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Higher order recoil corrections to energy levels of two–body systems

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Abstract

We have calculated a correction of order $m\,\alpha^7\,\ln^2\alpha$ to energy levels of the general two–body system of spin 1/2 particles with arbitrary masses. The result allows for the improved theoretical predictions of the $1S-2S$ and $2S-2P$ intervals in positronium. Further implications to the hydrogen–deuterium $1S-2S$ isotope shift are discussed also.

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I. INTRODUCTION

The study of recoil corrections in hydrogenic systems has a long history. In the nonrelativistic limit both masses m_1 and m_2 of a two–body system could be replaced by the single reduced mass $\mu = m_1 m_2/(m_1 + m_2)$. The treatment of relativistic effects is much more complicated. It would be incorrect the use of the Dirac equation with a reduced mass. In general recoil corrections could be described by the Bethe–Salpeter equation [1] or some other two–body effective equation (see e.g. [2]). which is usually obtained by the elimination of the relative time. Several corrections have been calculated in this approach. However, with the increasing order of α, the application of the BS equation increases in the complexity. In spite of these problems, it was possible to calculate many higher order corrections, for example, $m\,\alpha^6$ contributions to positronium hyperfine structure (HFS) [3]. In parallel, effective theories have been developed, to take advantage of a natural cancellation between various terms in the perturbation theory. Let us mention the NRQED (nonrelativistic quantum electrodynamics) introduced by Caswell and Lepage [4], which has inspired further developments like the effective Hamiltonian approach [5]. Using these methods, recoil corrections to order α^6 have been calculated for hydrogen, muonium and very recently [6–8] for the positronium atom. Recoil effects are especially dominant in positronium energy levels because of the absence of a heavy nucleus. On the other side, positronium has been intensively investigated experimentally. Several transition frequencies: for the ground state hyperfine splitting [9], for the $1s - 2s$ triplet interval [10] and for the fine structure ($n = 2$) [11] have been measured with a high precision. In this paper we calculate the complete double logarithmic correction in the next order i.e. $m\,\alpha^7 \ln^2 \alpha$, which we think, is the leading correction beyond the known terms. The annihilation term together with other spin dependent terms have already been derived few years ago in [12]. Very recently, a complete result has also been obtained by Melnikov and Yelkhovsky [13], and both results: our and this in [13] are in an agreement. This calculation significantly reduces uncertainty of theoretical predictions of the positronium Lamb shift and of the hydrogen–deuterium isotope shift.

II. THE METHOD OF THE CALCULATION OF $\ln^2 \alpha$ TERM

We apply a time ordered perturbation technique and calculate diagrams presented in Fig. 1. Since the Coulomb gauge is used, the exchange of Coulomb and transverse photons is considered separately. We have checked and verified that no further diagrams contribute to $\ln^2 \alpha$, except for the annihilation term. However, this term could be incorporated as an additional point–like interaction in the Breit Hamiltonian [14]. Since we are concentrated on $\ln^2 \alpha$ term only, the calculation is relative simple. One assumes that all momenta are of order $m\,\alpha$, and identifies logarithmic terms as ultraviolet or infrared divergences in the corresponding integrals. The actual regularizations of these divergences are not relevant, since they lead to the same $\ln^2 \alpha$ term, so we will often not write these regularizations explicitly. In the momentum space, the double logarithmic term $\ln^2 \alpha$ comes from the integration over two momenta. It is very convenient in the calculation to regularize separately these momenta by some cut–offs. So, one has

$$\int_{\epsilon\alpha}^{\delta\alpha} dk \int_0^{\lambda\alpha} dq\; f(k, q)\,, \tag{1}$$

where f is some function that comes from the matrix elements, which for example could be of the form $f = q/(k\,(q^2+\alpha^2))$. The parameter ϵ is assumed to be small. Parameters δ, λ are assumed to be large or infinitely large with the assumption that first the limit in λ and next in δ is performed. It is an assumption which is verified during the calculation that the lower cut-off is necessary only for one momentum, which we denote here by k. After all integrations on gets from self energy diagrams the logarithmic term of the form $\ln(\delta/\epsilon)\ln\lambda$ which is to be replaced by $\ln^2\alpha$. For exchange diagrams one gets $\ln(\mu/\epsilon)\ln\lambda$ which is replaced by $1/2\ln^2\alpha$. Additionally, for the so called self–energy seagull diagram we get $\ln^2\delta$, and it is replaced by $\ln^2\alpha$. It is an assumption of our calculations that no $\ln\delta\ln\lambda$ terms appear for the exchange diagrams. We have verified it for some diagrams, but were not able to prove it for the general case.

III. CONTRIBUTIONS TO $\ln^2\alpha$

In the following we neglect the spin dependent terms. These terms, contributing to hyperfine structure, have already been obtained in [12] and confirmed in [13]. They also may contribute to energy levels, but due to various internal cancellations, do not give $\ln^2\alpha$. In the framework of nonrelativistic QED one derives the following expressions for the energy shift of two–body system due to the self–energy ($\hbar = c = 1$)

$$E^S = e^2\int^{\delta\,\alpha}\frac{d^3k}{(2\,\pi)^3\,2\,k}\left(\delta^{ij}-\frac{k^i\,k^j}{k^2}\right)\langle\phi|e^{i\,\boldsymbol{k}\cdot\boldsymbol{r}_1}\,\frac{p_1^i}{m_1}\,\frac{1}{E-H-k}\,e^{-i\,\boldsymbol{k}\cdot\boldsymbol{r}_1}\,\frac{p_1^j}{m_1}|\phi\rangle+(1\to 2)\,, \quad (2)$$

and due to the exchange of transverse photon

$$E^E = -e^2\int\frac{d^3k}{(2\,\pi)^3\,2\,k}\left(\delta^{ij}-\frac{k^i\,k^j}{k^2}\right)\langle\phi|e^{i\,\boldsymbol{k}\cdot\boldsymbol{r}_1}\,\frac{p_1^i}{m_1}\,\frac{1}{E-H-k}\,e^{-i\,\boldsymbol{k}\cdot\boldsymbol{r}_2}\,\frac{p_2^j}{m_2}|\phi\rangle+(1\leftrightarrow 2)\,. \quad (3)$$

In the following we consider all contributions to energy levels in the order $m\,\alpha^7\,\ln^2\alpha$ that come from this expression and various relativistic corrections. We denote here and below by E^S the contribution from the self–energy diagram and by E^E a corresponding contribution coming from the exchange diagram.

A. retardation in the nonrelativistic self–energy and photon–exchange

The retardation contribution E^S_q is obtained from the fourth term in the following expansion of the resolvent

$$\frac{1}{E-H-k} = -\frac{1}{k}+\frac{H-E}{k^2}-\frac{(H-E)^2}{k^3}+\frac{(H-E)^3}{k^4}+\ldots\,, \quad (4)$$

The previous terms contribute at lower order in α. After this expansion the matrix elements become divergent. We can regularize Coulomb potential by

$$\frac{\alpha}{r}\to\frac{\alpha}{r}(1-e^{-\alpha\,\lambda\,r})\,, \quad (5)$$

to prevent these singularities. The retardation contribution then takes a form

$$E_q^S = e^2 \int_{\epsilon\,\alpha}^{\delta\alpha} \frac{d^3k}{(2\,\pi)^3\,2\,k} \left(\delta^{ij} - \frac{k^i\,k^j}{k^2}\right) \langle\phi|e^{i\,\boldsymbol{k}\cdot\boldsymbol{r}_1}\,\frac{p_1^i}{m_1}\,\frac{(H-E)^3}{k^4}\,e^{-i\,\boldsymbol{k}\cdot\boldsymbol{r}_1}\,\frac{p_1^j}{m_1}|\phi\rangle + (1\to 2)\,. \tag{6}$$

One can use the equation

$$e^{i\,\boldsymbol{k}\cdot\boldsymbol{r}_1}\,(H-E)e^{-i\,\boldsymbol{k}\cdot\boldsymbol{r}_1} = H - E + \frac{k^2}{2\,m_1} - \frac{\boldsymbol{p}_1\cdot\boldsymbol{k}}{m_1}\,, \tag{7}$$

to select in the numerator the terms proportional to the second power of k, since only these terms give $\ln(\delta/\epsilon)$.

$$\begin{aligned} E_q^S = {} & \frac{e^2}{m_1^2} \int_{\epsilon\,\alpha}^{\delta\alpha} \frac{d^3k}{(2\,\pi)^3\,2\,k^5} \left(\delta^{ij} - \frac{k^i\,k^j}{k^2}\right) \langle\phi|p^i \left[\frac{3\,k^2}{2\,m_1}\,(H-E)^2\right. \\ & + \left(\frac{\boldsymbol{p}\cdot\boldsymbol{k}}{m_1}\right)^2 (H-E) + \frac{\boldsymbol{p}\cdot\boldsymbol{k}}{m_1}\,(H-E)\,\frac{\boldsymbol{p}\cdot\boldsymbol{k}}{m_1} + (H-E)\left.\left(\frac{\boldsymbol{p}\cdot\boldsymbol{k}}{m_1}\right)^2\right] p^j|\phi\rangle + (1\to 2)\,. \end{aligned} \tag{8}$$

By commuting $H-E$ on right and on left one expresses all matrix elements by one term which logarithmic part is as follows:

$$\left\langle\frac{1}{(\mu\,\alpha\,r)^4}\right\rangle_\lambda \to -8\,\ln\lambda\,, \tag{9}$$

where $\boldsymbol{r} = \boldsymbol{r}_1 - \boldsymbol{r}_2$, $r = |\boldsymbol{r}|$ and μ is a reduced mass. After using the replacement $\ln(\delta/\epsilon)\,\ln\lambda \to \ln^2\alpha$ one obtains

$$E_q^S = \left(-\frac{32}{3}\,\mu + \frac{104}{3}\,\frac{\mu^3}{m_1\,m_2} - \frac{16}{3}\,\frac{\mu^5}{m_1^2\,m_2^2}\right)\frac{\alpha^7}{\pi}\,\ln^2\alpha\,. \tag{10}$$

The calculation of retardation in the photon exchange diagrams, proceeds in the similar way. One starts from the nonrelativistic formula for the energy shift due to the exchange of the transverse photon in (3), expand the resolvent to the third power of $H-E$ and obtain the following expression for the retardation contribution

$$\begin{aligned} E_q^E = {} & -\frac{e^2}{m_1\,m_2} \int_{\epsilon\,\alpha} \frac{d^3k}{(2\,\pi)^3\,2\,k^5} \left(\delta^{ij} - \frac{k^i\,k^j}{k^2}\right) \langle\phi|p_1^i\,e^{i\,\boldsymbol{k}\cdot\boldsymbol{r}_1}\,(H-E)^3 e^{-i\,\boldsymbol{k}\cdot\boldsymbol{r}_2}\,p_2^j|\phi\rangle \\ & + (1\leftrightarrow 2)\,. \end{aligned} \tag{11}$$

It is transformed to the more suitable form, using

$$e^{i\,\boldsymbol{k}\cdot\boldsymbol{r}_1}\,(H-E)^3\,e^{-i\,\boldsymbol{k}\cdot\boldsymbol{r}_2} = e^{i\,\boldsymbol{k}\cdot\boldsymbol{r}/2}\left[H - E + \frac{k^2}{8\,\mu} - \frac{\boldsymbol{p}\cdot\boldsymbol{k}}{2}\left(\frac{1}{m_1} - \frac{1}{m_2}\right)\right]^3 e^{i\,\boldsymbol{k}\cdot\boldsymbol{r}/2}\,. \tag{12}$$

Since we expect and search only for terms that contain $\ln\epsilon$, we select in the numerator only these, containing the second power of k. Other terms do not give $\ln\epsilon$ and therefore

$$\begin{aligned} E_q^E = {} & \frac{2\,e^2}{m_1\,m_2} \int_{\epsilon\,\alpha}^{\mu\alpha} \frac{d^3k}{(2\,\pi)^3\,2\,k^5} \left(\delta^{ij} - \frac{k^i\,k^j}{k^2}\right) \langle\phi|p^i\,e^{i\,\boldsymbol{k}\cdot\boldsymbol{r}/2}\left\{(H-E)^3 + \frac{3\,k^2}{8\,\mu}\,(H-E)^2\right. \\ & + \frac{1}{4}\left(\frac{1}{m_1} - \frac{1}{m_2}\right)^2 \left.\left[\boldsymbol{p}\cdot\boldsymbol{k}^2\,(H-E) + \boldsymbol{p}\cdot\boldsymbol{k}\,(H-E)\,\boldsymbol{p}\cdot\boldsymbol{k} + (H-E)\,\boldsymbol{p}\cdot\boldsymbol{k}^2\right]\right\} e^{i\,\boldsymbol{k}\cdot\boldsymbol{r}/2}\,p^j|\phi\rangle\,. \end{aligned} \tag{13}$$

For the same reasons we changed the upper cut-off in k, since it does not affect the logarithmic singularity in ϵ. All the matrix elements, except for the first one are calculated in the same way as in the case of the self-energy diagram. It is because we can neglect $e^{i\,\boldsymbol{k}\cdot\boldsymbol{r}/2}$ factors. The first term in braces in Eq. (13) is calculated as follows. One returns with the expansion to the complete resolvent with the nonregularized Coulomb potential

$$\Delta E_q^E = \frac{2\,e^2}{m_1\,m_2}\int\frac{d^3k}{(2\,\pi)^3\,2\,k}\left(\delta^{ij}-\frac{k^i\,k^j}{k^2}\right)\left\langle e^{i\,\boldsymbol{k}\cdot\boldsymbol{r}/2}\,p^i\frac{1}{E-H+k}\,p^j\,e^{i\,\boldsymbol{k}\cdot\boldsymbol{r}/2}\right\rangle\,. \tag{14}$$

This matrix element is calculated using the Gavrila-Costescu formula from [15]. The corresponding logarithmic part is:

$$\langle ...\rangle \approx -\frac{2}{5}\,\frac{\alpha^6}{k^2}\,\ln\left(\frac{(\mu\,\alpha)^2+k^2/4}{k}\right)\,\delta^{ij}\,. \tag{15}$$

The integration over k from $\mu\,\alpha^2$ to μ gives

$$\Delta E_q^E = \frac{8}{5}\,\frac{\mu^3}{m_1\,m_2}\,\frac{\alpha^7}{\pi}\,\ln^2\alpha\,. \tag{16}$$

After summing all terms one derives the following expression for the retardation in the transverse photon exchange diagram:

$$E_q^E = \left(-\frac{16}{15}\,\frac{\mu^3}{m_1\,m_2}+\frac{8}{3}\,\frac{\mu^5}{m_1^2\,m_2^2}\right)\,\frac{\alpha^7}{\pi}\,\ln^2\alpha\,. \tag{17}$$

B. correction to the current

For the further derivations we transform the initial expression to the more convenient form. The self–energy contribution could be now calculated in the dipole approximation:

$$E^S = e^2\int\frac{d^3k}{(2\,\pi)^3\,2\,k}\left(\delta^{ij}-\frac{k^i\,k^j}{k^2}\right)\,\langle\phi|\jmath_1^i\,\frac{1}{E-H-k}\,\jmath_1^j|\phi\rangle+(1\rightarrow 2)\,, \tag{18}$$

where $\jmath$, ϕ and H contain relativistic corrections, which are described later on. The $m\,\alpha^7\,\ln^2\alpha$ term is obtained from the second term in the expansion (4). With the proper integration limits E^S becomes

$$E^S = e^2\int_{\epsilon\,\alpha}^{\delta\,\alpha}\frac{d^3k}{(2\,\pi)^3\,2\,k^3}\left(\delta^{ij}-\frac{k^i\,k^j}{k^2}\right)\,\langle\phi|\jmath_1^i\,(H-E)\,\jmath_1^j|\phi\rangle+(1\rightarrow 2) \tag{19}$$

$$= \frac{\alpha}{3\,\pi}\,\ln\!\left(\frac{\delta}{\epsilon}\right)\langle\phi|[\boldsymbol{\jmath}_1\,;\,[H-E\,;\,\boldsymbol{\jmath}_1]]|\phi\rangle+(1\rightarrow 2)\,. \tag{20}$$

The analogous derivation for the exchange of single transverse photon leads to:

$$E^E = -e^2\int_{\epsilon\,\alpha}^{\mu\,\alpha}\frac{d^3k}{(2\,\pi)^3\,2\,k^3}\left(\delta^{ij}-\frac{k^i\,k^j}{k^2}\right)\,\langle\phi|\jmath_1^i\,(H-E)\,\jmath_2^j|\phi\rangle+(1\leftrightarrow 2) \tag{21}$$

$$= -\frac{\alpha}{3\,\pi}\,\ln\!\left(\frac{\mu}{\epsilon}\right)\langle\phi|[\boldsymbol{\jmath}_1\,;\,[H-E\,;\,\boldsymbol{\jmath}_2]]|\phi\rangle+(1\leftrightarrow 2)\,. \tag{22}$$

One can consider now, all relativistic corrections, separately. By the correction to the current we mean

$$\boldsymbol{j} = \frac{\boldsymbol{p}}{m} + \delta\boldsymbol{j}\,, \tag{23}$$

$$\delta\boldsymbol{j} = -\frac{p^2}{2\,m^3}\,\boldsymbol{p}\,. \tag{24}$$

It is obtained by expansion in p/m of the expression $\bar{u}(p)\boldsymbol{\gamma}\,u(p)$. The corresponding correction to electron self–energy is

$$E^S_j = -\frac{2\,\alpha}{3\,\pi}\,\ln\!\left(\frac{\delta}{\epsilon}\right)\langle\phi|\left[-\frac{p_1^2}{2\,m_1^3}\,\boldsymbol{p}_1\,;\,\left[H-E\,;\,\frac{\boldsymbol{p}_1}{m_1}\right]\right]|\phi\rangle + (1\to 2)\,. \tag{25}$$

The commutators in matrix element could be performed with the result:

$$\langle\phi|\ldots|\phi\rangle = \alpha^6\,\frac{\mu^5}{m_1^4}\,\langle\phi|\frac{1}{(\mu\,\alpha\,r)^4}|\phi\rangle\,, \tag{26}$$

and E_j becomes

$$E^S_j = \frac{16}{3}\left(\frac{\mu^5}{m_1^4} + \frac{\mu^5}{m_2^4}\right)\frac{\alpha^7}{\pi}\,\ln^2\alpha\,. \tag{27}$$

The calculation of contribution coming from the exchange of the transverse photon is analogous and leads to the result:

$$E^E_j = \frac{8}{3}\,\frac{\mu^5}{m_1\,m_2}\left(\frac{1}{m_1^2} + \frac{1}{m_2^2}\right)\frac{\alpha^7}{\pi}\,\ln^2\alpha\,. \tag{28}$$

C. correction to the Hamiltonian

The correction to Hamiltonian in the self–energy diagram gives a contribution of the form:

$$E^S_H = \frac{\alpha}{3\,\pi}\,\ln\!\left(\frac{\delta}{\epsilon}\right)\langle\phi|\left[\frac{\boldsymbol{p}_1}{m_1}\,;\,\left[\delta H\,;\,\frac{\boldsymbol{p}_1}{m_1}\right]\right]|\phi\rangle + (1\to 2)\,, \tag{29}$$

and in the photon exchange diagram it is

$$E^E_H = -\frac{\alpha}{3\,\pi}\,\ln\!\left(\frac{\mu}{\epsilon}\right)\langle\phi|\left[\frac{\boldsymbol{p}_1}{m_1}\,;\,\left[\delta H\,;\,\frac{\boldsymbol{p}_2}{m_2}\right]\right]|\phi\rangle + (1\leftrightarrow 2)\,. \tag{30}$$

Only few terms survive the commutators but only one gives the double log,

$$\delta H = \frac{\alpha}{2\,m_1\,m_2}\,p_1^i\left(\frac{\delta^{ij}}{r} + \frac{r^i\,r^j}{r^3}\right)p_2^j\,. \tag{31}$$

When inserted in the expression for E^S_H it becomes

$$E_H^S = \frac{\alpha}{3\,\pi}\,\ln\!\left(\frac{\delta}{\epsilon}\right)\,\frac{\alpha}{m_1^3\,m_2}\,\langle\phi|p_1^i\,\left[p_1^k\,;\,\left[\frac{1}{2\,r}\,\left(\delta^{ij}+\frac{r^i\,r^j}{r^2}\right)\,;\,p_1^k\right]\right]\,p_2^j|\phi\rangle + (1\leftrightarrow 2)\,. \tag{32}$$

The matrix element could be transformed to the form

$$\begin{aligned}\langle\phi|\ldots|\phi\rangle \;&=\; \langle\phi|p^i\,4\,\pi\,\delta_\perp^{ij}(r)\,p^j\,|\phi\rangle = (\mu\,\alpha)^2\,\langle\phi|\frac{r^i}{r}\,4\,\pi\,\delta_\perp^{ij}(r)\,\frac{r^j}{r}|\phi\rangle \\ &\to (\mu\,\alpha)^2\,\langle\phi|\frac{2}{r^3}|\phi\rangle \to 8\,\ln\lambda\,,\end{aligned} \tag{33}$$

where

$$\delta_\perp^{ij}(r) = \int\frac{d^3k}{(2\,\pi)^3}\,\left(\delta^{ij}-\frac{k^i\,k^j}{k^2}\right)\,e^{i\boldsymbol{k}\cdot\boldsymbol{r}} = \frac{2}{3}\,\delta^{ij}\,\delta^3(r) - \frac{1}{4\,\pi\,r^3}\,\left(\delta^{ij}-3\,\frac{r^i\,r^j}{r^2}\right)\,. \tag{34}$$

The correction from δH in the self–energy diagram is

$$E_H^S = \frac{8}{3}\,\left(\frac{\mu^5}{m_1^3\,m_2}+\frac{\mu^5}{m_2^3\,m_1}\right)\,\frac{\alpha^7}{\pi}\,\ln\!\left(\frac{\delta}{\epsilon}\right)\,\ln\lambda \to \frac{8}{3}\,\frac{\mu^5}{m_1\,m_2}\,\left(\frac{1}{m_1^2}+\frac{1}{m_2^2}\right)\,\frac{\alpha^7}{\pi}\,\ln^2\alpha\,. \tag{35}$$

The analogous calculation for the photon exchange diagram leads to

$$E_H^E = \frac{16}{3}\,\frac{\mu^5}{m_1^2\,m_2^2}\,\frac{\alpha^7}{\pi}\,\ln\!\left(\frac{\mu}{\epsilon}\right)\,\ln\lambda \to \frac{8}{3}\,\frac{\mu^5}{m_1^2\,m_2^2}\,\frac{\alpha^7}{\pi}\,\ln^2\alpha\,. \tag{36}$$

D. correction to the wave function

Correction to the wave function in the self–energy diagram gives:

$$\begin{aligned}E_\phi^S &= \frac{2\,\alpha}{3\,\pi}\,\ln\!\left(\frac{\delta}{\epsilon}\right)\,\langle\phi|\delta H\,\frac{1}{(E-H)'}\,\left[\frac{\boldsymbol{p}_1}{m_1}\,;\,\left[-\frac{\alpha}{r}\,;\,\frac{\boldsymbol{p}_1}{m_1}\right]\right]\,|\phi\rangle + (1\to 2) &(37)\\ &= \frac{2\,\alpha}{3\,\pi}\,\ln\!\left(\frac{\delta}{\epsilon}\right)\,\left(\frac{1}{m_1^2}+\frac{1}{m_2^2}\right)\,\langle\phi|\delta H\,\frac{1}{(E-H)'}\,4\,\pi\,\delta^3(r)|\phi\rangle\,, &(38)\end{aligned}$$

where $1/(H-E)'$ is a reduced Coulomb Green function and δH here is the spin independent part of the Breit Hamiltonian:

$$\delta H = -\frac{p^4}{8\,m_1^3}-\frac{p^4}{8\,m_2^3}+\frac{\pi\,\alpha}{2}\,\left(\frac{1}{m_1^2}+\frac{1}{m_2^2}\right)\,\delta^3(r) - \frac{\alpha}{2\,m_1\,m_2}\,p^i\,\left(\frac{\delta^{ij}}{r}+\frac{r^i\,r^j}{r^3}\right)\,p^j\,. \tag{39}$$

The logarithmic correction in these matrix elements has already been calculated in the context of positronium hyperfine structure in [5]

$$\begin{aligned}\langle\phi|\delta H\,\frac{1}{(E-H)'}\,4\,\pi\,\delta^3(r)|\phi\rangle &= 8\,\mu^5\,\alpha^6\,\ln\lambda\,\left[\frac{\mu}{2}\,\left(\frac{1}{m_1^3}+\frac{1}{m_2^3}\right)-\frac{1}{4}\,\left(\frac{1}{m_1^2}+\frac{1}{m_2^2}\right)+\frac{1}{m_1\,m_2}\right]\\ &= 2\,\mu^3\,\alpha^6\,\ln\lambda\,.\end{aligned} \tag{40}$$

The contribution from the correction to wave function becomes

$$E_\phi^S = \left(\frac{4}{3}\,\mu - \frac{8}{3}\,\frac{\mu^3}{m_1\,m_2}\right)\frac{\alpha^7}{\pi}\,\ln^2\alpha\,. \tag{41}$$

The corresponding contribution from the exchange diagrams is calculated as a second order correction to energy coming from $\delta H = H^{(4)}$ and $H^{(5)}$

$$E_\phi^E = 2\,\langle H^{(4)}\,\frac{1}{(E-H)'}\,H^{(5)}\rangle\,. \tag{42}$$

$H^{(5)}$ is an effective Hamiltonian that gives correction to energy at order $m\,\alpha^5\ln\alpha$ due to photon exchange:

$$H^{(5)} = -\frac{2}{3}\,\frac{\alpha^2\,\ln\alpha}{m_1\,m_2}\,\delta^3(r)\,. \tag{43}$$

Since the logarithmic singularities in $H^{(5)}$ are regularized separately from singularities in the matrix elements one should include an additional factor 1/2. The matrix element in Eq. (42) is the same as for self–energy case, so one obtains:

$$E_\phi = \frac{1}{3}\,\frac{\mu^3}{m_1\,m_2}\,\frac{\alpha^7}{\pi}\,\ln^2\alpha\,. \tag{44}$$

E. retardation in the seagull contribution

The seagull contribution comes from the interaction term $A^2/(2m)$. Let's consider first the exchange diagrams. There are six of them, which differ in the time ordering of emission or absorption of two-photons. The sum, after neglecting terms with no $\ln^2\alpha$, could be transformed to

$$E_S^E = -\frac{1}{3}\,\frac{e^2}{m_1^2\,m_2}\int_{\epsilon\alpha}^{\mu\alpha}\frac{d^3q}{(2\,\pi)^3}\,\frac{1}{q^3}\,\biggl\langle p^i\,(H-E)\,p^j\,\frac{\alpha}{2\,r}\left(\delta^{ij}+\frac{r^i\,r^j}{r^2}\right) + \frac{\alpha}{2\,r}\left(\delta^{ij}+\frac{r^i\,r^j}{r^2}\right)p^j\,(H-E)\,p^i\biggr\rangle + (1\leftrightarrow 2)\,. \tag{45}$$

After commuting $(H-E)$ on the left or right side of the expression, it is transformed to

$$E_S^E = \frac{2}{3}\,\frac{\mu^3}{m_1\,m_2}\,\frac{\alpha^7}{\pi}\,\ln\!\left(\frac{\mu}{\epsilon}\right)\left\langle\frac{1}{r^4}\right\rangle \to -\frac{8}{3}\,\frac{\mu^3}{m_1\,m_2}\,\frac{\alpha^7}{\pi}\,\ln^2\alpha\,. \tag{46}$$

The self energy diagrams with the seagull insertion after neglecting terms with no $\ln^2\alpha$ and several transformations, sum to:

$$E_S^S = \frac{1}{m_1^2\,m_2}\int^{\lambda\alpha}\frac{d^3q_1}{(2\,\pi)^3}\,\frac{e^2}{2\,q_1}\left(\delta^{ik}-\frac{q_1^i\,q_1^k}{q_1^2}\right)\int_{\epsilon\alpha}^{\delta\alpha}\frac{d^3q_2}{(2\,\pi)^3}\,\frac{e^2}{2\,q_2}\left(\delta^{kj}-\frac{q_2^k\,q_2^j}{q_2^2}\right) \frac{1}{q_2^2\,(q_1+q_2)}\left\langle e^{-i\boldsymbol{q}_1\cdot\boldsymbol{r}}\left[p^i\,;\,\left[\frac{\alpha}{r}\,;\,p^j\right]\right] + \text{h.c.}\right\rangle + (1\leftrightarrow 2)\,. \tag{47}$$

It could be further calculated using the following equation

$$\left(\delta^{ij} - \frac{q^i\,q^j}{q^2}\right)\left\langle e^{-i\boldsymbol{q}\cdot\boldsymbol{r}}\left[p^i\,;\,\left[p^j\,;\,\frac{\alpha}{r}\right]\right]\right\rangle \approx \frac{4\,\pi}{q}\,, \tag{48}$$

which holds in the limit of large q, so one obtains

$$E_S^S = -\frac{16}{3}\,\frac{\alpha^7}{\pi}\left[\ln\left(\frac{\delta}{\epsilon}\right)\,\ln\lambda - \frac{1}{2}\,\ln^2\delta\right]\frac{\mu^3}{m_1\,m_2} \to -\frac{8}{3}\,\frac{\mu^3}{m_1\,m_2}\,\frac{\alpha^7}{\pi}\,\ln^2\alpha\,. \tag{49}$$

F. other diagrams

There are further diagrams, which may contribute to $m\,\alpha^7\,\ln^2\alpha$ but they cancel out between themselves. First example is a family of diagrams involving triple seagull insertions. It consists of six diagrams and contributes at order $m\,\alpha^7$, but the $\ln^2\alpha$ terms exactly cancels out. The second family of diagrams involves the exchange of two photons. It has been partially accounted for in E_H^E, namely as a part of contribution coming from δH. The corrections beyond that do not show infrared singularity and therefore do not give $\ln^2\alpha$. The third and last family of diagrams is self–energy with the exchange of transverse photon. There are together 16 diagrams. Their sum gives a contribution which has been exactly included in E_H^S as a part of Hamiltonian correction. Therefore we state that there are no further contributions to $m\,\alpha^7\,\ln^2\alpha$ term.

IV. SUMMARY

The double logarithmic correction coming from self–energy diagrams equals to

$$E^S = E_q^S + E_j^S + E_H^S + E_\phi^S + E_S^S = \left(-4\,\mu + \frac{32}{3}\,\frac{\mu^3}{m_1\,m_2}\right)\frac{\alpha^7}{\pi\,n^3}\,\ln^2\alpha\,\delta_{l0}\,, \tag{50}$$

and from the exchange diagrams

$$E^E = E_q^E + E_j^E + E_H^E + E_\phi^E + E_S^E = \left(-\frac{11}{15}\,\frac{\mu^3}{m_1\,m_2}\right)\frac{\alpha^7}{\pi\,n^3}\,\ln^2\alpha\,\delta_{l0}\,, \tag{51}$$

where we could restore the n and l-dependence, since all corrections were governed by $\phi^2(0)$ or by $\phi'(0)\phi(0)$, which vanish for states with $l \neq 0$ and have $1/n^3$ dependence for nS states. These corrections sum to

$$E = E^S + E^E = \left(-4\,\mu + \frac{149}{15}\,\frac{\mu^3}{m_1\,m_2}\right)\frac{\alpha^7}{\pi\,n^3}\,\ln^2\alpha\,\delta_{l0}\,. \tag{52}$$

In comparison to the work of Melnikov and Yelkhovsky [13] we found an agreement separately for self–energy and exchange contributions, and it forms a significant test of these calculations. For the completion of results we present the spin dependent contribution which was first calculated in [12]. It is obtained as a spin dependent δH correction to the wave function. We have verified that although the self–energy seagull diagrams also contribute separately to $\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2\,\ln^2\alpha$, their sum vanishes. This correction equals to

$$E_{\rm hfs} = \left(-\frac{64}{9}\frac{\mu^3}{m_1\,m_2} + \frac{112}{9}\frac{\mu^5}{m_1^2 m_2^2}\right)\frac{\alpha^7}{\pi\,n^3}\,\ln^2\alpha\,\frac{\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2}{4}\,\delta_{l0}\,. \tag{53}$$

The spin independent correction, which we derived here, affects the 1S-2S transition in hydrogenic systems. In the limit of large nucleus mass one obtains

$$E(nS) = \frac{\mu^3}{m^2}\left[-1 + \frac{29}{60}\frac{m}{M} + O\Big(\frac{m}{M}\Big)^2\right]\frac{\alpha^7}{\pi\,n^3}\,\ln^2\alpha^{-2}\,. \tag{54}$$

The first term in brackets is in agreement with the known $\ln^2\alpha^{-2}$ term in the nonrecoil case. It was customary to assume a coefficient μ^3/m^2 [2], as one expected it to give the largest contribution to the recoil corrections. Our calculations confirms this assumption since 29/60 is indeed smaller than 3, as obtained by expansion of μ^3/m^2 coefficient in the m/M mass ratio. Its contribution to 1S-2S transition in hydrogen is about 1 kHz, which is relatively small in comparison to the uncertainty of about 30 kHz or more, coming from the poorly known proton charge radius or unknown higher order two–loop corrections. However, it is significant for the hydrogen-deuterium isotope shift of the 1S-2S transition, where the proton charge radius and two–loop corrections cancel out. This additional term contributes

$$\Delta\nu_{H-D}(1S-2S) = 0.48\ \text{kHz}\,, \tag{55}$$

which should be compared with the precision of the most recent measurement by the Garching group [16] $\nu = 670\,994\,334.64(15)$ kHz.

There are further contributions specific to positronium. They come from the annihilation diagrams and were obtained in [12]

$$E_{\rm ann} = -\frac{3}{8}\,m\,\frac{\alpha^7}{\pi\,n^3}\,\ln^2\alpha\,\frac{3+\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2}{4}\,\delta_{l0}\,. \tag{56}$$

The complete result for positronium is a sum of (52), (53) with $m_1 = m_2 = m$ and (56)

$$E = -\left(\frac{499}{480} + \frac{7}{8}\frac{\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2}{4}\right) m\,\frac{\alpha^7}{\pi\,n^3}\,\ln^2\alpha\,\delta_{l0}\,. \tag{57}$$

It contributes 1.16 MHz to the $1^3S_1 - 2^3S_1$ transition. The final theoretical predictions and measurements for this transition are

$$\nu(1S-2S)_{\rm the} = 1\,233\,607\,222.2(0.6)\ \text{MHz}\,, \tag{58}$$
$$\nu(1S-2S)_{\rm exp} = 1\,233\,607\,216.4(3.2)\ \text{MHz [10]}\,. \tag{59}$$

This correction affects also $2^3S_1 - 2^3P_J$ transitions by -0.17 MHz. Although current measurements are much less precise [11], a new project is underway by the Michigan group to re-measure $2S - 2P$ transitions with the much better accuracy, comparable with this correction. The natural continuation of this work would be the calculation of the single log and the constant terms. We think, however, it is a pretty difficulty task and the calculation presented here gives a rough estimate for remaining terms, which are assumed to be of the half of $\ln^2\alpha$ contribution. It gives 0.24 kHz uncertainty for the H-D(1S-2S) isotope shift, 0.6 MHz for the 1S-2S transition frequency in positronium, and 0.9 kHz for 2S-2P also in positronium.

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FIGURES

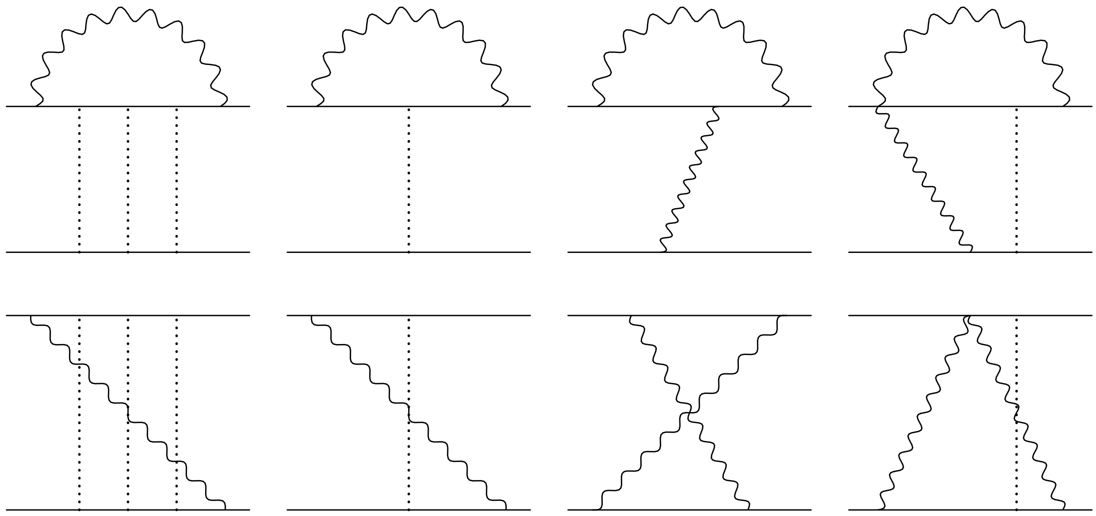

FIG. 1. Time ordered diagrams contributing to energy levels in order $m\,\alpha^7 \ln^2 \alpha$. The wavy line is a transverse photon and the dotted line denotes retardation, namely the term $(H-E)$ in the expansion in Eq. (4). Each diagram represents a whole class of diagrams that differ in time ordering of vertices.