of regularized contributions.

In fact, one usually starts from an exact expression which can be easily checked to have a finite value. Then one has to use different approximations to handle this expression at different scales. In this way some auxiliary parameter(s) are introduced which enable one to separate applicability domains for different approximations. Finally, a necessary condition for the sum of thus calculated contributions to be correct is its independence from any scale separating parameter.

In the present paper we successively pursue this line of reasoning for a recalculation of the order $(Z\alpha)^6m^2/M$ correction to hydrogen energy levels. We discuss only $S$ levels since for higher angular momenta levels the result is actually firmly established [4, 2]. As far as the controversy mentioned above concerns details of a regularization at the subatomic scale, the result’s dependence on a principal quantum number $n$ is also known. That’s why we perform all the calculations for the ground state and then restore the $n$ dependence in the final result.

To make the presentation self-contained we rederive some known results, using sometimes new approaches. In Sec.2 the general outline of the problem is given. Sections 3, 4 and 5 are devoted to the Coulomb, magnetic, and seagull contributions, respectively. The correspondence between various results is discussed in Conclusion. In Appendixes, we address a couple of minor computational issues.

Throughout the paper the Coulomb gauge of electromagnetic potentials and relativistic units $\hbar = c = 1$ are used. Leaving aside the radiative corrections we set $Z = 1$
in what follows.

2 General Outline

The first recoil correction to a bound state energy of the relativistic electron in the Coulomb field is an average value of the non-local operator, 

$$ \Delta E_{\text{rec}} = -\frac{1}{M} \int \frac{d\omega}{2\pi i} \left\langle \left( \vec{p} - \vec{D}(\omega, \vec{r}) \right) G(\vec{r}', \vec{r}|E + \omega) \left( \vec{p} - \vec{D}(\omega, \vec{r}) \right) \right\rangle, \quad (1) $$

taken over an eigenstate of the Dirac equation in the Coulomb field,

$$ H\psi(\vec{r}) = E\psi(\vec{r}), \quad H = \vec{\alpha}\vec{p} + \beta m - \frac{\vec{\alpha}}{r}. \quad (2) $$

In (1), \(\vec{p}\) is the electron momentum operator, \(\vec{D}(\omega, \vec{r})\) describes an exchange by the transverse (magnetic) quantum,

$$ \vec{D}(\omega, \vec{r}) = \int \frac{d^3k}{(2\pi)^3} e^{i\vec{k}\vec{r}} \frac{4\pi\alpha\vec{\alpha}_k}{k^2 - \omega^2}, \quad \vec{\alpha}_k \equiv \vec{\alpha} - \frac{\vec{k}(\vec{\alpha}\vec{k})}{k^2}, \quad (3) $$

while

$$ G(\vec{r}', \vec{r}|E + \omega) = \left( E + \omega - \vec{\alpha}\vec{p} - \beta m + \frac{\vec{\alpha}}{r'} \right)^{-1} \delta(\vec{r}' - \vec{r}) \quad (4) $$

is the Green’s function for the Dirac equation in the Coulomb field. The integration contour in (1) goes from the minus infinity to zero below the real axis, round zero from above and then proceeds to the plus infinity above the real axis.

As far as we are going to calculate the correction (1) perturbatively, i.e. as a power series in \(\alpha\), it proves convenient to decompose (1) into three parts,

$$ \Delta E_{\text{rec}} = C + M + S, \quad (5) $$

namely the Coulomb, magnetic and seagull contributions, corresponding to \(\vec{p}\vec{p}\), \(\vec{p}\vec{D} + \vec{D}\vec{p}\) and \(\vec{D}\vec{D}\) terms from (1) respectively.

3 Coulomb Contribution

It is natural to continuously transform the integration contour into the sum of two sub-contours, thus splitting the Coulomb contribution into two terms,

$$ C = \left\langle \frac{\vec{p}^2}{2M} \right\rangle - \frac{1}{M} \left\langle \vec{p}\Lambda\vec{p} \right\rangle, \quad (6) $$
where $\Lambda_-$ is the projector to the set of negative-energy Dirac-Coulomb eigenstates. The former term in (6) results from the integration along the upper half of the infinite circumference and its value is determined by the atomic scale $p \sim m_0$. Being the average of the local operator, this term can be easily calculated exactly. The latter term in (6) arises as an integral along the contour $C_-$, wrapping the half-axis $(-\infty, 0)$ in the counterclockwise direction. To the order we discuss, this term is completely saturated by momenta from the relativistic scale $p \sim m$. That’s why it can be calculated without any regularization [1, 2]:

$$-\frac{1}{M} \langle \bar{p} \Lambda_- \bar{p} \rangle \alpha^6 = \frac{m^2 \alpha^6}{M}. \quad (7)$$

4 Magnetic Contribution

Using the identity

$$\langle \bar{p}G\bar{D} + G\bar{D}\bar{p} \rangle = \frac{1}{\omega} \langle [\bar{p}, H]G\bar{D} + G[D, H] + \{\bar{p}, \bar{D}\} \rangle, \quad (8)$$

which follows directly from the equation for the Green’s function, we can extract from the general expression for the magnetic contribution,

$$\mathcal{M} = \frac{1}{M} \int \frac{d\omega}{2\pi i} \langle \bar{p}G\bar{D} + G\bar{D}\bar{p} \rangle, \quad (9)$$

its local part,

$$\frac{1}{M} \int_{C_-} \frac{d\omega}{2\pi i \omega} \langle \{\bar{p}, \bar{D}(\omega, \vec{r})\} \rangle = -\frac{1}{2M} \langle \{\bar{p}, \bar{D}(0, \vec{r})\} \rangle. \quad (10)$$

Due to the rapid convergency of the integral in (9) at the infinity, the integration contour can be reduced to $C_-$. By virtue of the virial relations (see [3] and references therein), the sum of local parts of the Coulomb and magnetic contributions takes a simple form [3]:

$$\left\langle \frac{p^2}{2M} - \frac{1}{2M} \{\bar{p}, \bar{D}(0, \vec{r})\} \right\rangle = \frac{m^2 - E^2}{2M}. \quad (11)$$

Physically, this contribution to the recoil correction is induced by an instantaneous part of the electron-nucleus interaction.

4.1 Long Distances

Immediate integration with respect to $\omega$ in (9) gives [2]:

$$\mathcal{M} = -\frac{\alpha}{M} \int \frac{d^3 \vec{k}}{(2\pi)^3} \left\langle \bar{p} \left( \sum_+ \frac{|m\rangle\langle m|}{k + E_m - E} - \sum_- \frac{|m\rangle\langle m|}{E - E_m + k} \right) \frac{4\pi \alpha \vec{k}}{k} e^{i\vec{k}\vec{r}} \right\rangle, \quad (12)$$

where $\sum_+(-)$ stands for the sum over discrete levels supplied by the integral over positive-(negative-) energy part of the continuous spectrum.
4.1.1 Positive Energies

In the leading nonrelativistic approximation, the first term in Eq. (12) reads,

\[ \mathcal{M}_+ = \frac{\alpha}{Mm} \int \frac{d^3 \vec{k}}{(2\pi)^3} \left\{ \bar{\psi} \mathcal{G} (\vec{r}', \vec{r}| E - k) \frac{4\pi e^{i\vec{k} \cdot \vec{r}}}{k} \psi \right\}, \tag{13} \]

where \( \mathcal{G} (\vec{r}', \vec{r}| E - k) \) is the Green’s function for the Schrödinger equation in the Coulomb field, and the average is taken now over the nonrelativistic wavefunction. For the ground state, we work with

\[ \psi (\vec{r}) = \sqrt{\frac{(m\alpha)^3}{\pi}} e^{-m\alpha r}, \quad E = -\frac{m\alpha^2}{2}. \tag{14} \]

Only \( p \)-wave term from the partial expansion,

\[ \mathcal{G} (\vec{r}', \vec{r}| \omega) = \sum_l (-1)^l (2l + 1) P_l (\vec{n}' \cdot \vec{n}) \mathcal{G}_l (r', r| \omega), \tag{15} \]

survives the integration over the angles:

\[ \mathcal{M}_+ = -\frac{m\alpha^3}{M\pi} \int_0^\infty dk \int_{-1}^1 dx (1 - x^2) \left\{ \mathcal{G}_1 (r', r| E - k) e^{ikx} \right\}. \tag{16} \]

For the nonrelativistic Green’s function in the Coulomb field we use the integral representation from the paper [10],

\[ \mathcal{G}_1 (r', r| -\frac{\kappa^2}{2m}) = \frac{im}{2\pi \sqrt{rr'}} \int_0^\pi ds \frac{\exp i \left\{ \frac{2m\alpha}{\kappa} s + \frac{2(r' + r)}{\tan s} \right\}}{1 - e^{2i\frac{m\alpha}{\kappa}}} J_3 \left( \frac{2\kappa \sqrt{rr'}}{\sin s} \right). \tag{17} \]

The integrals over \( r \) and \( r' \) in (13) are easily calculated after expanding the Bessel function into the power series. The result can be expressed in the form,

\[ \mathcal{M}_+ = \frac{2\kappa^5 \sqrt{m} \alpha^6}{M\pi} \int_0^\infty dk \int_{-1}^1 dx (1 - x^2) \int_C dt \frac{\frac{1}{(a - bt)^4}}{1 - e^{2\pi i \frac{m\alpha}{\kappa}}} \frac{1}{t}, \tag{18} \]

where \( \kappa = \sqrt{2m(k - E)} \), the contour \( C \) is the unit circumference \( |t| = 1 \) directed clockwise, and

\[ a = \left( 1 + \frac{m\alpha}{\kappa} \right) \left( 1 + \frac{m\alpha}{\kappa} - \frac{ik\kappa}{\kappa} \right), \quad b = \left( 1 - \frac{m\alpha}{\kappa} \right) \left( 1 - \frac{m\alpha}{\kappa} + \frac{ik\kappa}{\kappa} \right). \]

Integration by parts conveniently extracts from the last integral in (18) the terms nonvanishing at large momenta:

\[ \mathcal{M}_+ = -\frac{2\kappa^5 m^2 \alpha^5}{M\pi} \int_0^1 dy (1 - y^2) \int_{-1}^1 dx (1 - x^2) F(x, y), \tag{19} \]

where

\[ F(x, y) = \frac{2}{b(a - b)^3} - \frac{1 - y}{b^2(a - b)^2} - \frac{y(1 - y)}{ab^2(a - b)} + \frac{1 - y^2}{a^2b^2} - \frac{y(1 - y^2)}{a^3b} \int_0^1 dt \frac{t - y}{1 - \frac{b}{a} t}. \tag{20} \]
and the new integration variable $y \equiv m\alpha/\kappa$ is introduced. Since

$$\frac{k}{\kappa} = \frac{\alpha}{2} \frac{1 - y^2}{y},$$

(21)

to get a power series expansion of (19) with respect to $\alpha$ up to the first order, we need an expansion of the integrand with respect to $y$ also up to the first order (note that $a - b = 4y - 2ikx/\kappa$):

$$(1 - y^2)F(x, y) \approx \frac{2}{(a - b)^3} - \frac{1}{2(a - b)} + \frac{1}{2} - \frac{y^2}{2(a - b)} - \frac{y}{2} + y \ln(a - b).$$

(22)

Here the last term emerges as a result of expansion of the integral in (20),

$$\int_0^1 dt \, \frac{t^{-y}}{1 - \frac{2 t}{a}} = \frac{1}{1 - y} F\left(1, 1 - y; 2 - y; \frac{b}{a}\right),$$

(23)

where $F(1, 1 - y; 2 - y; b/a)$ is the Gauss hypergeometric function. Integrating now (22) first with respect to $x$, and then with respect to $y$ from 0 to some $y_0$ ($\alpha^{1/2} \ll y_0 \ll 1$), we obtain,

$$\int_0^{y_0} dy (1 - y^2) \int_{-1}^{1} dx (1 - x^2) F(x, y) \approx \pi \frac{\alpha}{32} - \frac{1}{48y_0^2} - \frac{1}{12} \ln \frac{4y_0^2}{\alpha} + \frac{1}{48} - \frac{1}{9} + \frac{2y_0}{3} + \frac{2y_0^2}{3} \ln 4y_0 - \frac{3y_0^2}{4} - \frac{\pi \alpha}{32}. $$

(24)

On the other hand, we can neglect $\alpha$ in $F(x, y)$ on the interval $[y_0, 1]$. In the sum of two integrals, the dependence on the auxiliary parameter $y_0$ disappears, and we come to the result,

$$\mathcal{M}_+ = \frac{m^2 \alpha^5}{M\pi} \left\{ - \frac{\pi}{\alpha^2} + \frac{8}{3} \ln \frac{1}{\alpha} + \frac{8}{3} \ln \frac{Ry}{\langle E \rangle_{1S}} + \frac{16}{3} \ln 2 + \frac{32}{9} - \pi \alpha \right\}. $$

(25)

Here the Bethe logarithm is introduced [11],

$$16 \int_0^{y_0} dy \, y \left( \frac{2 - y}{1 + y} \right)^2 \frac{1}{(1 + y)^4 (1 - y)} = \ln \frac{Ry}{\langle E \rangle_{1S}} + 2 \ln 2 + \frac{11}{6}. $$

(26)

In (25), the order $\alpha^4$ term is just the lowest-order contribution to (11), the order $\alpha^5$ terms are in accord with the result of Salpeter [12], while the order $\alpha^6$ term coincides with the retardation correction, found in [2], Eq.(14) by the different method.

It can be easily seen that the order $\alpha^6$ contribution to the positive-energy part of (12) is exhausted by the sum of those to (10) and (25). Actually, relativistic corrections are at least of the $\alpha^2$ relative order. The effect of retardation reveals itself starting from the $\alpha^5$ order (27). Hence the relativistic corrections to the retardation are at least of the $\alpha^7$ order.
4.1.2 Negative Energies

Virtual transitions into negative-energy states give rise to the second term in (12). In the leading nonrelativistic approximation, it equals

\[ M_\text{−} = \frac{\alpha^2}{4m^2 M} \left\langle \frac{d^3 \tilde{k}}{(2\pi)^3} \left\langle \frac{4\pi}{k'^2} \frac{4\pi}{k^2} \right\rangle \right. \]

(27)

where \( k' = \vec{k} - \vec{k}'(\vec{k}\vec{k}')/k'^2 \), \( \vec{k}' = \vec{p}' - \vec{p} - \vec{k} \), \( \vec{p} \) and \( \vec{p}' \) being the arguments of the wavefunction and its conjugate respectively. The integral over \( k \) diverges logarithmically (leading linear divergency vanishes due to the numerator which at \( k \to \infty \) becomes transverse to itself, and hence rises only like \( k \), not \( k^2 \)). To treat this divergency we use the following formal trick \[2\]: subtract from (27) the same expression with \( k'^2 + \lambda^2 \) substituted in place of \( k'^2 \). For \( \lambda \gg m\alpha \), the subtracted term is completely determined by a scale much less than the atomic one, so that we will find that term below using a relativistic approach.

The regularized version of (27) can be written in the form

\[ M_\text{−} - M_\text{r} = \frac{\alpha^2}{4m^2 M} \left\langle \left( \frac{4\pi}{k'^2} - \frac{4\pi}{k'^2} \right) \right. \]

(28)

In the coordinate representation, the integral above is

\[ \frac{in_j}{r^2} \left( \frac{\delta_{ij} - \partial_i \partial_j}{\lambda^2} \right) \frac{1 - e^{-\lambda r}}{r} = \frac{in_j}{r^2} \left( \frac{1}{\lambda^2} \right) e^{\lambda r}. \]

(29)

After substitution into (28) it gives

\[ M_\text{−} - M_\text{r} = \frac{\alpha^2}{4m^2 M} \left\langle 4\pi \delta(\vec{r}) \int_0^{\lambda} d\sigma \left( 1 - \frac{\sigma^2}{\lambda^2} \right) e^{\sigma r} \right. \]

(30)

Finally, the result of trivial calculation of the average over the ground state reads,

\[ M_\text{−} - M_\text{r} = \frac{m^2 \alpha^6}{M} \left( 2 \ln \frac{\varepsilon}{\alpha} - 1 \right), \]

(31)

where \( \varepsilon \equiv \lambda/2m \).

4.2 Short Distances

Since in the nonrelativistic approximation the subtracted term, \( M_\text{r} \), is ultraviolet divergent, we have to calculate it beyond this approximation, i.e. using a relativistic approach. It proves more convenient in this approach to postpone the integration over \( \omega \) to the last stage of calculation. As we will see below, the reversed order of integration
first over space variables, then over frequency) makes the calculations quite simple. The fee for the technical advantage is that a regulator contribution is calculated not only for the negative-, but for the positive-energy part of $\mathcal{M}$ also. Surely, the instantaneous contribution can be left aside, so that only two first terms from the r.h.s. of (3) are considered below.

For the subtracted term, we have the new expansion parameter, $m\alpha/\lambda$, and hence the Coulomb interaction during the single magnetic exchange can be treated perturbatively. The order $m\alpha^6/M$ contributions arise due to only two first terms of the Green’s function expansion in the Coulomb interaction, $G(0)$ and $G(1)$. Let us begin with the second contribution:

$$\mathcal{M}_G = \frac{2}{M} \int_{C_-} \frac{d\omega}{2\pi i} \frac{1}{\omega} \left\langle [\vec{p}, H] G^{(1)} \right\rangle. \quad (32)$$

Here

$$D^r = \int \frac{d^3\vec{k}}{(2\pi)^3} e^{i\vec{k}\vec{r}} \frac{4\pi\alpha\vec{\alpha}_k}{k^2 + \lambda^2 - \omega^2},$$

and we can neglect atomic momenta in comparison with $\lambda$ and $m$:

$$\mathcal{M}_G = -\frac{\alpha^3\psi^2}{\pi M} \int_{C_-} \frac{d\omega}{\omega} \left\langle \frac{4\pi\vec{p}'}{\Omega^2} \frac{2m + \omega + \vec{\alpha}\vec{p}'}{\frac{2\pi^2}{p^2} - \frac{\Omega^2}{p^2}} \frac{4\pi \omega + \vec{\alpha}\vec{p}}{q^2} \frac{4\pi\vec{\alpha}_p}{\frac{2\pi^2}{p^2} - \frac{2\pi^2}{p^2} - K^2} \right\rangle. \quad (33)$$

The notations of [2] are used: $\psi^2 \equiv |\psi(0)|^2$, the angle brackets denote here integrations over $\vec{p}$ and $\vec{p}'$ together with the average over the spinor $u_\alpha = \delta_{\alpha 1}$; $\vec{q} = \vec{p}' - \vec{p}$; and

$$K \equiv \sqrt{\omega^2 - \lambda^2}, \quad \Omega \equiv \sqrt{2m\omega + \omega^2}.$$

The average over the spin degrees of freedom gives

$$\langle (2m + \omega + \vec{\alpha}\vec{p}') (\omega + \vec{\alpha}\vec{p}) \vec{\alpha}_p \vec{p}'' \rangle = \omega \vec{p}''_p = \omega \vec{p}'_p \vec{q}. \quad (34)$$

Then, after transition to the coordinate representation we get

$$\mathcal{M}_G = \frac{2\alpha^3\psi^2}{mM} \int_{C_-} \frac{d\omega}{\omega} \int_0^\infty dr \left( \frac{e^{i\Omega r} - 1}{\Omega^2 r} \right) R_n \left[ \left( \delta_{ij} + \frac{\partial_i \partial_j}{\Omega^2} \right) e^{i\Omega r} - \frac{1}{r} - (\Omega \rightarrow K) \right]. \quad (35)$$

The integration over $r$ is simple but lengthy. It results in

$$\mathcal{M}_r = -\frac{\alpha^3\psi^2}{2mM} \int_{C_-} \frac{d\omega}{\omega} \left\{ \frac{K}{\Omega} - \frac{K^2}{\Omega^2} \ln \left( 1 + \frac{\Omega}{K} \right) + (\Omega \leftrightarrow K) + 2 \ln \left( 1 + \frac{K}{\Omega} \right) \right\}. \quad (36)$$

Here the contour of integration goes counterclockwise around the cut connecting points $-2m$ and $-\lambda$. According to the Feynman rules, $\Omega = i|\Omega|$, while $K = +(-)|K|$ on the lower (upper) edge of this cut. Since the integrand is regular at small $\omega$, we can put $\lambda = 0$ (recall that $\lambda \ll m$) and get

$$\mathcal{M}_G = \frac{\alpha^3\psi^2}{mM} \int_0^1 dx \left( \frac{\sqrt{1 - x}}{x^{3/2}} - \frac{1}{x^2} \arctan \sqrt{\frac{x}{1 - x}} - \frac{1}{\sqrt{x(1 - x)}} \right) = -\frac{3\pi\alpha^3\psi^2}{2mM}. \quad (37)$$
To calculate a contribution due to $G^{(0)}$ we have to account properly for the wavefunction’s short-distance behavior:

$$
\mathcal{M}_{\psi} = -\frac{\alpha^3 \psi^2}{\pi M} \int_{C_-} \frac{d\omega}{i\omega} \left( \left( \frac{4\pi \vec{p}'}{p'^2} + \frac{2m + \omega + \vec{\alpha} \vec{p}'}{p'^2 - \Omega^2} \right) \frac{4\pi \vec{\alpha}_q}{q^2 - K^2} \right.
$$

$$
+ \left. \left( \frac{4\pi \vec{\alpha}_p \cdot \vec{\omega} + \vec{\alpha} \vec{p}' \cdot 4\pi \vec{q}}{p'^2 - \Omega^2} \right) \frac{2m + \vec{\alpha} \vec{p}'}{p'^2} \right) \frac{4\pi}{p^2} \right). 
$$

(38)

Averaging over the spin part of the wavefunction, we obtain

$$
\mathcal{M}_{\psi}^r = -\frac{\alpha^3 \psi^2}{\pi M} \int \frac{d\omega}{i} \left( \left( \frac{4m}{\omega} + 1 \right) \frac{4\pi}{p'^2(p'^2 - \Omega^2)} \frac{4\pi}{q^2 - K^2} \frac{4\pi \vec{p}'^2}{p^4} \right.
$$

$$
- \left. \frac{4\pi}{(p'^2 - K^2)(p'^2 - \Omega^2)} \frac{4\pi}{q^2} \frac{4\pi \vec{p}'^2}{p^4} \right). 
$$

(39)

Again, the six-dimensional integral over $\vec{p}$ and $\vec{p}'$ turns into a simple integral over $r$ in the coordinate representation, and equals

$$
\mathcal{M}_{\psi}^r = \frac{2\alpha^3 \psi^2}{M} \int \frac{d\omega}{i} \left\{ \left( \frac{4m}{\omega} + 1 \right) \left[ \frac{1}{\Omega^2} \ln \left( 1 + \frac{\Omega}{K} \right) + \frac{1}{K^2} \ln \left( 1 + \frac{K}{\Omega} \right) - \frac{1}{\Omega K} \right] \right. 
$$

$$
+ \left. \frac{1}{2m\omega} \ln \frac{\Omega}{\Omega} \right\}. 
$$

(40)

Finally, the integration along the same contour as above gives for non-vanishing in the limit $\varepsilon \to 0$ terms:

$$
\mathcal{M}_{\psi}^r = \frac{m^2 \alpha^6}{M} \left( \frac{2}{\varepsilon} - \frac{32}{9\pi \sqrt{\varepsilon}} \int_0^\infty \frac{d\theta}{\sqrt{\cosh \theta}} + 2 \ln \frac{1}{\varepsilon} \right). 
$$

(41)

We see that as expected the logarithmic in $\varepsilon$ term cancels the corresponding one in (31). The more singular in $\varepsilon$ terms can only be the result of the regularization procedure applied to the positive-energy contribution (25). As far as the latter is non-singular at short distances, this procedure is actually unnecessary, i.e. it can produce only positive powers of $m\alpha/\lambda$. An explicit calculation can be found in Appendix A.

### 4.3 Total Magnetic Contribution

So, in the sum of all contributions due to a single magnetic exchange, any dependence on the scale separating parameter $\varepsilon$ cancels away, and we get

$$
\mathcal{M}_{\alpha^6} + \left\langle \frac{p^2}{2M} \right\rangle_{\alpha^6} = \frac{m^2 \alpha^6}{M} \left( -1 + 2 \ln \frac{1}{\alpha} - 1 - \frac{3}{2} \right). 
$$

(42)

Here $-1$ in the r.h.s. is due to the (long-distance) effect of retardation (see (25) and \[2\], Eq.(14)), $2 \ln \frac{1}{\alpha} - 1$ comes from the whole range of scales from $m\alpha$ to $m$, while $-3/2$ is the short-distance contribution.
5 Seagull Contribution

5.1 Long Distances

Again, the best suited way to analyze the atomic scale contribution is to begin from taking the integral with respect to $\omega$. It proves that in the order of interest, only positive-energy intermediate states are to be considered [2]:

$$S_+ = \frac{\alpha^2}{2M} \int \frac{d^3 \vec{k}}{(2\pi)^3} \left\{ \frac{4\pi}{2m} \frac{2\vec{p} \cdot \vec{k}'}{2m} \frac{4\pi}{k^2} \frac{2\vec{p} + i\vec{\sigma} \times \vec{k}}{2m} \right\}. \tag{43}$$

A simple power counting shows that only bilinear in $\vec{k}$ and $\vec{k}'$ term gives rise to the ultraviolet divergency. To regularize this divergency, we subtract from the divergent term the regulator contribution, which at large distances equals to

$$- \frac{\alpha^2}{4m^2 M} \left\{ \frac{4\pi}{k^2 + \lambda^2} \frac{4\pi}{k^2} \right\}, \tag{44}$$

while $m\alpha \ll \lambda, \lambda' \ll m$. In the coordinate representation, the regularized version of (43) is

$$S_+ - S_+^r = \frac{\alpha^2}{4m^2 M} \left\{ 2\frac{1}{r^2} \frac{\vec{p} \cdot \vec{p}'}{r^4} - \left( \nabla e^{-\lambda' r} \right) \left( \nabla e^{-\lambda r} \right) \right\}. \tag{45}$$

The average over the ground state reads ($\varepsilon' = \lambda' / 2m$):

$$S_+ - S_+^r = \frac{m^2 \alpha^6}{M} \left\{ 2\frac{\varepsilon'^2 + \varepsilon' \varepsilon + \varepsilon^2}{\alpha (\varepsilon' + \varepsilon)} + 1 - 2\ln \frac{\varepsilon' + \varepsilon}{\alpha} + \frac{2\varepsilon' \varepsilon}{(\varepsilon' + \varepsilon)^2} \right\}. \tag{46}$$

Here 1 appears due to the non-singular operator $\vec{p} r^{-2} \vec{p}'$. The first term in the curly brackets represents the regulator contribution to the previous order. In Appendix B, an appearance of this term as a short-distance contribution to the $m\alpha^5 / M$ order is shown explicitly. In what follows we calculate the subtracted term, whose non-relativistic version (44) is ultraviolet divergent, in the framework of a relativistic approach.

5.2 Short Distances

Just like in case of the single magnetic exchange, only two first terms of the Green’s function expansion in the Coulomb interaction contribute to the $m^2 \alpha^6 / M$ order. For the $G(1)$’s contribution we have,

$$S_G^r = \frac{\alpha^3 \psi^2}{2\pi M} \int_{C_-} \frac{d\omega}{i} \left\{ \frac{4\pi}{p^2 - K'^2} \frac{\omega + \alpha \vec{p}'}{p^2 - \Omega^2} \frac{4\pi}{q^2} \frac{\omega + \alpha \vec{p}}{p^2 - \Omega^2} \frac{4\pi}{K^2} \right\}. \tag{47}$$

Calculation along the same lines as in the case of $M^r_G$ gives the result

$$S_G^r = \frac{\pi \alpha^3 \psi^2}{Mm} (4 \ln 2 - 2), \tag{48}$$
which is non-singular in the limit $\lambda, \lambda' \to 0$.

As for the contribution due to $G(0)$, it can be extracted from

$$\frac{\alpha^3 \psi^2}{2\pi M} \int_{C_-} \frac{d\omega}{i} \left( \frac{4\pi \tilde{\alpha}^{\prime \prime} \omega + \tilde{\alpha}^{\prime \prime} q}{p^2 - K^2} \frac{4\pi \tilde{\alpha} q}{q^2 - K^2} \frac{2m + \tilde{\alpha} q}{(p^2 + \gamma^2)^2} 4\pi \right) + (\lambda \leftrightarrow \lambda'), \quad (49)$$

as a zeroth-order term of the Laurent series in $\gamma \equiv m\alpha$ (this series begins with an order $1/\gamma$ term describing the seagull contribution to $m^2 \alpha^5/M$ order at short distances discussed in Appendix B). The average over the spin part of the wavefunction is

$$\langle 2m\omega \tilde{\alpha}^{\prime \prime} \tilde{\alpha}_q + \tilde{\alpha}^{\prime \prime} \tilde{\alpha} q \tilde{\alpha} \tilde{\alpha} \rangle = -\left( \omega^2 + \left[ p^2 - \Omega^2 \right] \right) \left( 1 + \frac{(p' q)^2}{p^2 q^2} \right) + 2\tilde{p}' \tilde{q}. \quad (50)$$

The term in the square brackets can be omitted. In fact, the corresponding part of (49) does not depend on $m$ and hence (merely on dimensional grounds) contribute to the $m^2 \alpha^5/M$ order only. Then, the first term gives the non-singular in the limit $\lambda, \lambda' \to 0$ contribution:

$$-\omega^2 \left( 1 + \frac{(p' q)^2}{p^2 q^2} \right) \to \frac{\pi \alpha^3 \psi^2}{M m} (1 - 4 \ln 2). \quad (51)$$

Finally, analysis of the last term from (50) deserves more care since here we have the infrared singularity. Being integrated over the space variables, this term gives:

$$2\tilde{p}' \tilde{q} \to \frac{2\alpha^3 \psi^2}{M m} \int_{C_-} \frac{d\omega}{i\omega} \left\{ f(\Omega, K) - f(K', K) \right\}, \quad (52)$$

where

$$f(x, y) = \ln \left( 1 + \frac{x}{y} \right) - \frac{xy}{(x + y)^2} \quad (53)$$

(recall that $K' = \sqrt{\omega^2 - \lambda'^2}$). For $\varepsilon \ll 1$ we obtain

$$\frac{2\alpha^3 \psi^2}{M m} \int_{C_-} \frac{d\omega}{i\omega} f(\Omega, K) = \frac{\pi \alpha^3 \psi^2}{M m} \left( -2 \ln \frac{1}{\varepsilon} + 4 \ln 2 - 1 \right). \quad (54)$$

Calculation of the integral with $f(K', K)$ is a bit more cumbersome since it does not contain a small parameter. The contour $C_-$ for this integral encompasses in the counterclockwise direction the cut connecting the points $-\lambda$ and $-\lambda'$. Continuous deformation of $C_-$ leads to the following equation:

$$\int_{C_-} d\omega \ldots = \int_{C_+} d\omega \ldots - 2\pi i \text{Res}_{\omega=0} \ldots - 2\pi i \text{Res}_{\omega=\infty} \ldots, \quad (55)$$

where $\ldots$ stands for $f(K', K)/\omega$, and the contour $C_+$ goes in the clockwise direction around the cut connecting the points $\lambda$ and $\lambda'$. Using the evident relations,

$$\int_{C_+} d\omega \ldots = -\int_{C_-} d\omega \ldots, \quad (56)$$

$$\text{Res}_{\omega=0} \frac{1}{\omega} f(K', K) = f(\lambda', \lambda), \quad (57)$$

$$\text{Res}_{\omega=\infty} \frac{1}{\omega} f(K', K) = -\ln 2 + \frac{1}{4}, \quad (58)$$
we come to the result
\[
\frac{2\alpha^3\psi^2}{Mm} \int_{C_\infty} \frac{d\omega}{i\omega} f(K', K) = \frac{\pi \alpha^3\psi^2}{Mm} \left( 2 \ln \frac{2\epsilon}{\varepsilon + \varepsilon'} + \frac{2\varepsilon \varepsilon'}{(\varepsilon + \varepsilon')^2} - \frac{1}{2} \right). \tag{59}
\]

5.3 Total Seagull Contribution

As can be seen from (46), (48), (51), (54), and (59), the total seagull contribution to the \(m^2\alpha^6/M\) order does not depend on the scale separating parameters \(\lambda\) and \(\lambda'\), and equals
\[
S_{\alpha^6} = \frac{m^2\alpha^6}{M} \left( 1 - 2\ln \frac{2\alpha}{\varepsilon} + \frac{1}{2} + 4\ln 2 - 2 \right), \tag{60}
\]
where 1 comes from the long distances, \(4\ln 2 - 2\) from the short ones, while the remaining terms gain their values on the whole range of scales, from \(m\alpha\) to \(m\).

6 Conclusions

In complete accord with the result of Ref.[13], the total correction of the \(m^2\alpha^6/M\) order does not contain \(\ln \alpha\). It consists of two terms,
\[
\Delta E_{rec} = \left. \frac{m^2 - E^2}{2M} \right|_{\alpha^6} + \frac{m^2\alpha^6}{Mn^3} (2\ln 2 - 3). \tag{61}
\]
The former term is completely determined by the atomic scale and depends non-trivially on a principal quantum number \(n\),
\[
\left. \frac{m^2 - E^2}{2M} \right|_{\alpha^6} = \frac{m^2\alpha^6}{2Mn^3} \left( \frac{1}{4} + \frac{3}{4n} - \frac{2}{n^2} + \frac{1}{n^3} \right). \tag{62}
\]
As for the latter one, our calculations show that it has its origin at the scale of the order of \(m\).

The correction (61) shifts the hydrogen ground state by \(-16.4\) kHz and \(2S\) state by \(-1.9\) kHz. These figures are well comparable with the uncertainties of the recent Lamb shift measurements [14].

The result (61) differs from those obtained in Ref.[1, 3] and in Ref.[2]. Let us first discuss the origin of the difference in the latter case. In [2], it was erroneously assumed that the cancellation of singular operators at the atomic scale does not leave a non-vanishing remainder. The present calculation shows that due to a difference in details of a cut-off procedure used to regularize the average values of singular operators, some finite contributions do survive the cancellation process.

Unfortunately, the same error was repeated in Ref.[3]. The long-distance contribution was found there in the framework of some particular regularization scheme. Then it was
added to the short-distance contribution calculated in Refs. [1, 3] by completely different regularization procedures. The regularization dependence of the results obtained in [3] can be seen, for example, in Eq. (29) of Ref. [3], where the integration over \( k' \) being limited above by a parameter \( \sigma' \) gives rise to a finite (depending on \( \sigma'/\sigma \)) contribution to the result.

The error made in Ref. [1] is a computational one. It is caused by inaccurate treatment of the frequency dependence in the integral (42) of Ref. [1] (ironically, by an evident typographical error, just the important factors \( (\omega^2 - k_1^2)^{-1} \) and \( (\omega^2 - k_2^2)^{-1} \) are skipped in Eq. (42) of Ref. [1]). In what follows we rederive the result of the present work employing the regularization scheme used by the authors of Ref. [1].

First of all, the result for the long-distance contribution (46) of Ref. [1] ("the third term") is in accord with the result of the present work (1 in [1]).

As for the remaining contributions, let us begin with one general note. In their analysis of the integral (42), the authors of Ref. [1] use the symmetrization in \( \omega \), since, as they wrote, "generally there are three regions of photon energy \( \omega \sim \alpha^2, \omega \sim \alpha, \) and \( \omega \sim 1 \) that give a contribution and this middle region is almost eliminated by the symmetrization". In order not to discuss here whether the middle region is eliminated or not, we would like to recalculate the contributions of the first and the second terms in (43) of Ref. [1] without the symmetrization in \( \omega \). As far as the symmetrization procedure is no more than a technical trick, a result of calculation should not depend on whether this procedure is applied or not.

To get the high energy part of the first and second term contribution, we put \( \epsilon' = \epsilon = 0 \) in (49) and cut off the low energy end \( |\omega| < m\epsilon \) from the contour \( C_- \). Then the result for the short-distance (high energy) contribution to the integral (42) of Ref. [1] can be obtained:

\[
\Delta E = \frac{m^2 \alpha^6}{M^2} \ln \frac{\epsilon}{2}.
\]

The sum of the order \( m^2 \alpha^6/M \) contributions to Eqs. (51), (54) and (57) of Ref. [1] is two times smaller. An extra factor one half emerges there due to the symmetrization in \( \omega \), since the contribution of the contour \( C_+ \), wrapping the half-axis \( (m\epsilon, \infty) \), vanishes.

Turn now to the low energies. Only the second term of Eq. (43), Ref. [1], contributes there. According to (42) and (43) of Ref. [1], this contribution (with typos corrected) is,

\[
\Delta E = \frac{\alpha^2}{MM} \int_{C_L} \frac{d\omega}{2\pi i} \int \frac{d^3k_1}{(2\pi)^3} \int \frac{d^3k_2}{(2\pi)^3} \int \frac{d^3\vec{p}}{(2\pi)^3} \psi(\vec{p} + \vec{k}_1) 4\pi k_1 \frac{1}{k_1^2 - \omega^2} 2m\omega - p^2 \frac{4\pi k_2}{k_2^2 - \omega^2} \psi(\vec{p} + \vec{k}_2).
\]

Here the contour \( C_L \) goes from \(-m\epsilon\) to 0 below and then from 0 to \( m\epsilon \) above the real axis. Recall now that the high energy contribution (63) is calculated on the assumption that \( \epsilon \gg \alpha \). It means that in (64) we can neglect \( p^2 \) which is of the order of \((m\alpha)^2\), in
comparison with $2m\omega$ which will be shown below to be of the order of $m^2\alpha$. Then we can easily come to the coordinate representation and get,

$$\Delta E = \frac{\alpha^2}{2Mm^2} \int_{C_L} \frac{d\omega}{2\pi i} \frac{1}{\omega - 0} \left\langle \left( \nabla e^{i\omega |r|} \right)^2 - \frac{1}{r^4} \right\rangle.$$  \hspace{1cm} (65)

Since the integration contour does not wrap the zero point, we can safely add the operator $-1/r^4$ which is annihilated by the $\omega$ integration. The result of taking the average over the ground state is

$$\Delta E = -\frac{2m^2\alpha^6}{M} \int_{C_L} \frac{d\omega}{2\pi i} \frac{1}{\omega - 0} \left( 2 \ln \left( 1 - \frac{i|\omega|}{m\alpha} \right) + \frac{2i|\omega|}{m\alpha} \frac{1}{1 - \frac{|\omega|}{m\alpha}} + \frac{3}{2} \left( \frac{\omega}{m\alpha} \right)^2 \frac{1}{1 - \frac{|\omega|}{m\alpha}} \right).$$  \hspace{1cm} (66)

Here we see that the natural scale for $\omega$ is in fact $m\alpha$. Since $|\omega|$ is positive on the lower half of $C_L$, the integral above written in dimensionless units reads,

$$\Delta E = -\frac{m^2\alpha^6}{\pi M} \int_0^{\epsilon/\alpha} dx \left( \frac{4}{x} \arctan x - \frac{4}{1 + x^2} - 3 \frac{x^2}{1 + x^2} \right).$$  \hspace{1cm} (67)

The result of integration,

$$\Delta E = \frac{m^2\alpha^6}{M} \left( \frac{3}{\pi\alpha} - 2 \ln \frac{\epsilon}{\alpha} + \frac{1}{2} \right),$$  \hspace{1cm} (68)

being added to all the other seagull contributions, gives for the order $m^2\alpha^6/M$ seagull correction:

$$S_{\epsilon^6} = \frac{m^2\alpha^6}{M} \left( -2 \ln \frac{1}{\alpha} + 2 \ln 2 - \frac{1}{2} \right),$$  \hspace{1cm} (69)

in complete accord with the result $[60]$ of the present work.

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Appendix A

Extra terms in (41) should be canceled by the regulator counterpart of (13) which differs from (13) by $\sqrt{k^2 + \lambda^2}$ placed instead of $k$. Just like in the main text we approximate the sum over positive-energy intermediate states by the nonrelativistic Green’s function and the matrix element of $\vec{\alpha}$ by $\vec{p}/m$. Within this approximation, the regulator contribution is

$$\mathcal{M}_+ = \frac{\alpha}{Mm} \int \frac{d^3k}{(2\pi)^3} \left\langle \vec{p} \mathcal{G} \left( \vec{r}', \vec{r} | E - \sqrt{k^2 + \lambda^2} \right) - \frac{4\pi e^{ik\vec{r}}}{\sqrt{k^2 + \lambda^2}} \vec{p}_k \right\rangle.$$

(70)
After the transformations, the regulator version of the expression (18) is

\[
\mathcal{M}_r' = \frac{2^7 3m^5 \alpha^6}{M \pi} \int_0^\infty \frac{dk}{\kappa^5 \omega} \int_0^1 dx (1 - x^2) \int_C dt \frac{t^{1-m\alpha/\kappa}}{(a - bt)^4} \frac{1}{1 - e^{2\pi i m \kappa}},
\]

(71)

where \( \kappa = \sqrt{2m(\omega - E)}, \omega = \sqrt{k^2 + \lambda^2} \); the contour \( C \) and functions \( a \) and \( b \) are defined in the text. Only singular terms of the expansion (22) operate at distances of the order of \( \lambda^{-1} \). For those terms the integrals over \( k \) and \( x \) become elementary and give

\[
\mathcal{M}_r' = \frac{m^2 \alpha^6}{M} \left\{ -\frac{2}{\varepsilon^2} \left( \ln \frac{\varepsilon}{\alpha} - 1 \right) + \frac{2}{\varepsilon} - \frac{32}{9\pi \sqrt{\varepsilon}} \int_0^\infty \frac{d\theta}{\sqrt{\cosh \theta}} \right\}.
\]

(72)

So, the second and the third terms coincide with the corresponding terms in (41). The new singularity \( \sim \varepsilon^{-2} \) is nothing but the regulator contribution to the instantaneous part of the magnetic exchange (10):

\[
\frac{1}{2M} \langle \{ \vec{p}, \vec{D}^r(0, \vec{r}) \} \rangle \approx 4\pi \alpha \left\{ \frac{p_i' + p_i}{2m} \frac{p_j' + p_j}{2M} \frac{\delta_{ij} - q_i q_j / q^2}{q^2 + \lambda^2} \right\}
\]

(73)

\[
= \frac{2 m^2 \alpha^6}{M \varepsilon^2} \left( \ln \frac{\varepsilon}{\alpha} - 1 \right).
\]

Appendix B

The leading contribution to (49) is

\[
S^r = \frac{8m^3 \alpha^5}{M} \int_{C_-} \frac{d\omega}{2\pi i} \int \frac{d^3 \vec{p}}{(2\pi)^3} \frac{4\pi}{p^2 - \mathcal{K}^2} \frac{\omega}{p^2 - \Omega^2} \frac{4\pi}{\mathcal{K}^2}.
\]

(74)

After the integration with respect to \( \vec{p} \) it turns into

\[
S^r = \frac{m \alpha^5}{M \pi \varepsilon^2 - \varepsilon'^2} \int_{C_-} d\omega \omega \left( \frac{1}{\Omega + \mathcal{K}} - \frac{1}{\Omega + \mathcal{K}'} \right).
\]

(75)

Up to terms of the first order in \( \varepsilon, \varepsilon' \), one gets

\[
S^r = \frac{m^2 \alpha^5}{M \pi} \left( 3 - 2 \frac{\varepsilon^2 \ln(2/\varepsilon) - \varepsilon'^2 \ln(2/\varepsilon')}{\varepsilon^2 - \varepsilon'^2} - 2\pi \frac{\varepsilon'^2 + \varepsilon' \varepsilon + \varepsilon^2}{\varepsilon' + \varepsilon} \right).
\]

(76)

The last term compensates the leading contribution to (46).
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