Recoil Corrections of Order \((Z\alpha)^6(m/M)m\) to the Hydrogen Energy Levels Revisited

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Abstract

The recoil correction of order \((Z\alpha)^6(m/M)m\) to the hydrogen energy levels is recalculated and a discrepancy existing in the literature on this correction for the 1S energy level, is resolved. An analytic expression for the correction to the S-levels with arbitrary principal quantum number is obtained.

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I. INTRODUCTION

The calculation of the recoil corrections of order \((Z\alpha)^6(m/M)m\) to the hydrogen energy levels has a long history Refs. [1–6]. After initial disagreements consensus was achieved in Ref. [7], where one and the same result was obtained in two apparently different frameworks. The first, more traditional approach, used earlier in Refs. [2–4], starts with an effective Dirac equation in the external field. Corrections to the Dirac energy levels are calculated with the help of a systematic diagrammatic procedure. The other logically independent calculational framework, also used in Ref. [7], starts with an exact expression for all recoil corrections of the first order in the mass ratio of the light and heavy particles \(m/M\). This remarkable expression, which is exact in \(Z\alpha\), was first discovered by M. A. Braun [8], and rederived later in different ways in a number of papers Refs. [9,10,7].

The agreement on the \((Z\alpha)^6(m/M)m\) contribution achieved in [7] seemed to put an end to all problems connected with this correction. However, it was claimed in a recent work [11], that the result of [7] is in error. The discrepancy between the results of Refs. [7,11] is confusing since the calculation in [11] is performed in the same framework as the one employed in [7], namely it is based on a particularly nice form of the Braun formula obtained by the author earlier [10],

\[
\Delta E_{\text{rec}} = -\frac{1}{M} Re \int \frac{d\omega}{2\pi i} <n|\mathbf{p} - \hat{D}(\omega))G(E + \omega)(\mathbf{p} - \hat{D}(\omega))|n>,
\]

where summation over all intermediate states is understood, \(G(E + \omega)\) is the Coulomb-Green function in the Coulomb gauge, which in the momentum space has the form

\[
\hat{D}(\omega, k) = -4\pi Z\alpha(\alpha - \frac{k(\alpha k)}{k^2}) \frac{1}{\omega^2 - k^2 + i0} \equiv -4\pi Z\alpha \frac{\alpha_k}{\omega^2 - k^2 + i0},
\]

and

\[
\alpha_i = \gamma^0\gamma^i.
\]

Note that \(\hat{D}(\omega, k)\) is nothing more than the transverse photon propagator with the source at the proton position, and integration over the exchanged photon momentum \(k\) is implicit in the expression above. Below we will explicitly perform multiplication in the matrix element in Eq.(1). Respective contributions to the energy levels will be called Coulomb (corresponds to \(pp\)), magnetic (corresponds to \(p\hat{D}\) and \(\hat{D}p\)), and seagull (corresponds to \(\hat{D}\hat{D}\)).

It is the aim of this paper to resolve the above noted discrepancy on the recoil correction of order \((Z\alpha)^6(m/M)m\) to the \(1S\) energy level, and also to obtain this correction for the \(S\)-levels with arbitrary principal quantum number (it was earlier calculated only for \(n = 1, 2\) [7]).

II. TWO APPROACHES TO THE BRAUN FORMULA

Calculation of the recoil contribution of order \((Z\alpha)^6\) generated by the Braun formula was performed in [7] in a most straightforward way since separation of the high- and low-frequency contributions was made in the framework of the \(\epsilon\)-method developed by one of the
authors earlier [12]. Hence, not only were contributions of order \((Z\alpha)^6(m/M)m\) obtained in Ref. [7], but also linear in \(m/M\) parts of recoil corrections of orders \((Z\alpha)^4\) and \((Z\alpha)^5\) (ref. [13]) were reproduced for the 1S-state. Note that the Braun formula, despite its obvious advantages, in its present form sums only contributions linear in the mass ratio. Hence, old methods are more adequate for obtaining the proper mass dependence of the contributions of orders \((Z\alpha)^4\) and \((Z\alpha)^5\), which were worked out in Ref. [1]. Calculations in Ref. [7] turned out to be rather lengthy and tedious just because all corrections of previous orders in \(Z\alpha\) were reproduced.

The most significant feature of the recoil corrections of order \((Z\alpha)^6\), which made the whole approach of Ref. [11] possible, is connected with the absence of logarithmic recoil corrections of this order, as was proved in [6]. Unlike [7], the calculations in [11] are organized in such a way that one explicitly makes approximations inadequate for calculation of the contributions of the previous orders in \(Z\alpha\), significantly simplifying calculation of the correction of order \((Z\alpha)^6\). Due to absence of the logarithmic contributions of order \((Z\alpha)^6\), infrared divergences connected with the crude approximations inadequate for calculation of the contributions of the previous orders would be powerlike and can be safely thrown away. Next, absence of logarithmic corrections of order \((Z\alpha)^6\) means that it is not necessary to worry too much about matching the low- and high-frequency (long- and short-distance in terms of Ref. [11]) contributions, since each region will produce only nonlogarithmic contributions and correction terms would be suppressed as powers of the separation parameter. We would like to emphasize once more that this approach would be doomed if the logarithmic divergences were present, since in such a case one could not hope to calculate an additive constant to the log, since the exact value of the integration cutoff would not be known.

We are going to perform below calculation of the recoil contribution of order \((Z\alpha)^6\) in the framework of Ref. [11], and to discover the source of discrepancy between the results of Ref. [7] and Ref. [11]. In order to really implement such program we need to have a regular method to qualify all terms which will be thrown away. To this end we will use a slight generalization of the ordinary approach to calculation of the leading order contribution to the Lamb shift.

It may be proved that all corrections of order \((Z\alpha)^6(m/M)m\) are generated by the exchange of photons with momenta larger than \(m(Z\alpha)^2\), so we will consider below only this integration region. In the spirit of the common approach to the Lamb shift calculations we will split the integration region over the exchanged photon momenta (and when necessary over frequencies) with the help of an auxiliary parameter \(\sigma\) which satisfies the conditions

\[
mZ\alpha \ll \sigma \ll m, \tag{4}
\]

and we will call the photons with momenta smaller than \(\sigma\) low-frequency (or long-distance) photons, and the photons with momenta larger than \(\sigma\) will be called high-frequency (or short-distance) photons. Considering low-frequency photons we may expand over the ratio \(k/m\) since for such photons \(k/m \leq \sigma/m \ll 1\). On the other hand, for the high-

\[1\]Note that the apparent linear divergences in this region of the form \(\sigma/m\) are really parametrically small.
frequency photons $mZ\alpha/k \leq mZ\alpha/\sigma \ll 1$, and we may expand over this parameter. Note that for momenta of order $\sigma$ both expansions are valid simultaneously, and, hence, we may match the expansions and get rid of the auxiliary parameter $\sigma$. However, the problem under consideration is in a sense even simpler than calculation of the leading order contribution to the Lamb shift, and due to absence of the logarithmic contributions of order $(Z\alpha)^6(m/M)m$, precise matching of the high- and low-frequency contributions is unnecessary. Below we will consider calculation only of the low-frequency $(mZ\alpha < k < \sigma)$ contribution to the energy shift, since for the high frequency contribution the results of Ref. [7] and Ref. [11] nicely coincide.

III. MAIN RECOIL CONTRIBUTION

With the help of the Braun formula one may easily obtain an expression for the leading recoil correction which is linear in the mass ratio and which includes all terms of order $(Z\alpha)^4$ and lower (see Ref. [9]). To this end we rewrite the Coulomb contribution in Eq.(1) in the form

$$\Delta E_{Coul} = \frac{1}{2M} < n|p^2|n > - \frac{1}{M} < n|p\Lambda^{-}p||n >$$

$$\equiv \Delta E_{c1} + \Delta E_{c2}. \tag{5}$$

We also extract the nonretarded Breit part from the magnetic contribution in Eq.(1)

$$\Delta E_{magn} = \Delta E_{Br} + \Delta E_{magn,r}, \tag{6}$$

where

$$\Delta E_{Br} = -\frac{1}{2M} < n|p\hat{D}(0, k) + \hat{D}(0, k)p|n >, \tag{7}$$

and

$$\Delta E_{magn,r} = -\frac{1}{M} \int \frac{d\omega}{2\pi i} < n|[V, p]G(E + \omega)\hat{D}(\omega, k)$$

$$-\hat{D}(\omega, k)G(E + \omega)[V, p]|n > \frac{1}{\omega + i0}, \tag{8}$$

where $V$ is the Coulomb potential ($V = -Z\alpha/r$).

Now it is not difficult to check with the help of the virial relations (see, e.g., Ref. [14]), that the sum of the main part of the Coulomb term and of the Breit contribution acquires a very nice form

$$\Delta E_{c1} + \Delta E_{Br} = \frac{m^2 - E^2}{2M}, \tag{9}$$

where $E$ is the value of the energy given by the Dirac equation. As we will see below, all other recoil contributions to the energy level start at least with the term of order $(Z\alpha)^5$,
and, hence, the formula above correctly describes all contributions of order \((Z\alpha)^4\) and lower. However, this formula describes only contributions linear in the mass ratio. A more precise expression which takes into account corrections of higher order in \(m/M\), was obtained in Ref. [1].

It is easy to see that the expression in Eq.(9) also contains the correction of order \((Z\alpha)^6\), which for the \(nS\)-states has the form

\[
\Delta E_{GV} = \left(\frac{1}{8} + \frac{3}{8n} - \frac{1}{n^2} + \frac{1}{2n^3}\right) \frac{(Z\alpha)^6 m}{M} m. \tag{10}
\]

This contribution was originally obtained in Ref. [1].
The remaining part of the Coulomb contribution has the form

\[
\Delta E_{c2} = -\frac{1}{M} < n|p\Lambda_- p|n >. \tag{11}
\]

Let us check that this term leads to corrections of higher order than \((Z\alpha)^6\) when the intermediate momenta are of the atomic scale. We want to exploit the large (of order \(2m\)) value of the energy gap between positive and negative states in comparison with the typical energy splittings (of order \(m(Z\alpha)^2\)) in the positive energy spectrum. First, let us note that

\[
<n|p|V|\Lambda_-|p, V|n> = <n|p, H - E|\Lambda_-|p, H - E|n> \tag{12}
\]

\[
= -<n|p \sum m|m>(E_n - E_m)^2 p|n>.
\]

However, \((E_n - E_m)^2 > 4m^2(1 - c\alpha^2)\), and, hence,

\[
|<n|p, V|\Lambda_-|p, V|n> | = |<n|p \sum m|m>(E_n - E_m)^2 p|n> | \tag{13}
\]

\[
\geq |<n|p\Lambda_- p|n> |4m^2(1 - c\alpha^2).
\]

Then

\[
|<n|p\Lambda_- p|n> | \leq \frac{1}{4m^2(1 - c\alpha^2)} |<n|p, V|\Lambda_-|p, V|n> |. \tag{14}
\]

We know that at the atomic scale the Coulomb potential is of order \((Z\alpha)^2\), the momentum operators are of order \(Z\alpha\), and, hence, we explicitly have the factor \((Z\alpha)^6\). Note that this approach would not work if we had a projector on the positive energy states. In such a case the energy differences would be of order \((Z\alpha)^2\) themselves and we would not get any suppression, since the factors \((Z\alpha)^2\) would cancel in the numerator and denominator.

Returning to our case, it is easy to realize that the projector on the negative energy states leads to additional suppression in the nonrelativistic limit, and, hence, the term under consideration does not produce any contribution of order \((Z\alpha)^6\) at the atomic scale.

There is complete agreement between the results of Ref. [7] and Ref. [11] for the corrections discussed in this section.
IV. SEAGULL CONTRIBUTION

Following Ref. [11] let us again start with the Braun expression Eq. (1) for the seagull contribution and perform the integration by closing the contour each time around one of the transverse photon poles

\[
\Delta E_s = -\frac{1}{M} \int \frac{d\omega}{2\pi i} < n|\hat{D} (\omega, k) G(E + \omega) \hat{D} (\omega, k)| n > .
\]  

(15)

Substituting the pole representation for the Coulomb Green function we obtain in accordance with Ref. [11]

\[
\Delta E_s = \frac{(Z \alpha)^2}{2M} < n| \frac{4\pi \alpha_{k'}}{k'} ( \sum_m \frac{|m > < m|}{(E - k' - E_m)(E - k - E_m)} ) \left( 1 + \frac{E_m - E}{k' + k} \right) \] 

- \sum_m \frac{|m > < m|}{(E + k' - E_m)(E + k - E_m)} \left( 1 - \frac{E_m - E}{k' + k} \right) \frac{4\pi \alpha_k}{k} | n > .
\]

(16)

Let us consider positive- and negative-energy parts of this expression separately.

We may expand the positive energy part in \((E - E_m)/k\) and \((E - E_m)/k\), taking into account that in the low-frequency integration region \(mZ\alpha < k < \sigma\). In the first order of this expansion we get

\[
\Delta E_s^+ = \frac{(Z \alpha)^2}{2M} < n| \frac{4\pi \alpha_{k'}}{k'} \Lambda_+ \frac{4\pi \alpha_k}{k^2} | n > .
\]

(17)

Calculation of this contribution will be considered below. Let us turn to the negative-energy contribution. Energy differences are large for the negative energy contribution \(|E - E_m| \approx 2m(1 - c\alpha^2)\), so we expand the negative energy term in \(k/(E - E_m)\)

\[
\sum_m \frac{|m > < m|}{(E + k' - E_m)(E + k - E_m)} \left( 1 - \frac{E_m - E}{k' + k} \right)
\]

\[
= \sum_m \frac{|m > < m|}{E - E_m} \left( \frac{1}{k + k'} + \frac{(k + k')^2}{2(E - E_m)^3} \right).
\]

(18)

In accordance with Ref. [11] the terms linear in \(k/2m\) cancel, and the negative energy contribution acquires the form

\[
\Delta E_s^- = -\frac{(Z \alpha)^2}{4mM(1 + c\alpha^2)} < n| \frac{4\pi \alpha_{k'}}{k'} \Lambda_- \frac{1}{k + k'} \left( \frac{1}{2m(1 + c\alpha^2)} \right)^3 \frac{4\pi \alpha_k}{k} | n > .
\]

(19)

It may be shown (compare below consideration of the negative energy contribution in the case of the one transverse exchange) that the first term produces the contribution of order \((Z \alpha)^5\) while the second is of order \((Z \alpha)^7\). Only terms linear in \(k, k'\) are capable of producing contributions of order \((Z \alpha)^6\), but these terms cancel each other, as we have just seen.
Let us now return to the positive energy contribution. The idea of Ref. [11] is to consider matrix elements and to calculate them in the nonrelativistic approximation, which produces the leading low-frequency contribution. All matrix elements under consideration have common structure. In general they are the products of matrix elements of $\gamma$-matrices in the momentum space. Each such matrix element in the nonrelativistic limit may easily be reduced to an explicit function of momenta and $\sigma$-matrices, then transformed into coordinate space and calculated between Coulomb-Schroedinger wave functions.

We have performed an explicit calculation along these lines and obtained in complete accord with Ref. [11]

$$\Delta E^+_s = \frac{(Z\alpha)^2}{4m^2M} < n | 2\mathbf{p} \cdot \mathbf{p} + \frac{1}{r^4} - \frac{3\mathbf{p}^2 + 2\sigma\mathbf{l}}{2r^4} | n >. \quad (20)$$

This expression is singular at the origin. This singularity produces linear and logarithmic ultraviolet divergences in momentum space as well as a constant contribution, and hence the contribution under consideration cannot be calculated unambiguously in the general case. It is necessary to realize at this stage that the initial expression for the seagull contribution in Eq.(15) was defined unambiguously. Even separation of the integration region with the help of the auxiliary parameter $\sigma$ could not lead to an ultraviolet divergence in the low-frequency region since all momentum integrations are cut off from above by $\sigma$ and should generate not power divergent but power suppressed terms. It is clear that the apparent divergence is connected with our inaccurate calculation of the singularity at large momenta or small distances. Hence, we have to return to the initial momentum space expression for the positive energy seagull contribution and perform all calculations directly in the momentum space. The result of such a calculation may be later interpreted as an unambiguous prescription for the proper regularization of the coordinate space operators for the $S$-states.

Note, that for the non-$S$ states, wave functions vanish at the origin, the operators above are well defined on such wave functions, and lead to unambiguous results. Of course, any regularization at small distances will not influence the value of the non-$S$ matrix elements of the operator in Eq.(20), and will not influence the agreement between the $P$-level energy shift calculated in Ref. [11], and the same shift obtained earlier in another framework in Ref. [15].

**A. Accurate Calculation with Momentum Space Cutoff**

Direct calculation of the positive energy seagull contribution Eq.(16) in momentum space leads to the following expression for the $S$-state contribution

$$\Delta E^+_s = \frac{(Z\alpha)^2}{m^2M} \int \frac{d^3p\, d^3p\, d^3k\, d^3k}{(2\pi)^3(2\pi)^3(2\pi)^3} (2\pi)^3 \delta(p' - p - k') \frac{8\pi^2}{k^2k'^2} \quad (21)$$

$$\psi(p')[-\mathbf{p}' \cdot \mathbf{p} + \frac{(k'k)(p'k')(pk)}{k^2k'^2} - \frac{k'k}{2}]\psi(p) \equiv \Delta E_{s1} + \Delta E_{s2} + \Delta E_{1/4}.$$ 

The first two terms in the integrand do not rise too rapidly with $k$ and $k'$, and we may unambiguously calculate them using the Fourier transforms discussed above. For the first term we have
 functions/, and we may rewrite the expression above in the operator notation

\[ \Delta E_{s1} = -\frac{(Z\alpha)^2}{m^2 M} \int d^3r \frac{d^3p}{(2\pi)^3} \frac{d^3k}{(2\pi)^3} \frac{d^3k'}{(2\pi)^3} e^{i\mathbf{r} \cdot (\mathbf{p} + \mathbf{k} + \mathbf{k}' - \mathbf{p}' - \mathbf{r})} \frac{8\pi^2}{k^2 k'^2} \]  

(22)

\[ \psi(p') \mathbf{p}' \psi(p) = -\frac{(Z\alpha)^2}{2m^2 M} \int d^3r \frac{d^3p}{(2\pi)^3} \frac{d^3p'}{(2\pi)^3} e^{i\mathbf{r} \cdot (\mathbf{p} + \mathbf{k} + \mathbf{k}')/2} \psi(p') \mathbf{p}' \psi(p). \]

The remaining integration over \( p' \) and \( p \) simply returns us to the coordinate space wave functions, and we may rewrite the expression above in the operator notation\(^2\)

\[ \Delta E_{s1} = \frac{(Z\alpha)^2}{2m^2 M} \langle n | \mathbf{p} \frac{1}{r^2} \mathbf{p} | n \rangle. \]  

(23)

This contribution exactly reproduces the nonsingular operator obtained in the previous chapter.

Next we calculate the second contribution in the same manner as above

\[ \Delta E_{s2} = \frac{(Z\alpha)^2}{m^2 M} \int d^3r \int d^3p \frac{d^3p'}{(2\pi)^3} \frac{d^3k}{(2\pi)^3} \frac{d^3k'}{(2\pi)^3} e^{i\mathbf{r} \cdot (\mathbf{p} + \mathbf{k} + \mathbf{k}')/2} \psi(p') \frac{8\pi^2}{k^2 k'^2} \frac{(\mathbf{k}')(\mathbf{p}'k)(\mathbf{p}k)}{k^4 k'^4} \psi(p) \]

(24)

\[ = \frac{(Z\alpha)^2}{2m^2 M} \int d^3r \int d^3p \frac{d^3p'}{(2\pi)^3} \frac{d^3p}{(2\pi)^3} e^{i\mathbf{r} \cdot (\mathbf{p} + \mathbf{k} + \mathbf{k}')/2} \psi(p') \frac{\mathbf{p}'\mathbf{p}}{4r^2} \left( \delta_{ij} - \frac{r_i r_j}{r^2} \right) \left( \delta_{lm} - \frac{r_i r_m}{r^2} \right) \psi(p) \]

\[ = \frac{(Z\alpha)^2}{2m^2 M} \int d^3r \int d^3p \frac{d^3p'}{(2\pi)^3} \frac{d^3p}{(2\pi)^3} e^{i\mathbf{r} \cdot (\mathbf{p} + \mathbf{k} + \mathbf{k}')/2} \psi(p') \frac{1}{4r^2} \left( \mathbf{p}'\mathbf{p} - \frac{(\mathbf{p}'\mathbf{r})(\mathbf{p}\mathbf{r})}{r^2} \right) \psi(p). \]

Now we use the formula

\[ (\mathbf{r}'\mathbf{p}')(\mathbf{r}\mathbf{p}) = -[\mathbf{r} \times \mathbf{p}'][\mathbf{r} \times \mathbf{p}] + \mathbf{r}^2 (\mathbf{p}'\mathbf{p}), \]  

(25)

and omit the terms with the vector product since we are considering only \( S \)-states now. Then we obtain

\[ \Delta E_{s2} = 0. \]  

(26)

Next we have to calculate the third contribution, which corresponds to the \( 1/r^4 \) term in the naive result above in Eq.(20). This time we cannot use Fourier transformations over exchanged momenta for calculation of this integral, since this leads to a singular expression in coordinate space. So we first perform the safe Fourier transformations over the wave function momenta, and then directly evaluate the exchanged momenta integrals, taking into account that they are cut from above by \( \sigma \ll m \),

\[ \Delta E_{s3} = 0. \]

\(^2\)One has to take into account that the apparent sign of the expression below changes, since the momenta in the exponent have opposite signs.
\[ \Delta E_{1/r^4} = -\frac{(Z \alpha)^2}{m^2 M} \int \frac{d^3 k'}{(2\pi)^3} \frac{d^3 k}{(2\pi)^3} \frac{4\pi^2 (k'k)}{k'^2 k^2} \int d^3r e^{i(k+k')r} \frac{n(r)}{r} >. \] (27)

In order to preserve the transparency of the presentation we will perform the calculation only for \( n = 1 \) here. The general case of arbitrary principal quantum number will be considered at the end of the paper. We substitute explicit expressions for the 1S-wave functions in the formula above, and do the coordinate-space integral

\[ \Delta E_{1/r^4} = -\frac{(Z \alpha)^2}{m^2 M} |\psi(0)|^2 \int \frac{d^3 k'}{(2\pi)^3} \frac{d^3 k}{(2\pi)^3} \frac{4\pi^2 (k'k)}{k'^2 k^2} \int d^3r e^{i(k+k')r} e^{-2\gamma r} \] (28)

\[ = -\frac{64\pi^3 (Z \alpha)^2}{m^2 M} \gamma |\psi(0)|^2 \int \frac{d^3 k'}{(2\pi)^3} \frac{d^3 k}{(2\pi)^3} \frac{k'k}{k'^2 k^2[(k+k')^2 + (2\gamma)^2]^2}, \]

where \( \gamma = mZ\alpha. \)

Symmetrical integrals over the exchanged momenta are cut from above by the parameter \( \sigma. \) However, first integration, say over \( k', \) is convergent at high momenta and the cutoff may be safely ignored

\[ \Delta E_{1/r^4} = -\frac{16\pi (Z \alpha)^2}{m^2 M} \gamma |\psi(0)|^2 \int \frac{d^3 k}{(2\pi)^3} \int_0^\infty \frac{dk'}{k'^2} \int_0^1 dx \frac{k'kx}{[k^2 + k'^2 + 2kk'x + (2\gamma)^2]^2} \] (29)

\[ = -\frac{8\pi^2 (Z \alpha)^2}{m^2 M} \gamma |\psi(0)|^2 \int \frac{d^3 k}{(2\pi)^3} \frac{\arctan \frac{k}{2\gamma}}{k} - \frac{1}{2\gamma} = -\frac{4(Z \alpha)^2}{m^2 M} \gamma |\psi(0)|^2 \int_0^{\sigma} dk \frac{\arctan \frac{k}{2\gamma}}{k} - \frac{1}{2\gamma} \]

\[ = -\frac{(Z \alpha)^2}{m^2 M} \gamma |\psi(0)|^2 \frac{2\pi \ln \frac{\sigma}{2\gamma} - 2\frac{\sigma}{2\gamma}} {2\gamma}. \]

Nonlogarithmic term of order \((Z \alpha)^5\) in this expression is additionally suppressed by the small ratio \( \sigma/m, \) and may be safely ignored. Thus, we see that the properly regularized operator \( 1/r^4 \) in the seagull diagram does not generate a constant contribution. The logarithmic divergence above should cancel with the respective contribution of the one-transverse (magnetic) diagram.

V. MAGNETIC CONTRIBUTION

This time we start with the Braun expression for the one transverse photon in Eq.(1)

\[ \Delta E_{magn} = \frac{1}{M} \text{Re} \int \frac{d\omega}{2\pi i} <n |pG(E + \omega)\hat{D}(\omega, k) + \hat{D}(\omega, k)G(E + \omega)p|n> \] (30)

and first calculate the contour integral\(^3\)

\(^3\)Note that the overall minus sign is connected with the respective sign in the definition of the transverse propagator.
\[ \Delta E_{\text{magn}} = -\frac{Z\alpha}{2M} < n|p| \sum_+ \frac{|m > < m|}{k + E_m - E} - \sum_\pm \frac{|m > < m|}{E - E_m + k} \frac{4\pi \alpha k}{k^2} |n > + \text{h.c.} \]  

(31)

As we are again calculating the low-frequency corrections to the Breit potential let us expand the positive energy term in \((E_m - E)/k\)

\[ \Delta E_{\text{magn}}^+ \]  

(32)

\[ = -\frac{Z\alpha}{2M} < n|p| \sum_+ |m > < m| \left[ \frac{1}{k} - \frac{E_m - E}{k^2} + \frac{(E_m - E)^2}{k^3} + \ldots \right] \frac{4\pi \alpha k}{k} |n > + \text{h.c.} \]

The first term in this expansion may be written in the form

\[ \Delta E_{\text{magn1}}^+ = -\frac{Z\alpha}{2M} < n|p| \sum_+ |m > < m| \left[ \frac{4\pi \alpha_k}{k^2} \right] |n > + \text{h.c.} \]  

(33)

\[ = -\frac{Z\alpha}{2M} < n|p| \frac{4\pi \alpha_k}{k^2} |n > + \frac{Z\alpha}{2M} < n|p| \frac{4\pi \alpha_k}{k^2} |n > + \text{h.c.} \]

\[ = \Delta E_{\text{Br}} + \Delta E_{\text{magn1}}^+ , \]

and it is now evident that the first (Breit) term here coincides with that part of transverse exchange which cancels with the respective term in the Coulomb contribution.

Remaining positive-energy contributions are given by the expression

\[ \Delta E_{\text{magnr}}^+ = -\frac{Z\alpha}{2M} < n|p| \sum_+ |m > < m| \left[ -\frac{E_m - E}{k^2} + \frac{(E_m - E)^2}{k^3} + \ldots \right] \frac{4\pi \alpha_k}{k} |n > + \text{h.c.} \]  

(34)

\[ = \Delta E_{\text{magn2}}^+ + \Delta E_{\text{magn3}}^+ + \ldots \]

A. Positive Energy Contribution

In accordance with Ref. [11] one may check that the term \( \Delta E_{\text{magn2}}^+ \) does not lead to the contributions of order \((Z\alpha)^6\). We have

\[ \Delta E_{\text{magn2}}^+ = \frac{Z\alpha}{2M} < n|p| \sum_+ |m > < m| \left( E_m - E \right) \frac{4\pi \alpha_k}{k^3} |n > + \text{h.c.} \]  

(35)

\[ = -\frac{(Z\alpha)^2}{2M} < n|p| \frac{4\pi k'}{k^2} \Lambda_k \frac{4\pi \alpha_k}{k^3} |n > + \text{h.c.} \]

The simplest way to estimate this matrix element is to make a Fourier transformation. Then we need an infrared divergent Fourier transform of \(1/k^3\). All momentum integrals in the low-frequency region are cut off from below by \(m(Z\alpha)^2\), and it is easy to check that the
leading term in the infrared divergent Fourier transform generates a logarithmic divergent contribution of order \((Z\alpha)^5\) in accordance with Ref. [11]. The next terms vanish with the infrared cutoff and cannot produce contributions of order \((Z\alpha)^6\).

Let us turn now to the term \(\Delta E_{\text{magn}3}^+\). Naive calculation in the coordinate space in accordance with the result in Ref. [11] leads to the result

\[
\Delta E_{\text{magn}3}^+ = -\frac{Z\alpha}{2M} < n||p \sum (E_m - E)^2 |m > < m| \frac{4\pi \alpha_k}{k^4} |n > + h.c.
\] (36)

\[
= -\frac{(Z\alpha)^2}{4m^2 M} < n||2p \frac{1}{p^2} p - \frac{71^2}{2r^4} - \frac{\sigma l}{r^4} |n > .
\]

This expression contains only operators which are nonsingular at the origin for \(S\)-states. Hence, they are well defined, and there is no need for a careful momentum space consideration in this case.

**B. Negative Energy Contribution**

There are two negative-energy contributions connected with the magnetic term, one in Eq.(31), and the other in Eq.(33).

Let us consider first

\[
\Delta E_{\text{magn}}^- = \frac{Z\alpha}{2M} < n||p \sum \frac{|m > < m|}{E - E_m + k} \frac{4\pi \alpha_k}{k^4} |n > + h.c.
\] (37)

We have checked, in accordance with Ref. [11], that this term leads at most to contributions of order \((Z\alpha)^6\), and, hence, is of no interest.

We still have to calculate one more negative energy contribution, contained in Eq.(33)

\[
\Delta E_{\text{magn}1}^+ = \frac{Z\alpha}{2M} < n||p \sum \frac{|m > < m|}{E - E_m + k} \frac{4\pi \alpha_k}{k^4} |n > + h.c.
\] (38)

\[
= \frac{(Z\alpha)^2}{8m^2 M} < n||4\pi \alpha_k \frac{4\pi k(\alpha k)}{k^2} |n > + h.c.
\]

Naive calculation with the help of the Fourier transformation leads, in accordance with Ref. [11], to the expression

\[
\Delta E_{\text{magn}1}^- = \frac{(Z\alpha)^2}{4m^2 M} < n||4\pi \delta(r) - \frac{1}{r^4} |n > .
\] (39)

However, this expression, as in the case of the seagull contribution, contains singular operators at the origin, and does not have unambiguous meaning for the \(S\)-states. A more careful calculation, which explicitly takes into account a momentum space cutoff \(\sigma\), is needed.

First we transform the negative energy contribution in Eq.(38) to the form

\[
\Delta E_{\text{magn}1}^- = -\frac{Z\alpha}{4mM} < n||[p, V] \sum \frac{4\pi \alpha_k}{k^2} |n > + h.c.
\] (40)
Next we substitute the negative energy projection operator in the nonrelativistic approximation \( \Lambda_-(p) \approx 1/2 - (\alpha p + \beta m)/2m \) and use the trivial identity

\[
[p, V] \Lambda_- = \Lambda_- [p, V] - [\Lambda_-, [p, V]] = \Lambda_- [p, V] + \frac{\alpha p}{2m}, [p, V].
\]  

(41)

Note that the first term on the right hand side vanishes applied to the ket-vector, and the negative energy contribution reduces in the nonrelativistic approximation to

\[
\Delta E^{+}_{mag1-} = -\frac{Z\alpha}{2m^2 M} \int \frac{d^3k}{(2\pi)^3} <n|p_k[V] \frac{4\pi e^{ikr}}{k^2}|n>.
\]  

(42)

Then we use

\[
<n(r)|p_k = -i\gamma <n(r)\frac{r_k}{r},
\]  

(43)

and obtain

\[
\Delta E^{+}_{mag1-} = \frac{(Z\alpha)^2}{2m^2 M} \gamma \int \frac{d^3k}{(2\pi)^3} \int d^3r \psi(r) \frac{2(r_k r)}{r^4} \frac{4\pi e^{ikr}}{k^2}.
\]  

(44)

As in the case of the singular seagull contribution we will perform the calculation for \( n = 1 \) first, postponing consideration of the general case to the next chapter. We substitute explicit expressions for the wave functions and obtain

\[
\Delta E^{+}_{mag1-} = \frac{2\pi (Z\alpha)^2}{2m^2 M} \gamma |\psi(0)|^2 \int \frac{d^3k}{(2\pi)^3} \frac{4\pi}{k^2} \int_1^1 dx (1 - x^2) \int_0^\infty dr e^{-2\gamma r} e^{ikr}.
\]  

(45)

\[
= \frac{4\pi (Z\alpha)^2}{2m^2 M} \gamma^2 |\psi(0)|^2 \int \frac{d^3k}{(2\pi)^3} \frac{4\pi}{k^2} \left[ \frac{(4\gamma^2 + k^2) \arctan \frac{k}{2\gamma} - \frac{2}{k^2} \right],
\]

\[
= \frac{4\pi (Z\alpha)^2}{2m^2 M} \frac{(4\pi)^2}{(2\pi)^3} \gamma^2 |\psi(0)|^2 \int_0^\sigma dk \left[ \frac{(4\gamma^2 + k^2) \arctan \frac{k}{2\gamma} - \frac{2}{k^2} \right],
\]

\[
= \frac{\pi (Z\alpha)^2}{m^2 M} \gamma |\psi(0)|^2 [2 \ln \frac{\sigma}{2\gamma} - 1].
\]

Again, as in the case of the seagull contribution, this term may be understood as a proper regularization of the naive singular in the coordinate space operator from Eq.(39).
VI. CALCULATIONS FOR ARBITRARY PRINCIPAL QUANTUM NUMBER

The total low-frequency contribution for the 1S-state is given by the sum of the results in Eq.(10), Eq.(23), Eq.(29), Eq.(36) and Eq.(45)

\[ \Delta E_{\text{low-freq}}(1S) = -(Z \alpha)^6 \frac{m}{M} m, \] (46)

and coincides with the result obtained earlier for the low-frequency contribution in Ref. [7]. We see that the seagull and magnetic contributions partially cancel each other. This reflects cancellation of the 1/r^4 terms in the language of Ref. [11]. However, the contribution (−1) survives. This contribution is connected with the δ-function term in Ref. [11], and the error in Ref. [11] is due to an improper regularization of this contribution. Note that from the point of view of the coordinate representation after the Fourier transformation is done the proper regularization is highly nontrivial. One could never obtain this contribution with a naive ad hoc regularization in coordinate space.

The result in Eq.(46) is valid only for the 1S-state. We are going to generalize it to an arbitrary principal quantum number.

A. Seagull Contribution for Arbitrary nS-Level

The general expression for the wave function of an nS-level has the form

\[ \psi_n(r) = \left( \frac{\gamma^3}{\pi r^3} \right)^{1/2} e^{-\frac{\pi r}{n}} \left[ 1 - \frac{n-1}{n} \gamma r + \ldots \right]. \] (47)

Let us introduce \( \beta \equiv \gamma/n \). Almost all calculations above for \( n = 1 \) immediately turn into calculations for arbitrary \( n \) after substitution \( \gamma \to \beta \) [16]. The wave function has the form

\[ \psi_n(r) = \left( \frac{\beta^3}{\pi} \right)^{1/2} e^{-\beta r} \left[ 1 - (n-1)\beta r + \ldots \right] \equiv \psi_n(0) e^{-\beta r} \left[ 1 - (n-1)\beta r + \ldots \right]. \] (48)

Quadratic and higher order terms in \( r \) in the postexponential factor in the wave function do not produce any contribution to the energy level connected with the singular operator in the naive expression in Eq.(20), and we will ignore them below. The only difference between the general case and the case of \( n = 1 \) is connected with the linear term in the postexponential factor. Let us find out how it changes the result for the seagull contribution. First, let us write down the singular seagull contribution induced by the purely exponential part of the wave function for arbitrary \( n \) in the form

\[ \Delta E^{1/r^4}_s = -\frac{(Z \alpha)^2}{m^2 M} \left| \psi(0) \right|^2 \int \frac{d^3k}{(2\pi)^3} \frac{d^3k'}{(2\pi)^3} \frac{4\pi^2(k'k)}{k^2 k'^2} \int d^3r e^{i(k+k')r} e^{-2\beta r} \] (49)

\[ = -\frac{(Z \alpha)^2}{m^2 M} \left| \psi(0) \right|^2 \epsilon^{1/r^4}_s, \]

where
\[ \epsilon_s^{1/r^4} = 2\pi\beta \ln \frac{\sigma}{2\beta} \]  

The linear terms in the wave functions lead to an additional contribution

\[ \Delta E_{s,\text{corr}}^{1/r^4} = -\frac{(Z\alpha)^2}{m^2 M} |\psi(0)|^2 \int \frac{d^3k'}{(2\pi)^3} \frac{d^3k}{k'^2 k^2} \frac{4\pi^2 (k'k)}{k'^2 k^2} \int d^3r e^{i(k+k')r} e^{-2\beta/r} [-2(n-1)\beta] \]  

\[ = -\frac{(Z\alpha)^2}{m^2 M} |\psi(0)|^2 (n-1)\beta \frac{\partial}{\partial \beta} \epsilon_s^{1/r^4} = -\frac{(Z\alpha)^2}{m^2 M} |\psi(0)|^2 (n-1) [2\pi\beta \ln \frac{\sigma}{2\beta} - 2\pi \beta], \]

and the total seagull contribution to the energy shift is equal to

\[ \Delta E_{s,\text{tot}}^{1/r^4} = \Delta E_{s,\text{corr}}^{1/r^4} + \Delta E_{s,\text{corr}}^{1/r^4} = -\frac{(Z\alpha)^2}{m^2 M} |\psi(0)|^2 [\epsilon_s^{1/r^4} + (n-1)\beta \frac{\partial}{\partial \beta} \epsilon_s^{1/r^4}] \]  

\[ = -\frac{(Z\alpha)^2}{m^2 M} |\psi(0)|^2 [2\pi\gamma \ln \frac{\sigma}{2\beta} - 2\pi (n-1)\beta]. \]

**B. Magnetic Contribution for Arbitrary nS-Level**

As in the case of the seagull contribution the only difference of the general case from the case of \( n = 1 \) is connected with the linear term in the postexponential factor in the wave function. The purely exponential part of the wave function leads to the following singular magnetic contribution for arbitrary \( n \)

\[ \Delta E_{magn1-}^+ = \frac{(Z\alpha)^2}{m^2 M} |\psi(0)|^2 [2\pi\beta \ln \frac{\sigma}{2\beta} - \pi\beta] \equiv \frac{(Z\alpha)^2}{m^2 M} |\psi(0)|^2 \epsilon_{magn1-}^+. \]  

The new contribution induced by the linear term in the wave function has the form

\[ \Delta E_{magn1-.\text{corr}}^+ = -\frac{Z\alpha}{2m^2 M} \int \frac{d^3k}{(2\pi)^3} [(n-1)\beta] \{ <n|r|p_k|p, V|\frac{4\pi e^{ikr}}{k^2}|n> - <n|p_k|p, V|\frac{4\pi e^{ikr}}{k^2}|n> \} \]

\[ + <n|p_k|p, V|\frac{4\pi e^{ikr}}{k^2}|n> \}.

Next we write

\[ rP_k = P_k r - [P_k, r], \]  

and using the commutation relation

\[ [P_k, r] = -i \frac{P_k}{r}, \]

obtain
\[ \Delta E_{\text{magn}_{1,-}\text{cor}} = -\frac{Z \alpha}{2m^2 M} \int \frac{d^3 k}{(2\pi)^3} |-(n-1)\beta| < n|\frac{\mathbf{r}_k}{r}| \mathbf{p}, V| \frac{4\pi e^{ikr}}{k^2} |n > \]

\[ + < n|\mathbf{p}_k|\mathbf{p}, V| \frac{4\pi e^{ikr}}{k^2} 2r |n > \}.

\[ = -\frac{Z \alpha}{2m^2 M} \int \frac{d^3 k}{(2\pi)^3} (n-1) \{ < n|(-i\beta \frac{r_k}{r})| \mathbf{p}, V| \frac{4\pi e^{ikr}}{k^2} |n > \]

\[ -(n-1)\beta < n|\mathbf{p}_k|\mathbf{p}, V| \frac{4\pi e^{ikr}}{k^2} 2r |n > \} \]

\[ = \left( \frac{Z \alpha}{m^2 M} \right)^2 |\psi(0)|^2 (n-1) \left[ e_{\text{magn}_{1,-}}^+ + \beta \frac{\partial}{\partial \beta} \left( e_{\text{magn}_{1,-}}^+ \right) \right] \]

\[ = \left( \frac{Z \alpha}{m^2 M} \right)^2 |\psi(0)|^2 \left[ 2\pi \beta (n-1) \ln \frac{\sigma}{2\beta} - (n-1) \pi \beta - (n-1) 2\pi \beta \right] \]

\[ = \left( \frac{Z \alpha}{m^2 M} \right)^2 |\psi(0)|^2 \left[ 2\pi \beta (n-1) \ln \frac{\sigma}{2\beta} - 3(n-1) \pi \beta \right]. \]

Then the total singular magnetic contribution is equal to

\[ \Delta E_{\text{magn}_{1,-}\text{tot}} = \Delta E_{\text{magn}_{1,-}} + \Delta E_{\text{magn}_{1,-}\text{cor}} = \left( \frac{Z \alpha}{m^2 M} \right)^2 |\psi(0)|^2 \left[ 2\pi \gamma \ln \frac{\sigma}{2\beta} - \pi \beta - 3(n-1) \pi \beta \right] \]

VII. TOTAL RECOIL CORRECTION

The total low-frequency contribution of order \((Z \alpha)^6 (m/M)m\) for arbitrary \(nS\)-state is given by the sum of the terms in Eq.(10), Eq.(23), Eq.(52), Eq.(36) and Eq.(58)

\[ \Delta E_{\text{low-freq}} = \left( \frac{1}{8} + \frac{3}{8n} - \frac{1}{n^2} + \frac{1}{2n^3} \right) \frac{(Z \alpha)^6 m}{n^3 M} m + \frac{(Z \alpha)^2}{2m^2 M} < n|\mathbf{p} \frac{1}{r^2} \mathbf{p}|n > \]

\[ -\frac{(Z \alpha)^2}{m^2 M} |\psi(0)|^2 \left[ 2\pi \gamma \ln \frac{\sigma}{2\beta} - 2\pi (n-1) \beta - 2\sigma \right] - \frac{(Z \alpha)^2}{4m^2 M} < n|2\mathbf{p} \frac{1}{r^2} \mathbf{p}|n > \]

\[ +\frac{(Z \alpha)^2}{m^2 M} |\psi(0)|^2 \left[ 2\pi \gamma \ln \frac{\sigma}{2\beta} - \pi \beta - 3(n-1) \pi \beta \right]. \]
\[ \Delta E_{\text{tot}} = \left( \frac{1}{8} + \frac{3}{8n} - \frac{1}{n^2} + \frac{1}{2n^3} \right) (Z\alpha)^6 \frac{m}{M^m} + \frac{(Z\alpha)^6}{n^3} \frac{m}{M^m}. \]

Note that the last term connected with the naive singular operators in the coordinate space turned out to be state-independent.

To obtain the total recoil correction of order \((Z\alpha)^6(m/M)m\) it is also necessary to calculate the high-frequency (or short-distance) contribution to the energy shift. The simplest way is to use again the Braun formula Eq. (1), but this time in the Feynman gauge. This calculation is quite straightforward if one again uses the auxiliary parameter \(\sigma\) introduced above in order to qualify would be infrared divergences. Such a calculation was performed explicitly in ref. [11] and led to the result

\[ \Delta E_{\text{high-freq}} = (4\ln 2 - \frac{5}{2}) \frac{(Z\alpha)^6}{n^3} \frac{m}{M^m}, \]

in complete agreement with Ref. [7].

Then total correction of order \((Z\alpha)^6(m/M)m\) to the energy levels is given by the sum of the results in Eq. (59) and Eq. (60)

\[ \Delta E_{\text{tot}} = \left( \frac{1}{8} + \frac{3}{8n} - \frac{1}{n^2} + \frac{1}{2n^3} \right) (Z\alpha)^6 \frac{m}{M^m} + (4\ln 2 - \frac{7}{2}) \frac{(Z\alpha)^6}{n^3} \frac{m}{M^m}. \]

For \(n = 1, 2\) this result nicely coincides with the one obtained in Ref. [7].

In conclusion let us emphasize that discrepancies between the different results for the correction of order \((Z\alpha)^6(m/M)\) to the energy levels of the hydrogen-like ions are resolved and the correction of this order is now firmly established.

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