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RECOIL CORRECTION TO HYDROGEN ENERGY LEVELS: A REVISION

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Recent calculations of the order of $(Z\alpha)^4 \frac{m}{M}$ Ry pure recoil correction to the hydrogen energy levels are critically revised. The origins of errors made in the previous studies are elucidated. In the framework of a systematic approach, a new result is obtained for the 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 the S levels of hydrogen atom, which 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]. A different result for the same correction was subsequently obtained in Ref. [2]. While the same (exact in $Z\alpha$) starting expression for the pure recoil correction was employed in both papers, the methods of calculation and, in particular, the regularization schemes used were rather different. To resolve the discrepancy between the two results, an attempt was undertaken in Ref. [3] to prove the correctness of the earlier result of Ref. [1] by 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 for the difference between the result of Ref. [2] and that of Ref. [1]. This finding has led the authors of Ref. [3] to the conclusion that «discrepancies between the different results for the correction of the order of $(Z\alpha)^6(m/M)$ to the energy levels of the hydrogen-like ions are resolved and the correction of this order is now firmly established».

Assuming that the criticism of Ref. [3] is completely valid, we nevertheless cannot agree with the conclusion cited above. The point is that in emphasizing the importance of an explicit regularization of divergent expressions, the authors of Ref. [3] 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. Different approximations must then be used to handle this expression at different scales. In this way some auxiliary parameter(s), which enable us to separate the applicability domains for different approximations, are introduced. Finally, a necessary condition for the sum of the calculated contributions to be correct is its independence of any scale-separating parameter.

In the present paper we systematically pursue this line of reasoning for a recalculation of the order of $(Z\alpha)^6 m^2/M$ correction to the hydrogen energy levels. We discuss only the S levels since for higher angular-momentum levels the result has actually been firmly established [2, 4]. Since the controversy mentioned above concerns details of a regularization at the subatomic scale, the dependence of the results on the principal quantum number n is also known. We therefore 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. The general outline of the problem is given in Sec. 2. Sections 3, 4 and 5 deal with the Coulomb, magnetic, and seagull contributions, respectively. The correspondence between various results is discussed in Sec. 6. A couple of minor computational issues are addressed in the Appendices.

The Coulomb gauge of the electromagnetic potentials and relativistic units $\hbar = c = 1$ are used throughout the paper. 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 nonlocal operator [5–7, 1, 8],

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

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

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

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

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

and

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

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

Since we are going to calculate the correction (1) perturbatively, i.e., as a power series in α, we can decompose (1) into three parts:

$$\Delta E_{rec} = \mathcal{C} + \mathcal{M} + \mathcal{S}, \tag{5}$$

namely, the Coulomb, magnetic, and seagull contributions, which correspond to the **pp**, **pD** + **Dp**, and **DD** terms from (1), respectively.

3. COULOMB CONTRIBUTION

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

$$\mathcal{C} = \left\langle \frac{p^2}{2M} \right\rangle - \frac{1}{M} \langle \mathbf{p}\Lambda_- \mathbf{p} \rangle , \tag{6}$$

where Λ_- 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 $p \sim m\alpha$. 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. This term is completely saturated by momenta from the relativistic scale $p \sim m$. It can therefore be calculated without any regularization [1, 2]:

$$-\frac{1}{M} \langle \mathbf{p}\Lambda_- \mathbf{p} \rangle_{\alpha^6} = \frac{m^2\alpha^6}{M}. \tag{7}$$

4. MAGNETIC CONTRIBUTION

Using the identity

$$\langle \mathbf{p} G \mathbf{D} + \mathbf{D} G \mathbf{p} \rangle = \frac{1}{\omega} \langle [\mathbf{p}, H] G \mathbf{D} + \mathbf{D} G [H, \mathbf{p}] + \{\mathbf{p}, \mathbf{D}\} \rangle , \tag{8}$$

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

$$\mathcal{M} = \frac{1}{M} \int \frac{d\omega}{2\pi i} \langle \mathbf{p} G \mathbf{D} + \mathbf{D} G \mathbf{p} \rangle , \tag{9}$$

its local part,

$$\frac{1}{M} \int\limits_{C_-} \frac{d\omega}{2\pi i} \frac{1}{\omega} \langle \{\mathbf{p}, \mathbf{D}(\omega, \mathbf{r})\} \rangle = -\frac{1}{2M} \langle \{\mathbf{p}, \mathbf{D}(0, \mathbf{r})\} \rangle . \tag{10}$$

Due to the rapid convergence of the integral in (9) at infinity, we can reduce the integration contour to C_-. By virtue of the virial relations (see Ref. [9] and the references cited there), the sum of the local parts of the Coulomb and magnetic contributions takes a simple form [6]:

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

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 ω in (9) gives [2]:

$$\mathcal{M} = -\frac{\alpha}{M} \int \frac{d^3\mathbf{k}}{(2\pi)^3} \left\langle \mathbf{p} \left(\sum_{+} \frac{|m\rangle\langle m|}{k + E_m - E} - \sum_{-} \frac{|m\rangle\langle m|}{E - E_m + k} \right) \frac{4\pi \boldsymbol{\alpha}_k}{k} e^{i\mathbf{kr}} \right\rangle , \tag{12}$$

where $\sum_{+(-)}$ represents the sum over discrete levels supplied by the integral over the 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

$$\mathcal{M}_+ = \frac{\alpha}{Mm} \int \frac{d^3\mathbf{k}}{(2\pi)^3} \left\langle \mathbf{p}\, \mathcal{G}\left(\mathbf{r}', \mathbf{r}|E-k\right) \frac{4\pi e^{i\mathbf{kr}}}{k} \mathbf{p}_k \right\rangle, \tag{13}$$

where $\mathcal{G}\left(\mathbf{r}', \mathbf{r}|E-k\right)$ is the Green's function for the Schrödinger equation in the Coulomb field, and the average is taken over the nonrelativistic wave function. For the ground state we use

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

Only the p-wave term from the partial expansion

$$\mathcal{G}\left(\mathbf{r}', \mathbf{r}|\omega\right) = \sum_l (-)^l (2l+1) P_l(\mathbf{n}'\mathbf{n}) \mathcal{G}_l(r', r|\omega) \tag{15}$$

survives the integration over the angles:

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

For the nonrelativistic Green's function in the Coulomb field we use the integral representation from Ref. [10],

$$\mathcal{G}_1\left(r', r\left|-\frac{\kappa^2}{2m}\right.\right) = \frac{im}{2\pi\sqrt{r'r}} \int_0^\pi \frac{ds}{\sin s} \frac{\exp\left\{i\left[2(m\alpha/\kappa)s + \kappa(r'+r)/\operatorname{tg} s\right]\right\}}{1-\exp\left\{i2(m\alpha/\kappa)\pi\right\}} J_3\left(\frac{2\kappa\sqrt{r'r}}{\sin s}\right). \tag{17}$$

The integrals over r and r' in (16) can be easily calculated after expanding the Bessel function in a power series. The result can be expressed in the form

$$\mathcal{M}_+ = \frac{2^7 3 m^5 \alpha^6}{M\pi} \int_0^\infty \frac{dk\, k}{\kappa^5} \int_{-1}^{1} dx (1-x^2) \int_C dt \frac{t^{1-m\alpha/\kappa}}{(a-bt)^4} \frac{1}{1-\exp\left\{i2\pi m\alpha/\kappa\right\}}, \tag{18}$$

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

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

Integration by parts conveniently extracts from the last integral in (18) the terms which are non-vanishing at large momenta:

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

where

$$F(x,y)=\frac{2}{b(a-b)^3}-\frac{1-y}{b^2(a-b)^2}-\frac{y(1-y)}{ab^2(a-b)}+\frac{1-y^2}{a^2b^2}-\frac{y(1-y^2)}{a^3b}\int\limits_0^1\frac{dt\,t^{-y}}{1-(b/a)t}. \quad (20)$$

Here we introduced a new integration variable $y\equiv m\alpha/\kappa$. Since

$$\frac{k}{\kappa}=\frac{\alpha}{2}\frac{1-y^2}{y}, \quad (21)$$

a power series expansion of (19) with respect to α up to the first order can be achieved by expanding the integrand with respect to y up to the first order (note that $a-b=4y-2ikx/\kappa$):

$$(1-y^2)F(x,y)\approx\frac{2}{(a-b)^3}-\frac{1}{2(a-b)}+\frac{1}{2}-\frac{y^2}{2(a-b)}-\frac{y}{2}+y\ln(a-b). \quad (22)$$

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

$$\int\limits_0^1\frac{dt\,t^{-y}}{1-(b/a)t}=\frac{1}{1-y}F\left(1,1-y;2-y;\frac{b}{a}\right), \quad (23)$$

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

$$\int\limits_0^{y_0}dy(1-y^2)\int\limits_{-1}^{1}dx(1-x^2)F(x,y)\approx\frac{\pi}{32\alpha}-\frac{1}{48y_0^2}-\frac{1}{12}\ln\frac{4y_0^2}{\alpha}+\frac{1}{48}-$$
$$-\frac{1}{9}+\frac{2y_0}{3}+\frac{2y_0^2}{3}\ln 4y_0-\frac{3y_0^2}{4}-\frac{\pi\alpha}{32}. \quad (24)$$

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

$$\mathcal{M}_+=\frac{m^2\alpha^5}{M\pi}\left\{-\frac{\pi}{\alpha}+\frac{8}{3}\ln\frac{1}{\alpha}+\frac{8}{3}\ln\frac{\mathrm{Ry}}{\langle E\rangle_{1S}}+\frac{16}{3}\ln 2+\frac{32}{9}-\pi\alpha\right\}. \quad (25)$$

Here we introduce the Bethe logarithm [11]

$$16\int\limits_0^1 dy\,y\frac{F\left(1,1-y;2-y;((1-y)/(1+y))^2\right)-1}{(1+y)^4(1-y)}=\ln\frac{\mathrm{Ry}}{\langle E\rangle_{1S}}+2\ln 2+\frac{11}{6}. \quad (26)$$

In (25), the order α^4 term is the lowest-order contribution to (10), the order α^5 terms are in accord with the result of Salpeter [12], and the order α^6 term coincides with the retardation correction, found in Ref. [2], Eq. (14), by a different method.

It can be easily seen that the order α^6 contribution to the positive-energy part of (12) is exhausted by the sum of the contributions to (10) and (25). Actually, relativistic corrections are at least of the α^2 relative order. The retardation reveals itself beginning with the α^5 order (25). Hence the relativistic corrections for the retardation are at least of the order of α^7.

4.1.2. Negative Energies

Virtual transitions to the negative-energy states give rise to the second term in (12). In the leading nonrelativistic approximation, it is [2]

$$\mathcal{M}_- = \frac{\alpha^2}{4m^2M}\int \frac{d^3\mathbf{k}}{(2\pi)^3}\left\langle \frac{4\pi}{k'^2}\frac{4\pi\mathbf{k}^2_{k'}}{k^2}\right\rangle, \tag{27}$$

where $\mathbf{k}_{k'} = \mathbf{k} - \mathbf{k}'(\mathbf{k}\mathbf{k}')/k'^2$, and $\mathbf{k}' = \mathbf{p}' - \mathbf{p} - \mathbf{k}$; here $\mathbf{p}$ and $\mathbf{p}'$ are the arguments of the wave function and its conjugate, respectively. The integral over k diverges logarithmically (the leading linear divergence 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 divergence 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 find that term below by using a relativistic approach.

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

$$\mathcal{M}_- - \mathcal{M}^r_- = -\frac{\alpha^2}{4m^2M}\left\langle (p'_i - p_i)\int \frac{d^3\mathbf{k}}{(2\pi)^3}\frac{4\pi k_j}{k^2}\left(\delta_{ij} - \frac{k'_ik'_j}{k'^2}\right)\left(\frac{4\pi}{k'^2} - \frac{4\pi}{k'^2+\lambda^2}\right)\right\rangle. \tag{28}$$

In the coordinate representation, the integral above is

$$\frac{in_j}{r^2}\left(\delta_{ij} - \frac{\partial_i\partial_j}{\lambda^2}\right)\frac{1-e^{-\lambda r}}{r} = \frac{in_i}{r^2}\int\limits_0^{-\lambda} d\sigma\left(1 - \frac{\sigma^2}{\lambda^2}\right)e^{\sigma r}. \tag{29}$$

After substitution into (28) it gives

$$\mathcal{M}_- - \mathcal{M}^r_- = -\frac{\alpha^2}{4m^2M}\left\langle 4\pi\delta(\mathbf{r})\int\limits_0^{-\lambda} d\sigma\left(1 - \frac{\sigma^2}{\lambda^2}\right) + \frac{1}{r^2}\int\limits_0^{-\lambda} d\sigma\sigma\left(1 - \frac{\sigma^2}{\lambda^2}\right)e^{\sigma r}\right\rangle. \tag{30}$$

Finally, the result of a trivial calculation of the average over the ground state is

$$\mathcal{M}_- - \mathcal{M}^r_- = \frac{m^2\alpha^6}{M}\left(2\ln\frac{\varepsilon}{\alpha} - 1\right), \tag{31}$$

where $\varepsilon \equiv \lambda/2m$.

4.2. Short Distances

Since in the nonrelativistic approximation the subtracted term, $\mathcal{M}^r_-$, is ultraviolet divergent, we must calculate it beyond this approximation, i.e., using a relativistic approach. It is more convenient in this approach to postpone the integration over ω 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 price for the technical advantage is that a regulator contribution is calculated not only for the negative-energy part, but also for the positive-energy part of M. Surely, the instantaneous contribution can be put aside, so that only two first terms from the right-hand side of (8) are considered below.

For the subtracted term, we have the new expansion parameter, $m\alpha/\lambda$, and hence the Coulomb interaction during a 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:

$$\mathcal{M}_G^r = \frac{2}{M}\int\limits_{C_-} \frac{d\omega}{2\pi i}\,\frac{1}{\omega}\left\langle [\mathbf{p}, H] G^{(1)} \mathbf{D}^r \right\rangle. \qquad (32)$$

Here

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

and we can disregard the atomic momenta in comparison with λ and m:

$$\mathcal{M}_G^r = -\frac{\alpha^3\psi^2}{\pi M}\int\limits_{C_-} \frac{d\omega}{i\omega}\left\langle \frac{4\pi\mathbf{p}'}{p'^2}\,\frac{2m+\omega+\boldsymbol{\alpha}\mathbf{p}'}{p'^2-\Omega^2}\,\frac{4\pi}{q^2}\,\frac{\omega+\boldsymbol{\alpha}\mathbf{p}}{p^2-\Omega^2}\,\frac{4\pi\boldsymbol{\alpha}_p}{p^2-\mathcal{K}^2}\right\rangle. \qquad (33)$$

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

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

The average over the spin degrees of freedom gives

$$\langle (2m+\omega+\boldsymbol{\alpha}\mathbf{p}')(\omega+\boldsymbol{\alpha}\mathbf{p})\boldsymbol{\alpha}_p\mathbf{p}'\rangle = \omega\mathbf{p}'^2_p = \omega\mathbf{p}'_p\mathbf{q}. \qquad (34)$$

Then, after transition to the coordinate representation we obtain

$$\mathcal{M}_G^r = \frac{2\alpha^3\psi^2}{mM}\int\limits_{C_-}\frac{d\omega}{i\omega}\int\limits_0^\infty dr\left(\partial_i \frac{e^{i\Omega r}-1}{\Omega^2 r}\right) n_j \left[\left(\delta_{ij}+\frac{\partial_i\partial_j}{\Omega^2}\right)\frac{e^{i\Omega r}-1}{r} - (\Omega\to\mathcal{K})\right]. \qquad (35)$$

The integration over r is simple but lengthy. The result is

$$\mathcal{M}_G^r = -\frac{\alpha^3\psi^2}{2mM}\int\limits_{C_-}\frac{d\omega}{i\omega}\left\{\frac{\mathcal{K}}{\Omega} - \frac{\mathcal{K}^2}{\Omega^2}\ln\left(1+\frac{\Omega}{\mathcal{K}}\right) + (\Omega\leftrightarrow\mathcal{K}) + 2\ln\left(1+\frac{\mathcal{K}}{\Omega}\right)\right\}. \qquad (36)$$

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

$$\mathcal{M}_G^r = \frac{\alpha^3\psi^2}{mM}\int\limits_0^1 dx\left(\frac{\sqrt{1-x}}{x^{3/2}} - \frac{1}{x^2}\,\mathrm{arctg}\sqrt{\frac{x}{1-x}} - \frac{1}{\sqrt{x(1-x)}}\right) = -\frac{3}{2}\,\frac{\pi\alpha^3\psi^2}{mM}. \qquad (37)$$

To calculate the contribution due to $G^{(0)}$ we must account properly for the wave-function's short-distance behavior:

$$\mathcal{M}^{r}_{\psi} = -\frac{\alpha^3\psi^2}{\pi M}\int\limits_{C_-}\frac{d\omega}{i\omega}\left\langle\left(\frac{4\pi\mathbf{p}'}{p'^2}\,\frac{2m+\omega+\boldsymbol{\alpha}\mathbf{p}'}{p'^2-\Omega^2}\,\frac{4\pi\boldsymbol{\alpha}_q}{q^2-\mathcal{K}^2}\right.\right. + $$
$$\left.\left. + \frac{4\pi\boldsymbol{\alpha}_{p'}}{p'^2-\mathcal{K}^2}\,\frac{\omega+\boldsymbol{\alpha}\mathbf{p}'}{p'^2-\Omega^2}\,\frac{4\pi\mathbf{q}}{q^2}\right)\frac{2m+\boldsymbol{\alpha}\mathbf{p}}{p^2}\,\frac{4\pi}{p^2}\right\rangle. \tag{38}$$

Averaging over the spin part of the wave function, we obtain

$$\mathcal{M}^{r}_{\psi} = -\frac{\alpha^3\psi^2}{\pi M}\int\frac{d\omega}{i}\left\langle\left(\frac{4m}{\omega}+1\right)\frac{4\pi}{p'^2(p'^2-\Omega^2)}\,\frac{4\pi}{q^2-\mathcal{K}^2}\,\frac{4\pi\mathbf{p}_q^2}{p^4}\right. - $$
$$\left. - \frac{4\pi}{(p'^2-\mathcal{K}^2)(p'^2-\Omega^2)}\,\frac{4\pi}{q^2}\,\frac{4\pi\mathbf{p}_{p'}^2}{p^4}\right\rangle. \tag{39}$$

Again, the six-dimensional integral over $\mathbf{p}$ and $\mathbf{p}'$ turns into a simple integral over r in the coordinate representation. This integral is

$$\mathcal{M}^{r}_{\psi} = \frac{2\alpha^3\psi^2}{M}\int\frac{d\omega}{i}\left\{\left(\frac{4m}{\omega}+1\right)\left[\frac{1}{\Omega^2}\ln\left(1+\frac{\Omega}{\mathcal{K}}\right)+\frac{1}{\mathcal{K}^2}\ln\left(1+\frac{\mathcal{K}}{\Omega}\right)-\frac{1}{\Omega\mathcal{K}}\right]\right. + $$
$$\left. + \frac{1}{2m\omega}\ln\frac{\mathcal{K}}{\Omega}\right\}. \tag{40}$$

Finally, the integration along the same contour as above gives for the nonvanishing in the limit $\varepsilon\to 0$ terms

$$\mathcal{M}^{r}_{\psi} = \frac{m^2\alpha^6}{M}\left(\frac{2}{\varepsilon}-\frac{32}{9\pi\sqrt{\varepsilon}}\int\limits_0^\infty\frac{d\theta}{\sqrt{\operatorname{ch}\theta}}+2\ln\frac{1}{\varepsilon}\right). \tag{41}$$

We see that, as expected, the logarithmic in ε term cancels the corresponding term in (31). The more singular in ε terms can only be the result of the regularization procedure applied to the positive-energy contribution (25). Since the latter is nonsingular 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

In the sum of all contributions due to a single magnetic exchange any dependence on the scale separating parameter ε cancels out, and we obtain

$$\mathcal{M}_{\alpha^6} + \left\langle\frac{p^2}{2M}\right\rangle_{\alpha^6} = \frac{m^2\alpha^6}{M}\left(-1+2\ln\frac{1}{\alpha}-1-\frac{3}{2}\right). \tag{42}$$

Here -1 on the right-hand side is due to the (long-range) effect of retardation (see Eq. (25) and Ref. [2], Eq. (14)), $2\ln(1/\alpha)-1$ comes from the whole range of scales from $m\alpha$ to m, and $-3/2$ is the short-range contribution.

5. SEAGULL CONTRIBUTION

5.1. Long Distances

The best way to analyze the atomic scale contribution is to begin by taking the integral with respect to ω. It appears that in the order of interest only the positive-energy intermediate states should be considered [2]:

$$\mathcal{S}_+ = \frac{\alpha^2}{2M}\int\frac{d^3\mathbf{k}}{(2\pi)^3}\left\langle\frac{4\pi}{k'^2}\frac{2\mathbf{p'}_{k'} + i[\boldsymbol{\sigma}\mathbf{k}']}{2m}\frac{4\pi}{k^2}\frac{2\mathbf{p}_k + i[\boldsymbol{\sigma}\mathbf{k}]}{2m}\right\rangle. \tag{43}$$

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

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

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

$$\mathcal{S}_+ - \mathcal{S}_+^r = \frac{\alpha^2}{4m^2M}\left\langle 2\mathbf{p}\frac{1}{r^2}\mathbf{p} + \frac{1}{r^4} - \left(\nabla\frac{e^{-\lambda' r}}{r}\right)\left(\nabla\frac{e^{-\lambda r}}{r}\right)\right\rangle. \tag{45}$$

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

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

Here 1 appears due to the nonsingular operator $\mathbf{p}r^{-2}\mathbf{p}$. 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-range contribution to the $m\alpha^5/M$ order is shown explicitly. In what follows we calculate the subtracted term, whose nonrelativistic version (44) is ultraviolet divergent, in the framework of a relativistic approach.

5.2. Short Distances

Like in the 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

$$\mathcal{S}_G^r = \frac{\alpha^3\psi^2}{2\pi M}\int\limits_{C_-}\frac{d\omega}{i}\left\langle\frac{4\pi\boldsymbol{\alpha}_{p'}}{p'^2-\mathcal{K}'^2}\,\frac{\omega+\boldsymbol{\alpha}\mathbf{p}'}{p'^2-\Omega^2}\,\frac{4\pi}{q^2}\,\frac{\omega+\boldsymbol{\alpha}\mathbf{p}}{p^2-\Omega^2}\,\frac{4\pi\boldsymbol{\alpha}_p}{p^2-\mathcal{K}^2}\right\rangle. \tag{47}$$

Calculation along the same lines as in the case of $\mathcal{M}_G^r$ gives the result

$$\mathcal{S}_G^r = \frac{\pi\alpha^3\psi^2}{Mm}\left(4\ln 2 - 2\right), \tag{48}$$

which is nonsingular in the limit $\lambda, \lambda' \to 0$.

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

$$\frac{\alpha^3\psi^2}{2\pi M}\int\limits_{C_-}\frac{d\omega}{i}\left\langle\frac{4\pi\boldsymbol{\alpha}_{p'}}{p'^2-\mathcal{K}'^2}\,\frac{\omega+\boldsymbol{\alpha}\mathbf{p}'}{p'^2-\Omega^2}\,\frac{4\pi\boldsymbol{\alpha}_q}{q^2-\mathcal{K}^2}\,\frac{2m+\boldsymbol{\alpha}\mathbf{p}}{(p^2+\gamma^2)^2}\,4\pi\right\rangle+(\lambda\leftrightarrow\lambda') \tag{49}$$

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 the $m^2\alpha^5/M$ order at short distances discussed in Appendix B). The average over the spin part of the wave function is

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

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) contributes to the $m^2\alpha^5/M$ order only. The first term then gives the nonsingular contribution in the limit $\lambda,\lambda'\to 0$:

$$-\,\omega^2\left(1+\frac{(\mathbf{p}'\mathbf{q})^2}{p'^2q^2}\right)\;\to\;\frac{\pi\alpha^3\psi^2}{Mm}(1-4\ln 2)\,. \tag{51}$$

Finally, analysis of the last term in (50) deserves more attention since here we have the infrared singularity. Integrated over the space variables, this term gives

$$2\mathbf{p}'\mathbf{q}\to\frac{2\alpha^3\psi^2}{Mm}\int\limits_{C_-}\frac{d\omega}{i\omega}\left\{f(\Omega,\mathcal{K})-f(\mathcal{K}',\mathcal{K})\right\}, \tag{52}$$

where

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

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

$$\frac{2\alpha^3\psi^2}{Mm}\int\limits_{C_-}\frac{d\omega}{i\omega}f(\Omega,\mathcal{K})=\frac{\pi\alpha^3\psi^2}{Mm}\left(-2\ln\frac{1}{\varepsilon}+4\ln 2-1\right). \tag{54}$$

Calculation of the integral with $f(\mathcal{K}',\mathcal{K})$ is slightly 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 equation

$$\int\limits_{C_-}d\omega\ldots=\int\limits_{C_+}d\omega\ldots-2\pi i\operatorname*{Res}_{\omega=0}\ldots-2\pi i\operatorname*{Res}_{\omega=\infty}\ldots, \tag{55}$$

where $\ldots$ represents $f(\mathcal{K}',\mathcal{K})/\omega$, and the contour C_+ goes in the clockwise direction around the cut that connects the points λ and λ'. Using the evident relations,

$$\int\limits_{C_+}d\omega\ldots=-\int\limits_{C_-}d\omega\ldots, \tag{56}$$

$$\operatorname*{Res}_{\omega=0}\frac{1}{\omega}f(\mathcal{K}',\mathcal{K})=f(\lambda',\lambda)\,, \tag{57}$$

$$\operatorname*{Res}_{\omega=\infty}\frac{1}{\omega}f(\mathcal{K}',\mathcal{K})=-\ln 2+\frac{1}{4}\,, \tag{58}$$

we obtain

$$\frac{2\alpha^3\psi^2}{Mm}\int\limits_{C_-}\frac{d\omega}{i\omega}f(\mathcal{K}',\mathcal{K})=\frac{\pi\alpha^3\psi^2}{Mm}\left(2\ln\frac{2\varepsilon}{\varepsilon+\varepsilon'}+\frac{2\varepsilon\varepsilon'}{(\varepsilon+\varepsilon')^2}-\frac{1}{2}\right). \tag{59}$$

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 λ and λ'. The contribution is

$$\mathcal{S}_{\alpha^6}=\frac{m^2\alpha^6}{M}\left(1-2\ln\frac{2}{\alpha}+\frac{1}{2}+4\ln 2-2\right), \tag{60}$$

where 1 is the long-range contribution, $4\ln 2-2$ is the short-range contribution, and the remaining terms obtain their values on the whole range of scales from $m\alpha$ to m.

6. CONCLUSIONS

In complete agreement 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 nontrivially on the 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 term, 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 the $2S$ state by -1.9 kHz. These figures are comparable [14] or even exceed the uncertainties of the recent Lamb shift measurements [15].

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

Unfortunately, the same error was repeated in Ref. [3]. The long-range contribution was found there in the framework of some particular regularization scheme. It was then added to the short-range contribution calculated in Refs. [1, 2] by completely different regularization procedures. The regularization dependence of the results obtained in Ref. [3] can be seen, for example, in Eq. (29) of Ref. [3], where the integration over k', which is limited above by the parameter σ', gives rise to a finite (depending on σ'/σ) contribution to the result. This contribution was erroneously omitted from Eq. (29) of Ref. [3].

The error made in Ref. [1] is a computational error, which is caused by inaccurate treatment of the frequency dependence in the integral (42) of Ref. [1] (ironically, because of a typographical error, only 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 our result employing the regularization scheme used in Ref. [1].

First of all, the result for the long-range contribution (46) of Ref. [1] («the third term») is consistent with the result of our work (1 in Eq. (46)).

As for the remaining contributions, let us begin with one general comment. In their analysis of the integral (42), the authors of Ref. [1] use the symmetrization in ω, 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 the middle region is almost eliminated by the symmetrization». In order to avoid the discussion whether the middle region is eliminated or not, we will recalculate the contributions of the first and the second terms in Eq. (43) of Ref. [1] without the symmetrization in ω. Since the symmetrization procedure is no more than a technical trick, the result of a calculation should not depend on whether this procedure is applied or not.

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

$$\Delta E = \frac{m^2\alpha^6}{M} 2\ln\frac{\epsilon}{2}. \tag{63}$$

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

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

$$\Delta E = \frac{\alpha^2}{Mm} \int\limits_{C_L} \frac{d\omega}{2\pi i} \int \frac{d^3\mathbf{k}_1}{(2\pi)^3} \int \frac{d^3\mathbf{k}_2}{(2\pi)^3} \int \frac{d^3\mathbf{p}}{(2\pi)^3} \times \tag{64}$$
$$\times\, \psi(\mathbf{p}+\mathbf{k}_1) \frac{4\pi\mathbf{k}_1}{k_1^2 - \omega^2} \, \frac{1}{2m\omega - p^2} \, \frac{4\pi\mathbf{k}_2}{k_2^2 - \omega^2} \psi(\mathbf{p}+\mathbf{k}_2).$$

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

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

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

$$\Delta E = -\frac{2m^2\alpha^6}{M}\int\limits_{C_L}\frac{d\omega}{2\pi i}\,\frac{1}{\omega-0}\times$$
$$\times\left(2\ln\left(1-\frac{i|\omega|}{m\alpha}\right)+\frac{2i|\omega|}{m\alpha}\,\frac{1}{1-i|\omega|/m\alpha}+\frac{3}{2}\left(\frac{\omega}{m\alpha}\right)^2\frac{1}{1-i|\omega|/m\alpha}\right). \tag{66}$$

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

$$\Delta E = -\frac{m^2\alpha^6}{\pi M}\int\limits_0^{\epsilon/\alpha}dx\left(\frac{4}{x}\operatorname{arctg}x-\frac{4}{1+x^2}-3\frac{x^2}{1+x^2}\right). \tag{67}$$

The result of integration,

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

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

$$\mathcal{S}_{\alpha^6} = \frac{m^2\alpha^6}{M}\left(-2\ln\frac{1}{\alpha}+2\ln 2-\frac{1}{2}\right), \tag{69}$$

in complete agreement with our result (60).

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APPENDIX A

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

$$\mathcal{M}_+^r = \frac{\alpha}{Mm}\int\frac{d^3\mathbf{k}}{(2\pi)^3}\left\langle \mathbf{p}\,\mathcal{G}\left(\mathbf{r}',\mathbf{r}|E-\sqrt{k^2+\lambda^2}\right)\frac{4\pi e^{i\mathbf{kr}}}{\sqrt{k^2+\lambda^2}}\mathbf{p}_k\right\rangle. \tag{A.1}$$

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

$$\mathcal{M}_+^r = \frac{2^7 3m^5\alpha^6}{M\pi}\int\limits_0^\infty\frac{dk\,k^2}{\kappa^5\omega}\int\limits_{-1}^{1}dx(1-x^2)\int\limits_C dt\frac{t^{1-m\alpha/\kappa}}{(a-bt)^4}\frac{1}{1-\exp(2\pi i m\alpha/\kappa)}, \tag{A.2}$$

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

$$\mathcal{M}_+^r = \frac{m^2\alpha^6}{M}\left\{-\frac{2}{\varepsilon^2}\left(\ln\frac{\varepsilon}{\alpha}-1\right)+\frac{2}{\varepsilon}-\frac{32}{9\pi\sqrt{\varepsilon}}\int\limits_0^\infty \frac{d\theta}{\sqrt{\operatorname{ch}\theta}}\right\}. \tag{A.3}$$

The second and the third term therefore coincide with the corresponding terms in (41). The new singularity $\propto \varepsilon^{-2}$ is the regulator contribution to the instantaneous part of the magnetic exchange (10):

$$-\frac{1}{2M}\langle\{\mathbf{p},\mathbf{D}^r(0,\mathbf{r})\}\rangle \approx -4\pi\alpha\left\langle\frac{p_i'+p_i}{2m}\,\frac{p_j'+p_j}{2M}\,\frac{\delta_{ij}-q_iq_j/q^2}{q^2+\lambda^2}\right\rangle =$$
$$= -2\frac{m^2\alpha^6}{M\varepsilon^2}\left(\ln\frac{\varepsilon}{\alpha}-1\right). \tag{A.4}$$

APPENDIX B

The leading contribution to (49) is

$$\mathcal{S}^r = \frac{8m^3\alpha^5}{M}\int\limits_{C_-}\frac{d\omega}{2\pi i}\int\frac{d^3\mathbf{p}}{(2\pi)^3}\,\frac{4\pi}{p^2-\mathcal{K}'^2}\,\frac{\omega}{p^2-\Omega^2}\,\frac{4\pi}{p^2-\mathcal{K}^2}. \tag{B.1}$$

After the integration with respect to $\mathbf{p}$ it becomes

$$\mathcal{S}^r = \frac{m\alpha^5}{M\pi}\,\frac{1}{\varepsilon^2-\varepsilon'^2}\int\limits_{C_-} d\omega\,\omega\left(\frac{1}{\Omega+\mathcal{K}'}-\frac{1}{\Omega+\mathcal{K}}\right). \tag{B.2}$$

Up to terms of the first order in ε, ε' we obtain

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

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

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