Contributions to helium fine structure of order $m\,\alpha^7$

Krzysztof Pachucki[a,b] **and Jonathan Sapirstein**[c]

[a]Institute of Theoretical Physics, Warsaw University, Hoża 69, 00-681 Warsaw, Poland

[b] Institute for Theoretical Atomic and Molecular Physics, 60 Garden Street, Cambridge, MA 02138‡

[c] Department of Physics, University of Notre Dame, Notre Dame, Indiana 46556, USA.

Abstract. An effective Hamiltonian approach is used to analyze QED contributions to the fine structure of 2^3P_J levels in helium to order $m\,\alpha^7$. Formulas for leading contributions are derived and their numerical values presented.

1. Introduction

The fine structure of helium generally refers to the splitting of 2^3P_J energy levels for J=0,1, and 2. This intrinsically relativistic effect arises in leading order from the interaction of spins and orbital angular momentum, described by the Breit Hamiltonian. The value of this splitting has been measured with increasing precision over the years, and the most accurate results for the so-called large interval, $\nu_{01} = [E(2^3P_0)-E(2^3P_1)]/h$ and the small interval $\nu_{12} = [E(2^3P_1) - E(2^3P_2)]/h$ are

$$\begin{aligned}\nu_{01} &= 29\ 616.949\ 7(20)\mathrm{MHz}\ \ [1]\,,\\ \nu_{12} &= \ 2\ 291.174\ 0(14)\mathrm{MHz}\ \ [2].\end{aligned} \tag{1}$$

Because the splitting is proportional to α^2 Ry, these accurate measurements make helium a candidate for determining the fine structure constant providing that the higher order in α corrections can be sufficiently well understood.

To reach the necessary level of precision, which corresponds to α^5 Ry, an efficient approach to the two–electron bound state problem in QED is required. For neutral helium one wishes to take advantage of the fact that the fine structure constant α and $Z\,\alpha$ are small and perform an expansion of the binding energy in terms of them. It was recognized many years ago by Douglas and Kroll [3] that for the fine structure one can do this by expanding the kernel of the Bethe–Salpeter equation in powers of momenta. In this way one obtains effective operators which act as corrections to the Schrödinger Hamiltonian. To evaluate fine structure to order $m\,\alpha^6$ the first order expectation value of these operators along with the second order effect of the Breit Hamiltonian must

‡ temporary address

be considered. These calculations have been performed to high accuracy by Yan and Drake [4]. However, the operators derived by Douglas and Kroll were already rather singular, and only the fact that the wave function of triplet P states vanishes when $\vec{r}_1 = \vec{r}_2$ allowed the calculation to be carried out.

Application of the Douglas-Kroll method in the next order, $m\,\alpha^7$, leads to operators with divergent matrix elements even for triplet P states. This problem was met and solved recently in the calculation of $m\,\alpha^6$ contributions to helium S-levels [5] by using the concept of an effective Hamiltonian. However, for the fine structure problem the implementation of the method, which requires regulators that smooth the short-distance behavior of the theory, has not yet been fully worked out. Therefore, as a first step, we have chosen to calculate the numerically most significant part, which comes from two sources, the electron-nucleus interaction, and corrections to the two-electron Bethe logarithm. Another approach to the evaluation of these terms that has been given by Zhang [6], [7] will be discussed in the conclusions. We now describe our calculation.

2. Helium fine structure at order $m\,\alpha^7$

The fine structure in order $m\,\alpha^7$ can be written as

$$E^{(7)} = \langle H^{(7)}\rangle + 2\left\langle H^{(4)}\,\frac{1}{(E_0-H_0)'}\,H^{(5)}\right\rangle + E_L\,, \tag{2}$$

where E_L is a low energy part, with the photon energy restricted to be of order $m\,\alpha^2$, and $H^{(i)}$ is an effective Hamiltonian of order $m\,\alpha^i$. We present here a complete calculation of both E_L and the second order correction, and in addition evaluate the most numerically significant contribution in $H^{(7)}$. This is the one–loop radiative correction to the electron–nucleus interaction, which also contributes to hydrogen fine structure in order $m\,\alpha^7$ [8]. An artificial cut-off parameter is used to define the various terms, and we will explicitly demonstrate its cancellation in their sum.

2.1. Low energy part E_L

In the low energy part, the momenta of the photon that is emitted and reabsorbed is of order $m\,\alpha^2$. In the following we impose a cut off on the photon momentum denoted by $m\,\alpha\,\epsilon$. We assume that after expansion in α the limit $\epsilon\to 0$ is performed. E_L is further divided into two parts

$$E_L = E_{L1} + E_{L2}\,. \tag{3}$$

In the first part, E_{L1}, the electron current is simply $\boldsymbol{p}/m$ and we use the usual nonrelativistic formula for the energy shift, which is however to be corrected by relativistic effects,

$$\begin{aligned} E_{L1} = e^2 \int_0^{m\,\alpha\,\epsilon} &\frac{d^3k}{(2\,\pi)^3\,2\,k}\left(\delta^{ij}-\frac{k^i\,k^j}{k^2}\right) \\ &\times\delta\left\langle\phi\left|\frac{p_1^i+p_2^i}{m}\,\frac{1}{E-H-k}\,\frac{p_1^j+p_2^j}{m}\right|\phi\right\rangle. \end{aligned} \tag{4}$$

Here δ denotes the first order correction to ϕ, H and E due to δH, a spin dependent part of the Breit Hamiltonian $H^{(4)}$ (see Eq. (13)),

$$\begin{aligned}\delta H = &-\frac{3\,\alpha}{4\,m^2\,r^3}\,\boldsymbol{r}\times(\boldsymbol{p}_1-\boldsymbol{p}_2)\cdot\boldsymbol{s}+\frac{Z\,\alpha}{4\,m^2}\left(\frac{\boldsymbol{r}_1}{r_1^3}\times\boldsymbol{p}_1+\frac{\boldsymbol{r}_2}{r_2^3}\times\boldsymbol{p}_2\right)\cdot\boldsymbol{s}\\ &+\frac{\alpha}{2\,m^2\,r^3}\left(\boldsymbol{s}^2-\frac{3}{r^2}(\boldsymbol{s}\cdot\boldsymbol{r})^2\right).\end{aligned}\tag{5}$$

where $\boldsymbol{s}=(\boldsymbol{\sigma}_1+\boldsymbol{\sigma}_2)/2$, (the spin dependent part of the Breit Hamiltonian entering with a factor $(\boldsymbol{\sigma}_1-\boldsymbol{\sigma}_2)/2$ does not play a role in this calculation). After carrying out the k–integration and removing a term linearly dependent on ϵ, E_{L1} takes the form

$$\begin{aligned}E_{L1} = &-\frac{2\,\alpha}{3\,\pi\,m^2}\\ &\delta\left\langle\phi\left|(\boldsymbol{p}_1+\boldsymbol{p}_2)\,(H-E)\left\{\ln\left[\frac{2(H-E)}{m\,(Z\,\alpha)^2}\right]+\ln\left(\frac{Z^2\,\alpha}{2\,\epsilon}\right)\right\}(\boldsymbol{p}_1+\boldsymbol{p}_2)\right|\phi\right\rangle\end{aligned}\tag{6}$$

The $\ln Z^2\alpha$ term is separated out, as it has been previously calculated [9], and the $\ln 2\,\epsilon$ term will be shown to cancel with a similar contribution arising from the high energy part of the calculation.

The second part comes from a relativistic correction to the electron current. Spin dependent terms from the Coulomb and transverse photon exchange between the two electrons cancel out [10], but effects from an additional Coulomb exchange with the nucleus remain. This correction was originally calculated in [8] and is equal to

$$\begin{aligned}\delta\boldsymbol{j} = &\frac{\boldsymbol{p}}{m}\left(i\,\boldsymbol{k}\boldsymbol{r}-\frac{(\boldsymbol{k}\boldsymbol{r})^2}{2}\right)-\frac{1}{2\,m^3}\,\boldsymbol{p}\,p^2\\ &-\frac{1}{2\,m^2}\,\frac{Z\,\alpha}{r^3}\,\boldsymbol{r}\times\boldsymbol{\sigma}+\frac{1}{2\,m}\,\boldsymbol{k}\,\boldsymbol{r}\;\boldsymbol{k}\times\boldsymbol{\sigma}-\frac{i}{2\,m}\,\boldsymbol{k}\times\boldsymbol{\sigma}\,.\end{aligned}\tag{7}$$

One needs only the spin dependent part from both electrons, so

$$\begin{aligned}\delta\boldsymbol{j} = &\frac{1}{2\,m}\,\boldsymbol{k}\,\boldsymbol{r}_1\;\boldsymbol{k}\times\boldsymbol{\sigma}_1+\frac{1}{2\,m}\,\boldsymbol{k}\,\boldsymbol{r}_2\;\boldsymbol{k}\times\boldsymbol{\sigma}_2\\ &-\frac{1}{2\,m^2}\,\frac{Z\,\alpha}{r_1^3}\,\boldsymbol{r}_1\times\boldsymbol{\sigma}_1-\frac{1}{2\,m^2}\,\frac{Z\,\alpha}{r_2^3}\,\boldsymbol{r}_2\times\boldsymbol{\sigma}_2\,.\end{aligned}\tag{8}$$

The correction to energy involving δj has the form

$$\begin{aligned}E_{L2} = &\,e^2\int_0^{m\,\alpha\,\epsilon}\frac{d^3k}{(2\,\pi)^3\,2\,k}\left(\delta^{ij}-\frac{k^i\,k^j}{k^2}\right)\\ &\times 2\left\langle\phi\left|\delta j^i\,\frac{1}{E-H-k}\,\frac{p_1^j+p_2^j}{m}\right|\phi\right\rangle,\end{aligned}\tag{9}$$

and can be further simplified to

$$\begin{aligned}E_{L2} = &-\frac{\alpha}{3\,\pi\,m^2}\int_0^{m\,\alpha\,\epsilon}k\,dk\\ &\times\left\langle\phi\left|Z\,\alpha\left(\frac{\boldsymbol{r_1}\times\boldsymbol{\sigma}_1}{r_1^3}+\frac{\boldsymbol{r_2}\times\boldsymbol{\sigma}_2}{r_2^3}\right)\frac{1}{E-H-k}\,(\boldsymbol{p}_1+\boldsymbol{p}_2)\right|\phi\right\rangle.\end{aligned}\tag{10}$$

As a final expression one obtains

$$E_{L2} = \frac{i\,\alpha\,(Z\,\alpha)^2}{3\,\pi\,m^3} \times \left\langle \phi \middle| \left(\frac{\boldsymbol{r}_1}{r_1^3} + \frac{\boldsymbol{r}_2}{r_2^3}\right) \times \boldsymbol{s}\; \ln\left[\frac{2(H-E)}{m\,(Z\,\alpha)^2}\right] \cdot \left(\frac{\boldsymbol{r}_1}{r_1^3} + \frac{\boldsymbol{r}_2}{r_2^3}\right) \middle| \phi \right\rangle . \tag{11}$$

This completes the treatment of the low energy part E_L. We note that seagull terms, coming from the nonrelativistic form $A^2/(2\,m)$ do not contribute to the low energy part, as shown in [10].

2.2. Second order correction

The second order correction is

$$E_S = 2\left\langle H^{(4)}\,\frac{1}{(E-H)'}\,H^{(5)}\right\rangle . \tag{12}$$

$H^{(4)}$ is a Breit Hamiltonian

$$\begin{aligned} H^{(4)} = & -\frac{1}{8\,m^3}\,(p_1^4 + p_2^4) + \frac{Z\,\alpha\,\pi}{2\,m^2}\,[\delta^3(r_1) + \delta^3(r_2)] \\ & -\frac{\alpha}{2\,m^2}\,p_1^i\left(\frac{\delta^{ij}}{r} + \frac{r^i\,r^j}{r^3}\right)p_2^j + \frac{\alpha}{4\,m^2}\left(\frac{\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2}{r^3} - 3\,\frac{\boldsymbol{\sigma}_1\cdot\boldsymbol{r}\,\boldsymbol{\sigma}_2\cdot\boldsymbol{r}}{r^5}\right) \\ & +\frac{Z\,\alpha}{4\,m^2}\left[\frac{1}{r_1^3}\,\boldsymbol{r}_1\times\boldsymbol{p}_1\cdot\boldsymbol{\sigma}_1 + \frac{1}{r_2^3}\,\boldsymbol{r}_2\times\boldsymbol{p}_2\cdot\boldsymbol{\sigma}_2\right] \\ & +\frac{\alpha}{4\,m^2\,r^3}\,[(\boldsymbol{\sigma}_2 + 2\,\boldsymbol{\sigma}_1)\cdot\boldsymbol{r}\times\boldsymbol{p}_2 - (\boldsymbol{\sigma}_1 + 2\,\boldsymbol{\sigma}_2)\cdot\boldsymbol{r}\times\boldsymbol{p}_1] . \end{aligned} \tag{13}$$

$H^{(5)}$ is an effective Hamiltonian of order $m\,\alpha^5$

$$\begin{aligned} H^{(5)} = & \frac{\alpha}{\pi}\left\{\frac{Z\,\alpha}{4\,m^2}\left(\frac{1}{r_1^3}\,\boldsymbol{r}_1\times\boldsymbol{p}_1\cdot\boldsymbol{\sigma}_1 + \frac{1}{r_2^3}\,\boldsymbol{r}_2\times\boldsymbol{p}_2\cdot\boldsymbol{\sigma}_2\right)\right. \\ & -\frac{\alpha}{4\,m^2\,r^3}\,\boldsymbol{r}\times(\boldsymbol{p}_1 - \boldsymbol{p}_2)\cdot(\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2) \\ & \left.+\frac{\alpha}{4\,m^2}\left(\frac{\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2}{r^3} - 3\,\frac{\boldsymbol{\sigma}_1\cdot\boldsymbol{r}\,\boldsymbol{\sigma}_2\cdot\boldsymbol{r}}{r^5}\right)\right\} - \frac{7\,\alpha^2}{6\,\pi\,m^2}\,\frac{1}{r^3} \\ & +\frac{Z\,\alpha^2}{m^2}\,[\delta^3(r_1) + \delta^3(r_2)]\left[-\frac{4}{3}\,\ln(2\,\alpha\,\epsilon) + \frac{10}{9} - \frac{4}{15}\right] . \end{aligned} \tag{14}$$

$1/(E-H)'$ is a reduced Coulomb Green function that includes states with parity -1 and $l = 1, 2, 3$. The anomalous magnetic moment correction in $H^{(5)}$ has already been included in the calculations by Yan and Drake in [4]. The remaining part can be simplified to the form

$$E_S = 2\left\langle\phi\middle|\delta H\,\frac{1}{(E-H)'} \left\{-\frac{7\,\alpha^2}{6\,\pi\,m^2}\,\frac{1}{r^3} + \left(\frac{38}{45} - \frac{4}{3}\,\ln(2\,\alpha\,\epsilon)\right)\frac{Z\,\alpha^2}{m^2}\,[\delta^3(r_1) + \delta^3(r_2)]\right\}\middle|\phi\right\rangle , \tag{15}$$

where δH is given in Eq. (5).

2.3. One–loop radiative correction to the electron–nucleus interaction

This correction has previously been considered in the context of hydrogen fine structure [10]. It was derived in a form that can be directly used for the case of helium. It was also shown that radiative corrections can be incorporated by simply considering the electron on–shell form factors F_1, F_2 and the vacuum polarization (vp). The q^2 term from F_1 and vp gives

$$V_1 = \frac{i}{4\,m^2}\,\epsilon^{ijk}\,\sigma^i\,p^j\,4\,\pi\,Z\,\alpha\,\delta^3(r)\,p^k\,\frac{\alpha}{3\,\pi\,m^2}\left[-\ln(2\,\alpha\,\epsilon)+\frac{11}{24}-\frac{1}{5}\right]. \tag{16}$$

In this case ϵ is acting as a low-energy rather than a high energy cutoff. The q^2 term from F_2 is

$$V_2 = \frac{i}{2\,m^2}\,\epsilon^{ijk}\,\sigma^i\,p^j\,4\,\pi\,Z\,\alpha\,\delta^3(r)\,p^k\,\frac{\alpha}{12\,\pi\,m^2}\,. \tag{17}$$

The anomalous magnetic moment combined with relativistic corrections to the wave functions gives

$$V_3 = -\frac{1}{4\,m^2}\left(\frac{p^2}{2\,m^2}\,\frac{Z\,\alpha}{r^3}\,\boldsymbol{\sigma}\times\boldsymbol{r}\cdot\boldsymbol{p}+\frac{Z\,\alpha}{r^3}\,\boldsymbol{\sigma}\times\boldsymbol{r}\cdot\boldsymbol{p}\,\frac{p^2}{2\,m^2}\right)\frac{\alpha}{2\,\pi}\,. \tag{18}$$

One finally must account for the presence of two electrons, which leads to an additional factor of 2. The total electron-nucleus energy shift is

$$E_{EN} = 2\,\langle\phi|V_1+V_2+V_3|\phi\rangle = \frac{Z\,\alpha^2}{4\,\pi\,m^4}\,\Big\langle\phi\Big|$$
$$\left(\frac{91}{180}-\frac{2}{3}\,\ln(2\,\alpha\,\epsilon)\right)i\,\boldsymbol{s}\times\boldsymbol{p}_1\,4\,\pi\,\delta^3(r_1)\cdot\boldsymbol{p}_1-\frac{\boldsymbol{s}\times\boldsymbol{r}_1}{r_1^3}\cdot\boldsymbol{p}_1\,p_1^2\Big|\phi\Big\rangle \tag{19}$$

The logarithmic in α terms in Eq. (19) have already been calculated. The $\ln(2\,\epsilon)$ cancels out between E_L, E_{EN} and E_S. To show this, consider first the cutoff dependent part of Eq. (6), which can be written as

$$E_{L1}(\epsilon) = \frac{\alpha}{3\pi m^2}\,\ln(2\,\epsilon)\,\delta\langle\phi|[\boldsymbol{p}_1+\boldsymbol{p}_2;[H-E;\boldsymbol{p}_1+\boldsymbol{p}_2]]|\phi\rangle. \tag{20}$$

If the variation δ acts on the external wave functions, the double commutator reduces to a sum of delta functions, and cancels against the $\ln(2\,\epsilon)$ term from Eq. (15). If it instead acts on H one encounters the object $[\boldsymbol{p}_1+\boldsymbol{p}_2;[\delta H;\boldsymbol{p}_1+\boldsymbol{p}_2]]$, which after some manipulation can be seen to cancel the $\ln(2\epsilon)$ in Eq. (19).

3. Numerical calculation

We now numerically evaluate Σ, which is the following sum

$$\Sigma = E'_{L1}+E_{L2}+E'_S+E'_{EN}, \tag{21}$$

where prime denotes exclusion of logarithmic terms. In atomic units Σ is written as

$$E'_{L1} = -\frac{2}{3\,\pi}\,\delta\,\left\langle\phi\,\middle|\,(\boldsymbol{p}_1+\boldsymbol{p}_2)\,(H-E)\ln\left[\frac{2(H-E)}{Z^2}\right](\boldsymbol{p}_1+\boldsymbol{p}_2)\,\middle|\,\phi\right\rangle \tag{22}$$

$$E_{L2} = \frac{i\,Z^2}{3\,\pi}\,\Big\langle\phi\Big|\left(\frac{\boldsymbol{r}_1}{r_1^3}+\frac{\boldsymbol{r}_2}{r_2^3}\right)\times\boldsymbol{s}\,\ln\left[\frac{2(H-E)}{Z^2}\right]\cdot\left(\frac{\boldsymbol{r}_1}{r_1^3}+\frac{\boldsymbol{r}_2}{r_2^3}\right)\Big|\phi\Big\rangle, \tag{23}$$

$$E'_S = 2\Big\langle\phi\Big|\delta H\,\frac{1}{(E-H)'}\Big\{-\frac{7}{6\,\pi}\,\frac{1}{r^3}+\frac{38\,Z}{45}\,\left[\delta^3(r_1)+\delta^3(r_2)\right]\Big\}\Big|\phi\Big\rangle, \tag{24}$$

$$E'_{EN} = \frac{Z}{4\,\pi}\,\Big\langle\phi\Big|\frac{91}{180}\,i\,\boldsymbol{s}\times\boldsymbol{p}_1\,4\,\pi\,\delta^3(r_1)\cdot\boldsymbol{p}_1-\frac{\boldsymbol{s}\times\boldsymbol{r}_1}{r_1^3}\cdot\boldsymbol{p}_1\,p_1^2\Big|\phi\Big\rangle\,. \tag{25}$$

To numerically evaluate these expressions we follow the approach of Korobov [11]. We use the simplest possible basis set to expand triplet $P-$wave function in the form:

$$\boldsymbol{\phi}(r_1,r_2,r) = \sum_i v_i\,[\boldsymbol{r}_1\,\exp\left(-\alpha_i\,r_1-\beta_i\,r_2-\gamma_i\,r\right)-(1\leftrightarrow 2)]\,, \tag{26}$$

where α_i, β_i and γ_i are real and chosen in a uniform and random way with the conditions:

$$\begin{aligned}&A_1<\alpha_i<A_2, \beta_i+\gamma_i>\epsilon,\\ &B_1<\beta_i<B_2, \alpha_i+\gamma_i>\epsilon,\\ &C_1<\gamma_i<C_2,\ \alpha_i+\beta_i>\epsilon.\end{aligned} \tag{27}$$

Surprisingly, this basis set gives very accurate energy levels and wave functions. They can be further improved [12] by for example introducing two basis sets with independent A_i, B_i, C_i parameters. In this case, minimization with respect to this small set of global parameters with total length of basis set $N = 1200$ leads to the quite precise energy level for the triplet P-state

$$E(2^3P) = -2.133\,164\,190\,779\,283\,16(3)\,. \tag{28}$$

To obtain this result we used an inverse iteration method. Having precise wave functions, the matrix elements of various operators in Eqs. (22-25) can be calculated with the use of the integral

$$\frac{1}{16\,\pi^2}\int d^3r_1\int d^3r_2\,\frac{e^{-\alpha r_1-\beta r_2-\gamma r}}{r_1\,r_2\,r} = \frac{1}{(\alpha+\beta)(\beta+\gamma)(\gamma+\alpha)}\,, \tag{29}$$

and related terms obtained by differentiation or integration with respect to the appropriate parameters. The expectation values of operators involving spin-orbit and spin-spin terms is calculated using the formulas

$$\langle\boldsymbol{Q}\cdot\boldsymbol{s}\rangle_J = i\,\epsilon_{jki}\,\langle j|Q^k|i\rangle\,u_J\,, \tag{30}$$

$$\langle\boldsymbol{s}\cdot\hat{Q}\cdot\boldsymbol{s}\rangle_J = \langle j|Q^{ij}|i\rangle\,v_J\,, \tag{31}$$

where

$$\langle i|j\rangle = \delta^{ij}/3\,, \tag{32}$$

and

$$u_J = (1,1/2,-1/2)\,, \tag{33}$$

$$v_J = (-1,1/2,-1/10)\,, \tag{34}$$

for total angular momentum $J = 0,1,2$ respectively. While the electron-nucleus terms in E_{EN} could be calculated without too much effort, the second order terms require special considerations. They have been first calculated in the classic work of Lewis and Serafino [13] in the context of $m\,\alpha^6$ correction to helium fine structure, one order in α

less than the current calculations. It was pointed out by Yan and Drake [4] that some of their error estimates are too small. We confirm this, particularly for the term in Eq. (24) involving the spin orbit part of δH and $(\delta^3(r_1)+\delta^3(r_2))$, where we obtained a result three times larger

$$\left\langle \delta H_{LS}\,\frac{1}{(E-H)'}\,4\,\pi\,Z\,(\delta^3(r_1)+\delta^3(r_2))\right\rangle = -0.0915(2)\,u_J\,, \tag{35}$$

than the previously published result -0.0376 in [13]. This second order term is of particular importance, since it appears later on in the large k expansions of Bethe logs. We have calculated this second order term by expressing $E-H$ in Eq. (24) in the same basis set as external wave function ϕ. However, due to the high singularity of Dirac delta's and δH we also include two extra functions ϕ_L (on the left) and ϕ_R on the right hand side of $1/(E-H)'$:

$$\boldsymbol{\phi} = \boldsymbol{r}_1\,\psi - (1 \leftrightarrow 2)\,, \tag{36}$$

$$\boldsymbol{\phi}_R = \frac{\boldsymbol{r}_1}{r_1}\,\psi - (1 \leftrightarrow 2)\,, \tag{37}$$

$$\boldsymbol{\phi}_L = \frac{\boldsymbol{r}_1}{r_2}\,\psi - (1 \leftrightarrow 2)\,, \tag{38}$$

where first equation is a definition of ψ and ϕ is a 2^3P wave function.

The most computationally intensive part of the calculation was the evaluation of relativistic corrections to Bethe logs. Since E'_{L2} could not be calculated directly as in Eq. (23), we used a more convenient integral form:

$$E_{L2} = -\frac{\alpha}{3\,\pi}\int_0^\infty dk\,k^2\,L(k)\,, \tag{39}$$

$$L(k) = i\langle(\boldsymbol{p}_1+\boldsymbol{p}_2)\times\frac{1}{H+k-E}\,(\boldsymbol{p}_1+\boldsymbol{p}_2)\cdot\boldsymbol{s}\rangle\,. \tag{40}$$

While the value of this integral at $k=0$ serves as a simple test, the most crucial is the large $k-$asymptotics:

$$L(k) = \frac{1}{k^2}\left\{A+\frac{B}{k^{3/2}}+\frac{C\,\ln k}{k^2}+\frac{D}{k^2}+\frac{E}{k^{5/2}}+o\Big(\frac{1}{k^3}\Big)\right\}\,, \tag{41}$$

where

$$A = -\,Z\,\langle\Big(\frac{\boldsymbol{r}_1}{r_1^3}+\frac{\boldsymbol{r}_2}{r_2^3}\Big)\times(\boldsymbol{p}_1+\boldsymbol{p}_2)\cdot\boldsymbol{s}\rangle\,, \tag{42}$$

$$B = -\,i\,\frac{4\,\pi\,Z^2}{3\,\sqrt{2}}\,\langle\boldsymbol{p}_1\times\delta^3(r_1)\,\boldsymbol{p}_1\cdot\boldsymbol{s}+\boldsymbol{p}_2\times\delta^3(r_2)\,\boldsymbol{p}_2\cdot\boldsymbol{s}\rangle\,. \tag{43}$$

It is understood that A term is subtracted from the integral in Eq. (39). We calculate numerically values for $k=1,2,3$ up to 100. The value for larger k is obtained by fitting unknown higher order terms C, D, E in the expansion in Eq. (41). For k between 0 and 1, we integrated $L(k)$ analytically using spectral decomposition of H. Final numerical results are presented in Table I.

contribution	coeff. of $m\,\alpha^7$	ν_{01}[kHz]	ν_{12}[kHz]
E'_{EN}	$0.089507 u_J$	6.093	12.187
E'_{SL}	$0.02017(8) u_J$	1.373(5)	2.746(11)
E_{L2}	$-0.06755(5) u_J$	-4.599(3)	-9.197(7)
E'_{L1L}	$-0.0817(20) u_J$	-5.56(14)	-11.12(27)
E'_{SS}	$-0.04895(8) v_J$	9.997(16)	-3.999(6)
E'_{L1S}	$0.0959(4) v_J$	-19.586(82)	7.834(33)
Σ	$-0.0396(20) u_J$ $+0.0470(4) v_J$	-12.28(16)	-1.55(27)

Table 1. Numerical results in units of $m\,\alpha^7$ and in kHz for $m\,\alpha^7$ contributions to 2^3P_J fine structure. The first group comes from spin-orbit and the second from spin-spin interactions. $E'_{SL} + E'_{SS} = E'_S$ and $E'_{L1L} + E'_{L1S} = E'_{L1}$.

The Breit correction to Bethe logs E_{L1} is also calculated from the integral representation

$$E_{L1} \;=\; -\frac{2\,\alpha}{3\,\pi}\int dk\,k\,L(k)\,, \tag{44}$$

$$L(k) = 2\langle\phi|\delta H\,\frac{1}{(E-H)'}\,(p_1^i+p_2^i)\,\frac{1}{H+k-E}\,(p_1^i+p_2^i)|\phi\rangle + \tag{45}$$
$$\langle\phi|(p_1^i+p_2^i)\,\frac{1}{H+k-E}\,(\delta E-\delta H)\,\frac{1}{H+k-E}\,(p_1^i+p_2^i)|\phi\rangle\,.$$

One can prove that at $k=0$ the integrand $L(0)=0$. This serves as a useful test of the numerical evaluation of L. Moreover the large k asymptotics is:

$$L(k) = \frac{1}{k}\,\left\{A+\frac{B}{k}+\frac{C}{k^{3/2}}+\frac{D\,\ln k}{k^2}+\frac{E}{k^2}+o\Big(\frac{1}{k^{5/2}}\Big)\right\}\,, \tag{46}$$

with

$$A = 2\,\langle\delta H\,\frac{1}{(E-H)'}(\boldsymbol{p}_1+\boldsymbol{p}_2)^2\rangle\,, \tag{47}$$

$$B = \,-\,\langle\delta H\,\frac{1}{(E-H)'}\,4\,\pi\,Z\,(\delta^3(r_1)+\delta^3(r_2))\rangle$$
$$-\,\frac{i\,\pi\,Z}{2}\,\langle\boldsymbol{p}_1\times\delta^3(r_1)\,\boldsymbol{p}_1\cdot\boldsymbol{s}+\boldsymbol{p}_2\times\delta^3(r_2)\,\boldsymbol{p}_2\cdot\boldsymbol{s}\rangle\,. \tag{48}$$

Further terms in this expansion, namely C, D, E are obtained by fitting numerical values of $L(k)$ for $k=1,2,3,\ldots 100$. Since at small k a second order pole from 2^3S_1 state is present, we integrated $L(k)$ for k between 0 and 1 analytically. The spin orbit part E_{L1L} has the slowest numerical convergence and limits the precision of our calculations: all other contributions are obtained with at least 3 significant digits.

4. Summary

The goal of this paper has been to calculate the most numerically significant contribution to helium fine structure at order $m\,\alpha^7$. We have identified and calculated a set of terms that can be interpreted as the relativistic correction to the Bethe logarithm. Moreover we have carried out a complete calculation for the second order terms and the effective operators involving the electron-nucleus interaction. Each of these terms has a logarithmic dependence on a cutoff parameter ϵ, but we have shown that the sum is independent of ϵ.

Drake [14] has made available to us his compilation that includes lower order terms, mass polarization corrections, and the logarithmic terms in order $m\alpha^7$. He quotes 29 616.961 85(5)MHz for ν_{01} and 2 291.175 19(39) MHz for ν_{12}. Adding our results from Table 1, the present theoretical prediction for the splittings is

$$\begin{aligned} \nu_{01} &= 29\ 616.949\ 57(17)\mathrm{MHz}\,, \\ \nu_{12} &= \ 2\ 291.173\ 64(47)\mathrm{MHz}\,, \end{aligned} \tag{49}$$

where we have added our errors and Drakes in quadrature. The agreement with experiment is very good, which supports our assertion that we have identified the largest theoretical contributions in order $m\alpha^7$. We stress that the errors quoted are purely numerical, and no attempt to estimate the size of uncalculated terms has been made.

The agreement between theory and experiment found here is of course not surprising, since QED has been tested to high accuracy in many atomic systems. However, at this point we feel that it is premature to extract a value of the fine structure constant, which is the ultimate goal of studies of helium fine structure. This is because, as mentioned in the introduction, we have not yet derived all effective operators contributing to $H^{(7)}$, as a large number of terms involving electron-electron interactions have not been worked out in the effective Hamiltonian approach. These operators, along with the electron-nucleus terms treated here, have been studied by Zhang [6], [7]. They are tabulated as $\Delta E_i, i = 1-25$, in Eqs. (113), (114), and (115) in [6]. Were they to form a complete set, their numerical evaluation would then finish the calculation of helium fine structure to order $m\alpha^7$. However, we have found a number of discrepancies with this list. Firstly, it does not explicitly include the second order correction E_S, although the logarithmic part of that term was calculated by Zhang *et al.* in [9], and we agree on the total logarithmic contribution [10]. Secondly, when E_{EN} is treated, ΔE_2, which should correspond to the first term in Eq. (19), has a factor of 31 where we have 91. We would also get the factor 31 if we left out V_2, given by Eq. (19), so presumably neglect of that effect is the cause of this discrepancy. Thirdly, again in the term ΔE_2, there is a term denoted β' that should correspond to our formulas Eqs. (22) and (23): however, it is simple to see that these expressions are in disagreement, as we have even parity intermediate states whereas the intermediate states contributing to β' have odd parity. A preliminary investigation of certain electron-electron terms also indicates other possible discrepancies: in particular, ΔE_5 is sensitive to the electron-electron analog of V_2, and if that was also neglected the factor 29/5 should be modified. Therefore we stress that an independent derivation of $H^{(7)}$ operators is necessary in order to exploit the recent impressive experimental advances in the measurement of helium fine structure for a reliable determination of the fine structure constant α.

Acknowledgments

We wish to thank Vladimir Korobov for very fruitful advice on numerical methods and Gordon Drake for giving us unpublished numerical values for various fine structure terms. K.P. acknowledges support from Polish Committee for Scientific Research under contract No. 2P03B 057 18, and J.S from NIST precision measurement grant 60NANB6D0036 and NSF grant PHY98-70017.

References

[1] F. Minardi, G. Bianchini, P. Cancio Pastor, G. Giusfredi, F. S. Pavone, and M. Inguscio, Phys. Rev. Lett. **82**, 1112 (1999).
[2] C.H. Storry, M.C. George, and E.A. Hessels, Phys. Rev. Lett. **84**, 3274 (2000); J. Castillega, D. Livingston, A. Sanders, and D. Shiner, Phys. Rev. Lett. **84**, 4255 (2000).
[3] M. Douglass and N.M. Kroll, Ann. Phys. (N.Y) **82**, 89 (1974).
[4] Zong-Chao Yan and G.W.F. Drake, Phys. Rev. Lett. **74**, 4791 (1995).
[5] K. Pachucki, Phys. Rev. Lett. **84**, 4561 (2000).
[6] Tao Zhang, Phys, Rev. A **53**, 3896 (1996).
[7] Tao Zhang, Phys, Rev. A **54**, 1252 (1996).
[8] U. Jentschura and K. Pachucki, Phys. Rev. A **54**, 1853 (1996).
[9] Tao Zhang, Zong-Chao Yan and G.W.F. Drake, Phys. Rev. Lett. **77**, 1715 (1996).
[10] K. Pachucki, J. Phys. B **32**, 137 (1999).
[11] V.I. Korobov and S.V. Korobov, Phys. Rev. A **59**, 3394 (1999).
[12] V.I. Korobov, Phys. Rev. A **61**, 064503 (2000).
[13] M.L. Lewis and P.H. Serafino, Phys. Rev. **18**, 867 (1978).
[14] G.W.F. Drake, *private communication*.