Pure recoil corrections to hydrogen energy levels.

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The pure recoil correction to hydrogen–like energy levels is revisited. A new method for its evaluation is presented. We confirm, that the previous result [Doncheski,*et al*, Phys. Rev.A **43**, 2125 (1991)] of the $\frac{m^2}{M}(Z\alpha)^6$ contribution was missing some important terms. Our result is $\Delta E = \frac{m^2}{M}\,\frac{(Z\,\alpha)^6}{n^3}\,(4\,\log(2) - 7/2)$. A new value of the deuteron radius is obtained by comparing theory to the measurement of the hydrogen-deuterium isotope shift.

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I. INTRODUCTION

The recoil correction is the correction that comes from the finite mass of the nucleus. Since the electron–proton mass ratio is very small $m/M \approx 1/2000$, as a first approximation for the hydrogenic energy levels we can assume that the mass of the nucleus is infinite. This allows one to treat the nucleus as a static source of the Coulomb field. In such a case we have an exact solution of the Dirac equation. From that basis one can evaluate QED corrections: electron self–energy, vacuum polarization, etc. For the precise determination of hydrogenic energy levels we have to include also, the effects that come from finite nuclear mass. In the nonrelativistic approximation, the mass dependence is contained in the reduced mass μ of two–body system, but the situation is more complex in the full relativistic theory. As a starting point one usually considers a Bethe–Salpeter equation [1], which gives a full description of the two body system. Unfortunately, this equation is not easily tractable, and the limit of infinite nuclear mass, i.e. the Dirac equation, is obtained only upon resummation of an infinite series for the kernel of the Bethe–Salpeter equation. Thus it seems to be more convenient to develop an effective three–dimensional equation, at least for the evaluation of some subset of recoil corrections, that is equivalent to the Bethe–Salpeter equation and takes advantage of the small electron–proton mass ratio. One such a method has been developed by Grotch and Yennie [2] many years ago. Using this method, one can calculate all the pure recoil corrections, (i.e. without a photon loop on the fermion line), that contribute to hydrogen Lamb shift $E(2S-2P)$ at the level of one kHz. According to this method, the leading mass correction, (through $(Z\alpha)^4$ order) is obtained from the effective hamiltonian, by treating the proton nonrelativistically, with Coulomb and Breit interactions taken into account:

$$H_{\rm eff} = \boldsymbol{\alpha}\,\mathbf{p} + \beta\,m + \frac{p^2}{2M} + V_{\rm eff}\,, \tag{1}$$

$$\tilde{V}_{\rm eff}(p,p') = -\frac{e^2}{(\mathbf{p}-\mathbf{p}')^2}\left(1 + \frac{\boldsymbol{\alpha}_\perp\cdot(\mathbf{p}+\mathbf{p}')}{\mathbf{2M}}\right)\,, \tag{2}$$

where $\boldsymbol{\alpha}_\perp$ is the component of $\boldsymbol{\alpha}$ perpendicular to $\mathbf{p}-\mathbf{p}'$, m and M is the electron and the proton mass respectively. For simplicity we set $Z=1$ in Eq. (2) and below since we are dealing with hydrogen, but in the final results we restore the dependence on Z since results are applicable for $Z \neq 1$.

The approach of Ref. [2] has been refined and through α^4 order, but with the exact mass dependence, the energy levels of hydrogen (excluding the hyperfine structure) are [3]

$$E = \mu\,[f(n,j)-1] - \frac{\mu^2}{2\,(M+m)}\,[f(n,j)-1]^2 + \frac{\alpha^4\,\mu^3}{2\,n^3\,M^2}\,\left(\frac{1}{j+\frac{1}{2}} - \frac{1}{l+\frac{1}{2}}\right)(1-\delta_{l0})\,, \tag{3}$$

where $f(n,j)$ is a dimensionless Dirac energy and μ is the reduced mass. The exact mass dependence of the pure recoil correction in α^5 order was first worked out by Salpeter [4]. Using the Bethe–Salpeter formalism, he obtained the following result

$$\Delta E = \frac{\mu^3}{m\,M}\,\frac{\alpha^5}{\pi\,n^3}\left\{\frac{2}{3}\,\delta_{l0}\,\ln(\frac{1}{\alpha}) - \frac{8}{3}\,\ln(k_0(n)) - \frac{1}{9}\,\delta_{l0} - \frac{7}{3}\,a_n \right.$$
$$\left. -\frac{2}{M^2-m^2}\,\delta_{l0}\,\left[M^2\,\ln\left(\frac{m}{\mu}\right) - m^2\,\ln\left(\frac{M}{\mu}\right)\right]\right\}, \tag{4}$$

where

$$a_n = -2\,\left(\ln(\frac{2}{n}) + (1+\frac{1}{2}+\ldots+\frac{1}{n}) + 1 - \frac{1}{2\,n}\right)\,\delta_{l0} + \frac{1-\delta_{l0}}{l\,(l+1)\,(2\,l+1)}\,, \tag{5}$$

and $\ln(k_0(n))$ is the Bethe logarithm. In α^6 order, the m/M correction has been calculated by Doncheski, Grotch and Erickson in [5] using the effective potential method, with the following result

$$\Delta E = \frac{m^2}{M}\,\frac{\alpha^6}{n^3}\,\left(\frac{5}{2} - \ln(\frac{2}{\alpha}) + 2\,\ln(\frac{1}{\alpha}) - 4.25\right)\,. \tag{6}$$

It has been found that this result omits some important terms. Khriplovich and coworkers [6] calculated the exact mass dependence of the logarithmic term for the case of arbitrary masses, and found that the $\log(\alpha)$ term should be absent from eq. (6). We confirm here the Khriplovich result. We found that the Doncheski *et.al* calculation [5] missed some terms in the seagull contribution coming from the lower components of the wave function. We checked, both analytically and numerically, that these terms exactly cancel the $\log(\alpha)$ coefficient. We also correct the single transverse term.

II. DERIVATION OF FORMULAS

Our method takes advantage of the small electron–proton mass ratio. Because we are interested only in the first term in the m/M expansion, we may treat the proton nonrelativistically, i.e. its hamiltonian is the following

$$H = \frac{(\mathbf{P}+e\,\mathbf{A})^2}{2\,M}\,, \tag{7}$$

where $\mathbf{P}$ is the proton momentum, and $\mathbf{A}(R)$ is an electromagnetic vector potential in the Coulomb gauge at the proton position R. The O(m/M) term is obtained by taking the matrix element of this hamiltonian in the electron state ψ_R

$$\Delta E = \langle\psi_R|\frac{(\mathbf{P}+e\,\mathbf{A})^2}{2\,M}|\psi_R\rangle\,, \tag{8}$$

where ψ_R is an electron eigenstate of the QED hamiltonian in the external Coulomb field positioned at R. When we apply the perturbation theory, this formal expression contains also the radiative recoil contribution, which could easily be subtracted out by neglecting the terms with the photon emission and absorption by the same particle (electron or proton). We derive below the *exact* (without expansion in $Z\,\alpha$) expressions for the pure recoil correction. These relevant formulae were first derived by Shabaev [7] from the Bethe–Salpeter formalism.

In the derivation we first expand the expression in (8):

$$\begin{aligned}\Delta E &= \langle\psi_R|\frac{\mathbf{P}^2}{2\,M}|\psi_R\rangle + \langle\psi_R|\frac{\mathbf{P}}{M}\,e\,\mathbf{A}|\psi_R\rangle + \langle\psi_R|\frac{(e\,\mathbf{A})^2}{2\,M}|\psi_R\rangle \\ &= E_C + E_T + E_S\,,\end{aligned} \tag{9}$$

where E_C is a Coulomb, E_T is a single transverse, and E_S is a seagull contribution.

The Coulomb contribution is

$$E_C = \langle\psi_R|\frac{\mathbf{P}^2}{2\,M}|\psi_R\rangle\,. \tag{10}$$

Since we neglect photon loops on the fermion line, the state ψ_R here, is the eigenstate of the second quantized Dirac hamiltonian in the external Coulomb field. Therefore, we have one electron in, let us assume, state ϕ^S and a filled Dirac sea of states ϕ^n, so

$$E_C = \langle \ldots, \phi^3_R, \phi^2_R, \phi^1_R, \phi^S_R | \frac{\mathbf{P}^2}{2\,M} | \phi^S_R, \phi^1_R, \phi^2_R, , \phi^3_R, \ldots \rangle$$

$$= -\frac{\triangle_{R'}}{2\,M} \det \begin{pmatrix} \langle \phi^S_R | \phi^S_{R'} \rangle & \langle \phi^S_R | \phi^1_{R'} \rangle & \ldots \\ \langle \phi^1_R | \phi^S_{R'} \rangle & \langle \phi^1_R | \phi^1_{R'} \rangle & \ldots \\ \vdots & \vdots & \langle \phi^2_R | \phi^2_{R'} \rangle \end{pmatrix} , \tag{11}$$

where we introduced R' to move the differentiation $\mathbf{P}^2$ out of the matrix element. Since, after the R' differentiation we put $R' = R$

$$E_C = -\frac{\triangle_{R'}}{2\,M} \left(\langle \phi^S_R | \phi^S_{R'} \rangle + \sum_n \langle \phi^n_R | \phi^n_{R'} \rangle \right) + \sum_n \frac{\triangle_{R'}}{2\,M} \langle \phi^n_R | \phi^S_{R'} \rangle \langle \phi^S_R | \phi^n_{R'} \rangle \,. \tag{12}$$

We can omit the first sum in the above, because it does not depend on the electron state. Since $\phi_S(R, r) = \phi_S(r - R)$, we can make the replacement $P^i \rightarrow -p^i$,

$$E_C = \langle \phi^S | \frac{\mathbf{p}^2}{2\,M} | \phi^S \rangle - 2\,\frac{1}{2\,M} \sum_n \langle \phi^n | \mathbf{p} | \phi^S \rangle \langle \phi^S | \mathbf{p} | \phi^n \rangle \tag{13}$$

$$= \frac{1}{2\,M}\, \langle \phi^S | \mathbf{p} (P_+ - P_-) \mathbf{p} | \phi^S \rangle \,, \tag{14}$$

where P_+ and P_- are projection operators onto positive, negative energy subspace of the Dirac hamiltonian. In this way we derived the formula for the Coulomb contribution E_C.

The single transverse contribution E_T is:

$$E_T = \frac{1}{M} \langle \psi_R | \mathbf{P}\, e\, \mathbf{A} | \psi_R \rangle \,. \tag{15}$$

In the Furry picture, in the external potential

$$V(\mathbf{r}, t) = \Theta(t) V(\mathbf{r} - \mathbf{R}) + \Theta(-t) V(\mathbf{r} - \mathbf{R}') \,, \tag{16}$$

where $V(r) = -\alpha/r$, the single transverse contribution reads:

$$E_T = \frac{-i\,\partial^i_{R'}}{M} \int d^4y\; i\, G^{ij}(R - y) \langle \psi_R | i\, e^2\, j^j(y) | \psi_{R'} \rangle \tag{17}$$

$$= -\frac{e^2}{M} \int d^4y\;\; G^{ij}(R - y)\; \left\{ \Theta(y) \langle \psi_R | j^j(y)\, P^i | \psi_R \rangle + \Theta(-y) \langle \psi_R | P^i\, j^j(y) | \psi_R \rangle \right\} \,, \tag{18}$$

where G^{ij} are spatial components of the photon propagator in Coulomb gauge,

$$G^{ij}(x) = \int \frac{d\omega}{2\,\pi} \int \frac{d^3k}{(2\,\pi)^3} \left(\delta^{ij} - \frac{k^i\, k^j}{k^2} \right) \frac{1}{\omega^2 - k^2}\, e^{i\,(\omega\, x^0 - \mathbf{k}\,\mathbf{x})} \tag{19}$$

The matrix element

$$\langle \psi_R | j^j(y)\, P^i | \psi_R \rangle = \sum_n \langle \psi_R | j^j(y) | \psi_n \rangle\, \langle \psi_n | P^i | \psi_R \rangle \tag{20}$$

could be written as a sum over all possible states $|\psi_n\rangle$.

$$\begin{aligned} \langle \psi_R | j^j(y)\, P^i | \psi_R \rangle = & \\ & \sum_{n+} \langle \ldots, \phi_2, \phi_1, \phi_S | j^j(y) | \phi_n, \phi_1, \phi_2, \ldots \rangle \\ & \cdot \langle \ldots, \phi_2, \phi_1, \phi_n | P^i | \phi_S, \phi_1, \phi_2, \ldots \rangle + \\ & \sum_{n+ \neq S, m-} \langle \ldots, \phi_2, \phi_1, \phi_S | j^j(y) | \phi_S, \phi_1, \ldots, \overset{\overset{m}{\vee}}{\phi_n}, \ldots \rangle \end{aligned}$$

$$\cdot\langle\ldots,\overset{\overset{m}{\vee}}{\phi_n},\ldots,\phi_1,\phi_S|P^i|\phi_S,\phi_1,\phi_2,\ldots\rangle \tag{21}$$

$$= \sum_{n+}(\bar\phi_S\gamma^j\,\phi_n)(y)\,\langle\phi_n|P^i|\phi_S\rangle - \sum_{m^-}(\bar\phi_m\gamma^j\,\phi_S)(y)\,\langle\phi_S|P^i|\phi_m\rangle$$
$$+\left\{\sum_{n^+,m^-}(\bar\phi_m\gamma^j\,\phi_n)(y)\,\langle\phi_n|P^i|\phi_m\rangle\right\}, \tag{22}$$

where $+,-$ denotes positive, negative energy eigenstates in the above sums respectively. The last term in the above does not depend on state ϕ_S, so we simply drop it out. The single transverse contribution reads now:

$$E_T = -\frac{e^2}{M}\int d^4y\; G^{ij}(y)$$
$$\cdot\left\{\Theta(y_0)\left(\sum_{n+}(\bar\phi_S\gamma^j\,\phi_n)(y)\,\langle\phi_n|P^i|\phi_S\rangle - \sum_{m^-}(\bar\phi_m\gamma^j\,\phi_S)(y)\,\langle\phi_S|P^i|\phi_m\rangle\right) + \Theta(-y_0)\Big(c.c.\Big)\right\} \tag{23}$$

The summation over states gives Dirac–Coulomb propagators. We obtain for the single transverse contribution:

$$E_T = -\frac{e^2}{M}\int\frac{d\omega}{2\,\pi\,i}\int\frac{d^3k}{(2\,\pi)^3}\,\delta_\perp^{ij}\,\frac{1}{k^2}\,\left\{\langle\bar\phi_S|\gamma^j\,e^{i\,k\,r}\,S_F(E_S-\omega)\,\gamma^0\,p^i|\phi_S\rangle + c.c.\right\}\,, \tag{24}$$

where $\delta_\perp^{ij} = \delta^{ij} - \frac{k^i\,k^j}{k^2}$.

The seagull (or double transverse) contribution is the following:

$$E_S = \langle\psi_R|\frac{e^2}{2\,M}\mathbf{A}^2(R)|\psi_R\rangle\,. \tag{25}$$

For its evaluation we use a Furry picture in the external Coulomb potential, and obtain

$$E_S = \frac{e^4}{2\,M}\,(-i)^2\frac{1}{2}\int d^4y_1\int d^4y_2\;T\langle 0|\mathbf{A}^2(0)\,A^i(y_1)\,A^j(y_2)|0\rangle\;T\langle\psi|j^i(y_1)\,j^j(y_2)|\psi\rangle \tag{26}$$

$$= -\frac{e^4}{M}\int\frac{d\omega}{2\,\pi\,i}\int\frac{d^3k_1}{(2\,\pi)^3}\int\frac{d^3k_2}{(2\,\pi)^3}\,\frac{1}{\omega^2-k_1^2}\,\frac{1}{\omega^2-k_2^2}\,\delta_{1\perp}^{ki}\,\delta_{2\perp}^{kj}$$
$$\langle\bar\phi_S|\gamma^i\,e^{-i\,k_1\,r}\,S_F(E_S-\omega)\,\gamma^j\,e^{i\,k_2\,r}|\phi_S\rangle\,. \tag{27}$$

The above closed formulae will be used in the next section for the calculation of recoil corrections. We have also derived them by using the S–matrix formalism but the presented method, is simpler and conceptionally new.

III. THE LEADING ORDER CONTRIBUTION

The recoil contribution, through α^4 order is obtained from the Coulomb E_C and the single transverse E_T using the following approximations. In eq. (14) for E_C we neglect P_- and replace P_+ by unity

$$E_C = \frac{1}{2\,M}\langle\phi|\,\mathbf{p}^2|\phi\rangle\,. \tag{28}$$

In the single transverse contribution eq. (24) we replace the Dirac propagator $S_F(E-\omega)$ by $1/(\omega - i\,\epsilon)$, and obtain the so called Breit term:

$$E_T = -\frac{e^2}{M}\int\frac{d\omega}{2\,\pi\,i}\int\frac{d^3k}{(2\,\pi)^3}\delta_\perp^{ij}\,\frac{1}{\omega^2-k^2}\,\frac{(-1)}{\omega-i\,\epsilon}\,\left\{\langle\bar\phi|\gamma^j\,e^{-i\,k\,r}\,p^i|\phi\rangle + c.c.\right\}$$
$$= -\frac{4\,\pi\,\alpha}{M}\,\langle\bar\phi|\gamma^j\,p^i\,\frac{1}{8\,\pi\,r}\,\left(\delta^{ij}+\frac{r^i\,r^j}{r^2}\right)\,|\phi\rangle\,. \tag{29}$$

The sum of these terms, after some manipulation gives

$$\Delta E = \frac{m^2-E^2}{2\,M}\,, \tag{30}$$

where E is the Dirac energy. This simple result is valid through α^4 order.

IV. THE HIGHER ORDER CORRECTIONS

After separation of the leading order terms we are left with the following expressions. The Coulomb contribution

$$E'_C = -\frac{1}{M}\,\langle\phi|\mathbf{p}P_-\mathbf{p}|\phi\rangle \tag{31}$$

could be transformed upon the identity

$$(\not p - m - \gamma^0\,V)\,\mathbf{p}\phi = \gamma^0\,[\mathbf{p},V]\,\phi \tag{32}$$

to the form

$$E'_C = \frac{1}{M}\int\frac{d\omega}{2\,\pi\,i}\,\frac{1}{(\omega-i\,\epsilon)^2}\langle\bar\phi|[\mathbf{p},V]\,\gamma^0\,S(E-\omega)\,\gamma^0\,[\mathbf{p},V]|\phi\rangle\,. \tag{33}$$

The single transverse contribution after the separation is:

$$E'_T = -\frac{e^2}{M}\int\frac{d\omega}{2\,\pi\,i}\,\frac{1}{\omega-i\,\epsilon}\int\frac{d^3k}{(2\,\pi)^3}\,\delta^{ij}_\perp\,\frac{1}{\omega^2-k^2}\,\langle\bar\phi|\gamma^i\,e^{i\,k\,r}\,S_F(E-\omega)\,\gamma^0\,[p^i,V]|\phi\rangle\,. \tag{34}$$

The seagull contribution remains the same

$$\begin{aligned} E_S = -\frac{e^4}{M}\int\frac{d\omega}{2\,\pi\,i}\int\frac{d^3k_1}{(2\,\pi)^3}\int\frac{d^3k_2}{(2\,\pi)^3}\,\frac{1}{\omega^2-k_1^2}\,\frac{1}{\omega^2-k_2^2}\,\delta^{ki}_{1\perp}\,\delta^{kj}_{2\perp} \\ \langle\bar\phi|\gamma^i\,e^{-i\,k_1\,r}\,S_F(E-\omega)\,\gamma^j\,e^{i\,k_2\,r}|\phi\rangle\,. \end{aligned} \tag{35}$$

The evaluation of higher order corrections is a more complicated problem due to the fact that both small and large photon energies ω contribute through α^6. This is the reason why we used the ϵ–method introduced in [8]. Except for some terms in E_T it is sufficient to consider up to three photon exchange to obtain corrections through α^6 order. We perform the calculation for the 1S state, and later evaluate the difference $\Delta E(1S) - n^3\Delta E(nS)$, which we found to be exactly zero in α^6 order.

A. the Coulomb contribution

In contrast to E_T and E_S the calculation of the Coulomb contribution E_C, proceeds in straightforward way. The α^5 term is obtained by putting both wave functions ϕ on mass shell in (33), $\phi(r)\to\phi(0)$, and neglecting the Coulomb potential in the Dirac propagator,

$$\Delta E = -\frac{4}{3}\,\frac{m^2}{M}\,\frac{\alpha^5}{\pi}\,. \tag{36}$$

The α^6 term comes from the single potential term of the Dirac propagator, with both wave functions on mass shell

$$\Delta E = \frac{1}{2}\,\frac{m^2}{M}\,\alpha^6\,. \tag{37}$$

and from the Coulomb correction to one of the wavefunction $\phi(r)\to(\not p - m)^{-1}\,V\,\phi(0)$

$$\Delta E = \frac{1}{2}\frac{m^2}{M}\alpha^6\,. \tag{38}$$

The complete Coulomb contribution is a sum of (36,37,38)

$$E_C = \frac{m^2}{M}\left(-\frac{4}{3}\,\frac{\alpha^5}{\pi}+\alpha^6\right)\,, \tag{39}$$

in agreement with [5].

B. the seagull contribution

The seagull contribution E_S (35) is more difficult to evaluate, since it gives terms logarithmic in α. Thus we present more details of its evaluation. We use the method presented in detail in [8].

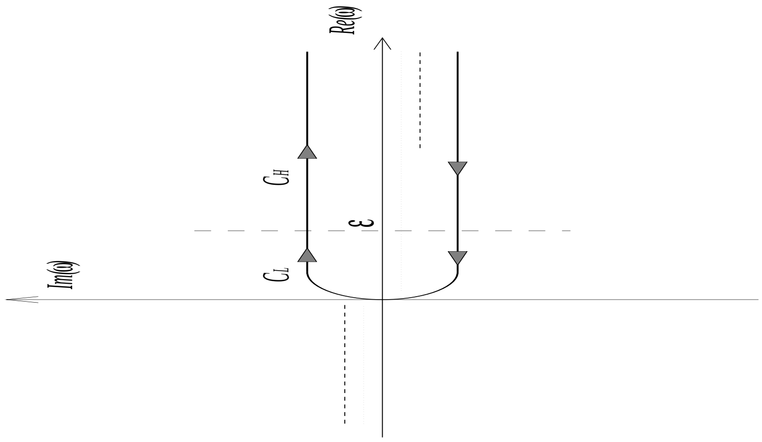

FIG. 1. The contour of ω–integration on the complex plain. C_L is the low energy part and C_H is the high energy part. The dashed line denotes the branch cut from the fermion propagator and dotted line from the photon propagator.

The contour of ω integration is deformed according to Fig. 1, and divided into two parts. In the high energy part C_H we expand the electron propagator in the Coulomb field, put the binding energy equal to zero, perform momentum integrals, expand in α and afterwards in ϵ. The terms divergent in ϵ will cancel out with the low energy part (the contour C_L), where we could perform the nonrelativistic approximation. For the terms in α^6 order the contour of ω–integration is again deformed according to Fig. 2. It so happens that the branch cuts from photon and fermion propagators cancel out and the expression under the ω–integral is an analytic function on the left hand side of the complex plane, i.e. for $\Re(\omega) < 0$.

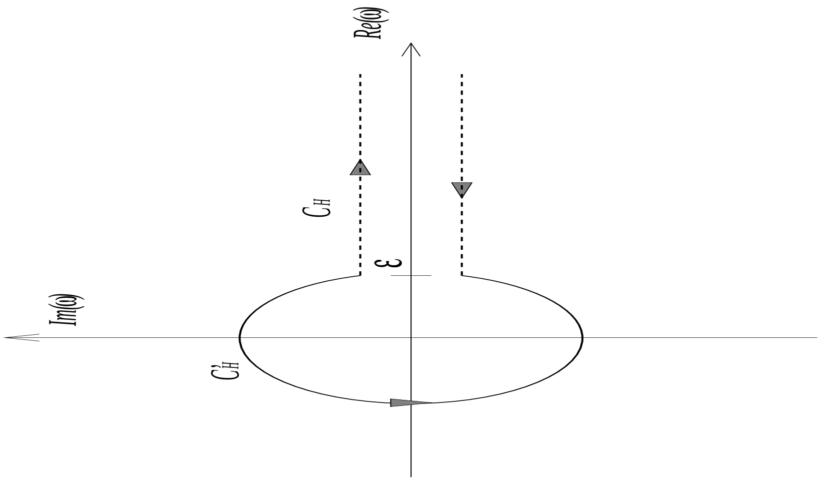

FIG. 2. C'_H is a deformation of the C_H contour, used in the evaluation of α^6 correction. The branch cuts from the fermion and photon propagators cancels out on the left hand side of complex ω plain.

First we consider the term with the one Coulomb vertex from the electron propagator in the seagull contribution (35). The contribution from the C_L contour is zero. In the C_H contour we put $E = m$, both wave functions on mass shell and set $m = 1$. Then

$$\Delta E = \frac{4\,\pi\,\alpha}{M}\,\phi(0)^2 \int \frac{d\omega}{2\,\pi\,i} \int \frac{d^3k_1}{(2\,\pi)^3} \int \frac{d^3k_2}{(2\,\pi)^3}\;\frac{1}{\omega^2 - k_1^2}\,\frac{1}{\omega^2 - k_2^2}$$

$$\frac{1}{(\mathbf{k}_1 - \mathbf{k}_2)^2}\,\frac{1}{X^2 + k_1^2}\,\frac{1}{X^2 + k_2^2}\left\{\omega^2\left(1 + \frac{(\mathbf{k}_1\mathbf{k}_2)^2}{k_1^2\,k_2^2}\right) + 2\,\mathbf{k}_1\mathbf{k}_2\right\}, \tag{40}$$

where $X = \sqrt{2\,\omega - \omega^2}$. After the k_1, k_2, ω integrals are done, the result is

$$\Delta E = \frac{m^2}{M}\,\alpha^6\,(4\,\ln(2) - 2)\,, \tag{41}$$

in agreement with [5].

The remaining terms which contribute through α^6 order are those with the free fermion propagator in eq. (35). After performing traces they are:

$$\Delta E = \frac{e^4}{M}\int\frac{d\omega}{2\,\pi\,i}\int\frac{d^3k_1}{(2\,\pi)^3}\int\frac{d^3k_2}{(2\,\pi)^3}\int\frac{d^3p}{(2\,\pi)^3}\,\phi(\mathbf{p}+\mathbf{k}_1)\,\phi(\mathbf{p}+\mathbf{k}_2)\frac{1}{X^2+p^2}\,\delta^{ki}_{1\perp}\,\delta^{kj}_{2\perp}\,T^{ij}\,, \tag{42}$$

$$T^{ij} = -(\omega + \frac{p^2}{2})\,\delta^{ij} + \frac{1}{2}(\delta^{ij}\mathbf{k}_1\mathbf{k}_2 - k_1^i k_2^j) + 2\,p^i\,p^j \tag{43}$$

$$= -\omega\,\delta^{ij} + \frac{1}{2}\,(-\delta^{ij}\,p^2 + \delta^{ij}\mathbf{k}_1\mathbf{k}_2 - k_1^i k_2^j) + 2\,p^i\,p^j\,. \tag{44}$$

We use the grouping in eq.(43) for the C_L contour and eq.(44) for the C_H contour. Before the ω–integration it is convenient to symmetrize in ω. The reason for this is the fact, that generally there are three regions of photon energy $\omega \sim \alpha^2, \omega \sim \alpha, \omega \sim 1$, that give a contribution, and this middle region is almost eliminated by the symmetrization (except for the first term in (44)). We assume in this subsection, that ϵ contains one power of α, i.e. $\epsilon = \alpha\,\epsilon'$ On the C_L contour, in the deep nonrelativistic region, all momenta have one power of α, and the photon energy is of order α^2. We can neglect ω^2 in the photon propagator. Then

$$\int_{C_L}\frac{d\omega}{2\,\pi\,i}\,\frac{1}{2}\left(\frac{1}{2\,\omega+p^2} + \frac{1}{-2\,\omega+p^2}\right) = \frac{1}{4}\,\Theta(\sqrt{2\,\epsilon} - p)\,. \tag{45}$$

The first term in eq. (43) does not give contribution on C_L contour, the third term is:

$$\Delta E = \frac{e^4}{2\,M}\langle\phi|p^j\,\frac{1}{8\,\pi\,r}\,\left(\delta^{kj}+\frac{r^k\,r^j}{r^2}\right)\,\frac{1}{8\,\pi\,r}\,\left(\delta^{ki}+\frac{r^k\,r^i}{r^2}\right)\,p^i|\phi\rangle = \frac{m^2}{M}\,\alpha^6\,. \tag{46}$$

The second term in eq. (43) is

$$\Delta E = \frac{e^4}{M}\int^{\sqrt{2\,\epsilon}}\frac{d^3p}{(2\,\pi)^3}\,\frac{d^3k_1}{(2\,\pi)^3}\,\frac{d^3k_2}{(2\,\pi)^3}\,\phi(\mathbf{p}+\mathbf{k}_1)\,\phi(\mathbf{p}+\mathbf{k}_2)\,\frac{1}{k_1^2}\,\frac{1}{k_2^2}\,\frac{\mathbf{k}_1\,\mathbf{k}_2}{4} \tag{47}$$

$$= \frac{\alpha^6}{M}\,\frac{2}{\pi}\int_0^{\sqrt{\frac{2\,\epsilon}{\alpha^2}}}dp\,\left(\frac{\arctan(p)}{p}-1\right)^2 = \frac{m^2}{M}\,\alpha^6\,\left(2\,\ln(2)-\ln\left(\frac{2\,\epsilon}{\alpha^2}\right)\right)\,. \tag{48}$$

On the C_H contour, the third term in eq. (44) does not contribute. In the evaluation of the second term in (44) we put one wave function on mass shell, and in the second wave function neglect α in the denominator. This can be done in two ways, so we have an additional factor 2,

$$\Delta E = 2\,\frac{(4\,\pi\,\alpha)^3}{M}\,\phi(0)^2\int_{C_H}\frac{d\omega}{2\,\pi\,i}\,\frac{d^3k_1}{(2\,\pi)^3}\,\frac{d^3k_2}{(2\,\pi)^3}\,\frac{1}{\omega^2-k_1^2}\,\frac{1}{\omega^2-k_2^2}$$
$$\frac{1}{k_1^2}\,\frac{1}{(\mathbf{k}_1-\mathbf{k}_2)^4}\,\frac{1}{X^2+k_2^2}\,\left(2\,k_1^2\,(\mathbf{k}_1\,\mathbf{k}_2)-k_1^2\,k_2^2-(\mathbf{k}_1\,\mathbf{k}_2)^2\right)\,. \tag{49}$$

After the k_1 and k_2 integrals are done, the expression is:

$$\Delta E = \frac{\alpha^6}{M}\,\left(-2+\frac{4}{\omega}+\frac{2}{t}-\frac{2}{\omega\,t}+\frac{2\,\log(t)}{\omega}-\frac{4\,\log(1+t)}{\omega^2}\right)\,\frac{1}{2}\,, \tag{50}$$

where $t=\sqrt{-\omega^2}/\sqrt{2\,\omega-\omega^2}$. The additional factor 1/2 at the end of eq. (50), is due to symmetrization in ω, and the fact that the term with $-\omega$ is exactly zero on the C_H contour. The ω–integration is done along the contour C'_H of Fig. 2,

$$\Delta E = \frac{\alpha^6}{M}\,\left(\frac{3}{2}+\frac{1}{2}\,\ln\left(\frac{\epsilon}{2}\right)\right)\,. \tag{51}$$

The first term in eq. (44) is again subdivided into three pieces

$$\Delta E = -\frac{e^4}{M}\int_{C_H}\frac{d\omega}{2\,\pi\,i}\,\frac{d^3p}{(2\,\pi)^3}\,\frac{d^3k_1}{(2\,\pi)^3}\,\frac{d^3k_2}{(2\,\pi)^3}\,\phi(\mathbf{p}+\mathbf{k}_1)\,\phi(\mathbf{p}+\mathbf{k}_2)\,\frac{1}{\omega^2-k_1^2}\,\frac{1}{\omega^2-k_2^2}$$
$$\cdot\left(\frac{2\,\omega}{X^2+p^2}-\frac{1}{2}\,\frac{(\mathbf{k}_1\times\mathbf{k}_2)^2}{k_1^2\,k_2^2}-\left(\frac{\omega}{X^2+p^2}-\frac{1}{2}\right)\frac{(\mathbf{k}_1\times\mathbf{k}_2)^2}{k_1^2\,k_2^2}\right)\,. \tag{52}$$

The first piece, in the above, becomes after k and p integration

$$\Delta E = -4\,\frac{\alpha^5}{M}\int_{C_H}\frac{d\omega}{2\,\pi\,i}\,\frac{\omega}{(w+\alpha)(w+\alpha+X)}\,, \tag{53}$$

where $w=\sqrt{-\omega^2}$. After symmetrizing in ω, performing integration, expanding in α and afterwards in ϵ' we found

$$\Delta E = \frac{m^2}{M}\,\left(\frac{\alpha^5}{\pi}\,2\,(1+\ln(2\,\alpha))-\alpha^6\,2\right)\,. \tag{54}$$

In the second piece of eq. (52) we first integrate with respect to p, next in k_1, k_2 and finally in ω. The result is

$$\Delta E = \frac{m^2}{M}\,\frac{\alpha^5}{\pi}\,\frac{8}{3}\,(1-\ln(2))\,. \tag{55}$$

In the third piece of eq. (52), we use the same method as in (49,50,51)

$$\Delta E = 2 \frac{(4\,\pi\,\alpha)^2}{M}\, 8\,\pi\,\alpha\,\phi(0)^2 \int_{C_H} \frac{d\omega}{2\,\pi\,i}\, \frac{d^3k_1}{(2\,\pi)^3}\, \frac{d^3k_2}{(2\,\pi)^3}$$

$$\frac{1}{\omega^2-k_1^2}\,\frac{1}{\omega^2-k_2^2}\,\frac{1}{(\mathbf{k}_1-\mathbf{k}_2)^4}\,\left(\frac{\omega}{X^2+k_2^2}-\frac{1}{2}\right)\frac{(\mathbf{k}_1\times\mathbf{k}_2)^2}{k_1^2\,k_2^2} \tag{56}$$

$$= \frac{m^2}{M}\frac{\alpha^6}{2}\left(1+\ln\left(\frac{\epsilon}{2}\right)\right)\,, \tag{57}$$

where implicitly symmetrization in ω is assumed in the above expression.

At this point the evaluation of seagull contributions is complete. The result for E_S is the sum of (41,46,48,51,54,55,57)

$$E_S = \frac{m^2}{M}\left\{\frac{\alpha^5}{\pi}\left[\frac{14}{3}-\frac{2}{3}\ln(2)+2\,\ln(\alpha)\right]+\alpha^6\,[-1+4\,\ln(2)+2\,\ln(\alpha)]\right\}\,. \tag{58}$$

Some explanation of the difference between the α^6 term of (58) and the corresponding term of Ref. [5] is needed. Since (58) is for the $1S$ state, while Ref. [5] does the $2S$ state, we expect some state dependence beyond the usual $1/n^3$ term. Eq.(4.24) of Ref. [5] is the correct seagull expression if one is working to order α^5 (see (4.27) of Ref. [2] RMP) but it is incorrect as a starting point for the α^6 terms since it was derived by setting the lower components of the wave function to zero.

C. the single transverse contribution

The single transverse contribution E_T' (34) is subdivided into three part:

$$E_T' = B_L + B_I + B_H\,, \tag{59}$$

$$B_L = -\frac{e^2}{M}\int_{C_L}\frac{d\omega}{2\,\pi\,i}\,\frac{1}{\omega-i\,\epsilon}\int\frac{d^3k}{(2\,\pi)^3}\,\frac{\delta_\perp^{ij}}{\omega^2-k^2}\langle\bar\phi|\gamma^i\,S_F(E-\omega)\,\gamma^0\,[p^i,V]|\phi\rangle + c.c. \tag{60}$$

$$B_I = -\frac{e^2}{M}\int_{C_L}\frac{d\omega}{2\,\pi\,i}\,\frac{1}{\omega-i\,\epsilon}\int\frac{d^3k}{(2\,\pi)^3}\,\frac{\delta_\perp^{ij}}{\omega^2-k^2}\langle\bar\phi|\gamma^i\,(e^{i\,k\,r}-1)\,S_F(E-\omega)\,\gamma^0\,[p^i,V]|\phi\rangle + c.c. \tag{61}$$

$$B_H = -\frac{e^2}{M}\int_{C_H}\frac{d\omega}{2\,\pi\,i}\,\frac{1}{\omega-i\,\epsilon}\int\frac{d^3k}{(2\,\pi)^3}\,\frac{\delta_\perp^{ij}}{\omega^2-k^2}\langle\bar\phi|\gamma^i\,e^{i\,k\,r}\,S_F(E-\omega)\,\gamma^0\,[p^i,V]|\phi\rangle + c.c. \tag{62}$$

where B_L is a low $\omega\sim\alpha^2$, B_I is an intermediate $\omega\sim\alpha$, and B_H is a high $\omega\sim 1$ energy contribution.

Since at the end we expand in ϵ, we can rewrite B_L using the identity (32)

$$B_L = \frac{e^2}{M}\int^\epsilon\frac{d^3k}{(2\,\pi)^3}\,\delta_\perp^{ij}\,\frac{1}{2\,k}\,\langle\phi|\gamma^i\,S_F(E-k)\,\gamma^0\,p^i|\phi\rangle + c.c.\,, \tag{63}$$

and apply a nonrelativistic approximation:

$$B_L = \frac{4}{3}\,\frac{e^2}{M}\int^\epsilon\frac{d^3k}{(2\,\pi)^3}\,\frac{1}{2\,k}\,\langle\phi|\mathbf{p}\,\frac{1}{E-k-H}\,\mathbf{p}|\phi\rangle\,. \tag{64}$$

This integral could be expressed in terms of Bethe logarithms $\ln(k_0)$, and was calculated in [8], eqs. (6.15, 6.17, 6.19),

$$B_L = \frac{m^2}{M}\,\frac{\alpha^5}{\pi}\left(\frac{8}{3}\,\ln(\frac{2\,\epsilon}{\alpha^2})+\frac{64}{3}\sqrt{\frac{\alpha^2}{2\,\epsilon}}-\frac{8}{3}\,\ln(k_0)\right)\,. \tag{65}$$

The intermediate energy part B_I is

$$B_I = 2\frac{e^2}{M}\int^\epsilon\frac{d^3k}{(2\,\pi)^3}\,\delta_\perp^{ij}\,\frac{1}{2\,k^2}\,\langle\bar\phi|\gamma^j\,(e^{i\,k\,r}-1)\,S_F(E-k)\,\gamma^0\,[p^i,V]|\phi\rangle\,. \tag{66}$$

Because of the presence $e^{i\,k\,r}-1$ we can expand in kinetic, potential, and binding energy without creating a divergence,

$$B_I = 2\frac{e^2}{M}\int^{\epsilon}\frac{d^3k}{(2\,\pi)^3}\,\delta_{\perp}^{ij}\,\frac{1}{2\,k^2}$$
$$\langle\phi|p^j\,(e^{i\,k\,r}-1)\,\left[\frac{1}{k^2}\left(\frac{p^2}{2}+V-E\right)-\left(\frac{1}{k}+\frac{1}{2}\right)\right]\,[p^i,V]|\phi\rangle\,. \tag{67}$$

After integration with respect to angles, r, and finally in k, B_I is

$$B_I = \frac{m^2}{M}\,\left(\frac{\alpha^5}{\pi}\,\left(\frac{32}{9}-\frac{8}{3}\,\ln\!\left(\frac{\epsilon}{2\,\alpha}\right)\right)+\alpha^6\,\left(-2-\frac{4}{\epsilon}+2\,\ln\!\left(\frac{\epsilon}{2\,\alpha}\right)\right)\right)\,. \tag{68}$$

The high energy part B_H is calculated in the same way as it was previously in (49–51). B_{H1} is calculated by neglecting V in the fermion propagator, and next by putting one wave function on mass shell, and neglecting α in the denominator of the second $\phi(p)$. The result is

$$B_{H1} = \frac{m^2}{M}\,\alpha^6\,\left(-\frac{32}{3}\sqrt{\frac{2}{\epsilon}}+\frac{4}{\epsilon}+2\,\ln\!\left(\frac{2}{\epsilon}\right)\right)\,. \tag{69}$$

B_{H2} is a single Coulomb correction from the fermion propagator. Here we put both wave functions on mass shell, perform all integrals to obtain:

$$B_{H2} = -\frac{m^2}{M}\,\alpha^6\,\frac{3}{2}\,. \tag{70}$$

The complete single transverse contribution E_T' is the sum of (65,68,69,70)

$$E_T' = \frac{m^2}{M}\left\{\alpha^6\,\left[-\frac{7}{2}-2\,\ln(\alpha)\right]+\right.$$
$$\left.\frac{\alpha^5}{\pi}\,\left[\frac{32}{9}+\frac{16}{3}\,\ln(2)-\frac{8}{3}\,\ln(\alpha)-\frac{8}{3}\,\ln(k_0)\right]\right\}\,. \tag{71}$$

This differs from the result presented in [5]. A recalculation of eq. (4.20) of that paper reveals an additional contribution beyond (4.21) which cannot be accounted for by the high momentum approximation. When this is added, the factor 9/4 of (4.22) in [5] is replaced by 6/4.

The total recoil correction ΔE is

$$\Delta E = E_C' + E_T' + E_S$$
$$= \frac{m^2}{M}\left\{\frac{\alpha^5}{\pi}\left[\frac{62}{9}+\frac{14}{3}\,\ln(2)-\frac{2}{3}\,\ln(\alpha)-\frac{8}{3}\,\ln(k_0)\right]+\alpha^6\left[-\frac{7}{2}+4\,\ln(2)\right]\right\}\,. \tag{72}$$

This result is valid for the 1S state. The state dependent corrections of α^6 order are connected with small photon energy, namely (46,47) and (67). Considering the difference $\Delta E(1S) - n^3\,E(nS)$, where we can expand the fermion propagator in kinetic and potential energy, (the divergent terms cancel out in this combination), we find that this difference is exactly zero. Thus the corresponding S state correction for arbitrary n is known. The α^6 correction corresponding to the one given in (72) is expected to be neglible for 2P state.

V. CONCLUSIONS

We have calculated higher order pure recoil corrections to hydrogenic energy levels. The correction in α^5 order eq. (72) agrees with the general result (4) for arbitrary masses, and in α^6 order is

$$\Delta E(nS) = \frac{m^2}{M}\,\frac{(Z\,\alpha)^6}{n^3}\,\left(4\,\ln(2)-\frac{7}{2}\right)\,, \tag{73}$$

which is different from the previous result of [5]. The correction of eq. (73) gives -7.4 kHz for the 1S state and -1 kHz for 2S state, (compared to the previous -3 kHz for 2S). Let us now consider the current situation for the Lamb shift taking (73) into account. Recently all the six sets of gauge invariant diagrams have been evaluated for the two-loop binding corrections to the Lamb shift. Five of these sets have independently been calculated by two groups

[9], [10] and these produce 4.7 kHz for the $n = 2$ Lamb shift. The last or sixth set has been completed in [11] with a large contribution of $-41(1)$ kHz. Taking these into account and adding the higher order correction to the one–loop electron self–energy, that has been obtained by extrapolation of P. Mohr's data [12] we obtain for the Lamb shift with the newer proton radius $r_p = 0.862(12)$ [13]

$$E_L(2S_{1/2} - 2P_{1/2}) = 1\,057\,838(6)\,\mathrm{kHz}\,, \tag{74}$$

$$E_L(4S - 2S) - \frac{1}{4}\,E_L(2S - 1S) = 868621(5)\,\mathrm{kHz}\,. \tag{75}$$

The older proton radius $r_p = 0.805(11)$ [14] will give a result which is 18 kHz smaller for the $n = 2$ Lamb shift of Eq. (74) and 16 kHz smaller for Eq. (75).

Comparing this with the experimental results:

$$E_L(2S_{1/2} - 2P_{1/2}) = 1\,057\,845(9)\,\mathrm{kHz}\;[15]\,, \tag{76}$$

$$E_L(2S_{1/2} - 2P_{1/2}) = 1\,057\,851(2)\,\mathrm{kHz}\;[16]\,, \tag{77}$$

$$E_L(2S_{1/2} - 2P_{1/2}) = 1\,057\,839(12)\,\mathrm{kHz}\;[17]\,, \tag{78}$$

$$E_L(4S - 2S) - \frac{1}{4}\,E_L(2S - 1S) = 868630(12)\,\mathrm{kHz}\;[18]\,. \tag{79}$$

we find satisfactory agreement with the experiments of [15], [17], and [18] if the larger proton radius is used, although it should be pointed out that it is necessary to confirm by an independent group the result for the binding two–loop correction [11], because it is unexpectedly large. If we include the $(\frac{\alpha}{\pi})^2\,(Z\,\alpha)^6\,\ln^3(Z\,\alpha)$ correction of Ref. [19], which was estimated to be -3.6 kHz for 2S state, the agreement will be less satisfactory. We prefer not include this correction, until the remaining corrections of that order have also been determined.

From the very precise measurement of the hydrogen-deuterium isotope shift [20] performed by the Hänsch group in Garching.

$$E_D(2S - 1S) - E_H(2S - 1S) = 670\,994\,337(22)\,\mathrm{kHz} \tag{80}$$

we can determine the deuteron charge radius. The theoretical value for this isotope shift [21], with the recently calculated nuclear polarizability correction [22] but without the nuclear size correction, is

$$[E_D(2S - 1S) - E_H(2S - 1S)]' = 670999549(14)\,, \tag{81}$$

where the error comes from the electron–proton mass ratio.

We take this opportunity to correct a previous paper of one of us (K.P.) [21]. The first correction is due to the terms calculated in the present paper while the second is due to the fact that the deuteron has spin 1 rather than spin 1/2. For a spin 1 particle the zitterbewegung term is not present [23] and this means that we should subtract from formula (3) above, which is valid for an electron interacting with a spin 1/2 nucleus, the expression

$$\Delta E = \frac{\mu^3\,\alpha^4}{2\,M^2\,n^3}\,\delta_{l0}\,, \tag{82}$$

where M is the deuteron mass. It changes the isotope shift by 11 kHz.

Using the expression for the nuclear size correction

$$\Delta E = \frac{2}{3\,n^3}\,\alpha^4\,\mu^3\langle r^2\rangle\,, \tag{83}$$

we find for the difference in the square of the charge radii of the deuteron and proton

$$r_{ch}^2 - r_p^2 = 3.805(19)\mathrm{fm}^2\,, \tag{84}$$

which gives for the deuteron charge radius (with $r_p = 0.862(12)$ fm)

$$r_{ch} = 2.133(6)\mathrm{fm}\,. \tag{85}$$

These results are in disagreement with the charge radius difference obtained from electron scattering experiments, (see [24] and references therein)

$$r_{ch}^2 - r_p^2 = 3.728(12)\mathrm{fm}^2\,, \tag{86}$$

but is in agreement with the radius obtained on the basis of nucleon–nucleon scattering data [25] (deuteron matter radius plus the Darwin term),

$$r_{ch}^2 - r_p^2 = 3.787(4)\mathrm{fm}^2\,. \tag{87}$$

This means that the interpretation of low energy electron–deuteron scattering data may require an additional analysis to obtain the correct charge radius.

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