

Helium fine structure theory for determination of α

Krzysztof Pachucki

Institute of Theoretical Physics, University of Warsaw, Hoza 69, 00-681 Warsaw, Poland

E-mail: krp@fuw.edu.pl

Vladimir A. Yerokhin

Center for Advanced Studies, St. Petersburg State Polytechnical University,
Polytekhnicheskaya 29, St. Petersburg 195251, Russia

E-mail: yerokhin@pcqnt1.phys.spbu.ru

Abstract. We present a recent progress in the calculation of helium fine-structure splitting of the 2^3P_J states, based on the quantum electrodynamic theory. Apart from the complete evaluation of $m\alpha^7$ and $m^2/M\alpha^6$ corrections, we have performed extensive tests by comparison with all experimental results for light helium-like ions and with the known large nuclear charge asymptotics of individual corrections. Our theoretical predictions are still limited by the unknown $m\alpha^8$ term, which is conservatively estimated by 1.7 kHz. However, comparison with the latest experimental result for the $2^3P_0 - 2^3P_2$ transition [M. Smiciklas and T. Shiner, Phys. Rev. Lett. (2010), in print] suggests that the higher-order contribution is in fact much smaller than the theoretical estimate. This means, that spectroscopic determination of α can be significantly improved, if the another measurement of the $2^3P_0 - 2^3P_2$ transition in helium-like Li^+ or Be^{2+} ion is performed.

1. Introduction

The quantum electrodynamic (QED) theory of atomic energy levels has achieved such a precision level which make possible determination of nuclear properties, like the charge radius, the magnetic dipole, or even the nuclear polarizability from the measured atomic spectra. If the nuclear structure effects are negligible or can be eliminated, one may obtain fundamental constants from comparison of theoretical predictions with experimental results. The most important examples include the Rydberg constant determined from the hydrogen spectroscopy, the electron mass derived from the bound-electron g factor in hydrogen-like ions, and α obtained from the helium fine structure. As it was first pointed out by Schwartz in 1964 [1], the splitting of the 2^3P_J levels in helium can be used for an accurate determination of the fine structure constant α . The attractive features of the fine structure as compared to other atomic transitions are, first, the long lifetime of the metastable 2^3P_J levels (roughly two orders of magnitude larger than that of the $2p$ state in hydrogen) and, second, the relative simplicity of the theory. Schwartz's suggestion stimulated a sequence of calculations [2, 3, 4, 5], which resulted in a theoretical description of the helium fine structure complete up to order $m\alpha^6$ (or α^4 Ry) and a value of α accurate to 0.9 ppm [6].

The present experimental precision for the fine-structure intervals in helium is sufficient for a determination of α with an accuracy of 14 ppb from Refs. [7, 8] and even 5 ppb from Ref. [9].

In order to match this level of accuracy in theoretical description of the fine structure, the complete calculation of the next-order, $m\alpha^7$ contribution and an estimation of the higher-order effects is needed. The work towards this end started in 1990s and extended over two decades [10, 11, 12, 13, 14, 15, 16, 17, 18, 19]. In 2006, the first complete evaluation of the $m\alpha^7$ correction to the helium fine structure was reported by one of us (KP) [20]. However, the numerical results presented there were in disagreement with the experimental values by more than 10 standard deviations (σ).

In our recent investigations [21, 22], we recalculated, using formulae from Ref. [20], all effects up to order $m\alpha^7$ to the fine structure of helium and performed calculations for helium-like ions with nuclear charges Z up to 10. The calculations were extensively checked by studying the hydrogenic ($Z \rightarrow \infty$) limit of individual corrections and by comparing them with the results known from the hydrogen theory. We found several problems in previous numerical calculations and in the meantime, the experimental value of the $2^3P_1 - 2^3P_2$ transition was changed by 3σ [8]. As a result, the present theoretical predictions are in agreement with the latest experimental data for the fine-structure intervals in helium, as well as with the most of experimental data available for light helium-like ions. Our calculation of the $m\alpha^7$ correction for the fine-structure splitting in light helium-like atoms was reported in Refs. [22, 23]. In this paper, we present a detailed description of all corrections to helium fine structure and a summary of numerical results.

2. QED theory of the helium fine-structure

According to the quantum electrodynamic theory (QED) energy levels of atomic system are a function of the fine structure constant α and the electron-nucleus mass ratio. We omit possible nuclear structure effects, as their contribution to the helium fine-structure is negligible. The fine-structure splitting $E_{\text{fs}}(\alpha)$ can be expanded in powers of α ,

$$E_{\text{fs}} = E_{\text{fs}}^{(4)} + E_{\text{fs}}^{(5)} + E_{\text{fs}}^{(6)} + E_{\text{fs}}^{(7)} + O(\alpha^8). \quad (1)$$

The expansion terms $E_{\text{fs}}^{(n)} \equiv m\alpha^n \mathcal{E}^{(n)}$ are of order $m\alpha^n$. They implicitly depend on the electron-nucleus mass ratio and may additionally involve powers of $\ln \alpha$. The advantage of this approach, is that each of the expansion terms is expressed as the expectation value of some effective Hamiltonian, as presented in the following. For convenience, we first consider the infinite nuclear mass limit, and then account for the finite nuclear mass corrections separately.

The dominant contribution to the helium fine structure is induced by the spin-dependent part of the Breit-Pauli Hamiltonian, which is, for an infinitely heavy nucleus,

$$\begin{aligned} H_{\text{fs}} &= \frac{1}{4} \left(\frac{\vec{\sigma}_1 \cdot \vec{\sigma}_2}{r^3} - 3 \frac{\vec{\sigma}_1 \cdot \vec{r} \vec{\sigma}_2 \cdot \vec{r}}{r^5} \right) (1 + a_e)^2 \\ &+ \frac{Z}{4} \left[\frac{1}{r_1^3} \vec{r}_1 \times \vec{p}_1 \cdot \vec{\sigma}_1 + \frac{1}{r_2^3} \vec{r}_2 \times \vec{p}_2 \cdot \vec{\sigma}_2 \right] (1 + 2a_e) \\ &+ \frac{1}{4r^3} \left\{ [(1 + 2a_e) \vec{\sigma}_2 + 2(1 + a_e) \vec{\sigma}_1] \cdot \vec{r} \times \vec{p}_2 \right. \\ &\quad \left. - [(1 + 2a_e) \vec{\sigma}_1 + 2(1 + a_e) \vec{\sigma}_2] \cdot \vec{r} \times \vec{p}_1 \right\}, \quad (2) \end{aligned}$$

where $\vec{r} = \vec{r}_1 - \vec{r}_2$. The above Hamiltonian includes the effect of the anomalous magnetic moment (amm) a_e , which is given by [24] (neglecting small vacuum-polarization corrections coming from particles heavier than electron)

$$a_e = \frac{\alpha}{2\pi} - 0.328\,478\,966 \left(\frac{\alpha}{\pi}\right)^2 + 1.181\,241\,457 \left(\frac{\alpha}{\pi}\right)^3 - 1.914\,4(35) \left(\frac{\alpha}{\pi}\right)^4 + \dots \quad (3)$$

Expanding the amm prefactors in Eq. (2), H_{fs} can be written as a sum of operators contributing to different orders in α ,

$$H_{\text{fs}} = H_{\text{fs}}^{(4)} + \alpha H_{\text{fs}}^{(5)} + \alpha^2 H_{\text{fs,amm}}^{(6)} + \alpha^3 H_{\text{fs,amm}}^{(7)} + \dots \quad (4)$$

Here, $H_{\text{fs}}^{(4)}$ and $H_{\text{fs}}^{(5)}$ are the complete effective Hamiltonians to order $m\alpha^4$ and $m\alpha^5$, respectively, whereas $H_{\text{fs,amm}}^{(6)}$ and $H_{\text{fs,amm}}^{(7)}$ are the amm parts of the corresponding higher-order operators. The contributions to the fine structure are

$$\mathcal{E}^{(4)} = \langle H_{\text{fs}}^{(4)} \rangle + O(m/M), \quad (5)$$

$$\mathcal{E}^{(5)} = \langle H_{\text{fs}}^{(5)} \rangle + O(m/M), \quad (6)$$

where expectation values are calculated with the corresponding eigenstate of the nonrelativistic Hamiltonian H_0

$$H_0 = \frac{p_1^2 + p_2^2}{2} - \frac{Z}{r_1} - \frac{Z}{r_2} + \frac{1}{r}. \quad (7)$$

The finite nuclear mass corrections up to order $m\alpha^5$ are conveniently divided into three parts, termed as the mass scaling, the mass polarization, and the recoil operators. The effect of the mass scaling is accounted for by including the prefactor $(m_r/m)^3$ into the operator H_{fs} , where m_r is the reduced mass for the electron-nucleus system. The effect of the mass polarization can be accounted for to all orders by evaluating expectation values of all operators on the eigenfunctions of the Schrödinger Hamiltonian with the mass-polarization operator $(m_r/M)\vec{p}_1 \cdot \vec{p}_2$ included. The third effect is induced by the recoil addition to the Breit-Pauli Hamiltonian,

$$H_{\text{fs,rec}} = \frac{Z}{2} \frac{m}{M} \left[\frac{\vec{r}_1}{r_1^3} \times (\vec{p}_1 + \vec{p}_2) \cdot \vec{\sigma}_1 + \frac{\vec{r}_2}{r_2^3} \times (\vec{p}_1 + \vec{p}_2) \cdot \vec{\sigma}_2 \right] (1 + a_e). \quad (8)$$

3. The spin-dependent $m\alpha^6$ contribution

The $m\alpha^6$ contribution to the helium fine structure is a sum of the second-order perturbation corrections induced by the Breit-Pauli Hamiltonian and the expectation value of the effective fine-structure Hamiltonian to this order, $H_{\text{fs}}^{(6)}$,

$$\mathcal{E}^{(6)} = \left\langle H_{\text{fs}}^{(4)} \frac{1}{(E_0 - H_0)'} H_{\text{fs}}^{(4)} \right\rangle + 2 \left\langle H_{\text{nf}}^{(4)} \frac{1}{(E_0 - H_0)'} H_{\text{fs}}^{(4)} \right\rangle + \left\langle H_{\text{fs}}^{(6)} + H_{\text{fs,amm}}^{(6)} \right\rangle. \quad (9)$$

Here, $1/(E_0 - H_0)'$ is the reduced Green function and $H_{\text{nf}}^{(4)}$ is the spin-independent part of the Breit-Pauli Hamiltonian,

$$H_{\text{nf}}^{(4)} = -\frac{1}{8} (p_1^4 + p_2^4) + \frac{Z\pi}{2} [\delta^3(r_1) + \delta^3(r_2)] - \frac{1}{2} p_1^i \left(\frac{\delta^{ij}}{r} + \frac{r^i r^j}{r^3} \right) p_2^j, \quad (10)$$

where we omitted a term with $\delta^3(r)$ since it vanishes for the triplet states. $H_{\text{fs}}^{(6)}$ consists of 15 operators first derived by Douglas and Kroll (DK) [2] in the framework of the Salpeter equation. These operators were later rederived using much simpler the effective field method in Ref. [15]. The result is

$$H_{\text{fs}}^{(6)} = \sum_{i=1}^{15} B_i, \quad (11)$$

where B_i are given in Table 1.

Table 1. Effective operators contributing to $H_{\text{fs}}^{(6)}$ (left column) and H_H (right column)

Operator $\times m \alpha^6$	Operator $\times m \alpha^7 / \pi$
$B_1 = -\frac{3Z}{8} p_1^2 \frac{\vec{r}_1}{r_1^3} \times \vec{p}_1 \cdot \vec{\sigma}_1$	$H_1 = -\frac{Z}{4} p_1^2 \frac{\vec{r}_1}{r_1^3} \times \vec{p}_1 \cdot \vec{\sigma}_1$
$B_2 = -Z \frac{\vec{r}_1}{r_1^3} \times \frac{\vec{r}}{r^3} \cdot \vec{\sigma}_1 (\vec{r} \cdot \vec{p}_2)$	$H_2 = -\frac{3Z}{4} \frac{\vec{r}_1}{r_1^3} \times \frac{\vec{r}}{r^3} \cdot \vec{\sigma}_1 (\vec{r} \cdot \vec{p}_2)$
$B_3 = \frac{Z}{2} \frac{\vec{r}}{r^3} \cdot \vec{\sigma}_1 \frac{\vec{r}_1}{r_1^3} \cdot \vec{\sigma}_2$	$H_3 = \frac{3Z}{4} \frac{\vec{r}}{r^3} \cdot \vec{\sigma}_1 \frac{\vec{r}_1}{r_1^3} \cdot \vec{\sigma}_2$
$B_4 = \frac{1}{2r^4} \vec{r} \times \vec{p}_2 \cdot \vec{\sigma}_1$	$H_4 = \frac{1}{2r^4} \vec{r} \times \vec{p}_2 \cdot \vec{\sigma}_1$
$B_5 = -\frac{1}{2r^6} \vec{r} \cdot \vec{\sigma}_1 \vec{r} \cdot \vec{\sigma}_2$	$H_5 = -\frac{3}{4r^6} \vec{r} \cdot \vec{\sigma}_1 \vec{r} \cdot \vec{\sigma}_2$
$B_6 = \frac{5}{8} p_1^2 \frac{\vec{r}}{r^3} \times \vec{p}_1 \cdot \vec{\sigma}_1$	$H_6 = \frac{1}{4} p_1^2 \frac{\vec{r}}{r^3} \times \vec{p}_1 \cdot \vec{\sigma}_1$
$B_7 = -\frac{3}{4} p_1^2 \frac{\vec{r}}{r^3} \times \vec{p}_2 \cdot \vec{\sigma}_1$	$H_7 = -\frac{1}{4} p_1^2 \frac{\vec{r}}{r^3} \times \vec{p}_2 \cdot \vec{\sigma}_1$
$B_8 = -\frac{i}{4} p_1^2 \frac{1}{r} \vec{\sigma}_1 \cdot (\vec{p}_1 \times \vec{p}_2)$	$H_8 = -\frac{Z}{4r} \frac{\vec{r}_1}{r_1^3} \times \vec{p}_2 \cdot \vec{\sigma}_1$
$B_9 = -\frac{3i}{4} p_1^2 \frac{1}{r^3} \vec{r} \cdot \vec{p}_2 \vec{r} \times \vec{p}_1 \cdot \vec{\sigma}_1$	$H_9 = -\frac{i}{2} p_1^2 \frac{1}{r^3} \vec{r} \cdot \vec{p}_2 \vec{r} \times \vec{p}_1 \cdot \vec{\sigma}_1$
$B_{10} = \frac{3i}{8r^5} \vec{r} \times (\vec{r} \cdot \vec{p}_2) \vec{p}_1 \cdot \vec{\sigma}_1$	$H_{10} = \frac{3i}{4r^5} \vec{r} \times (\vec{r} \cdot \vec{p}_2) \vec{p}_1 \cdot \vec{\sigma}_1$
$B_{11} = -\frac{3}{16r^5} \vec{r} \times (\vec{r} \times \vec{p}_1 \cdot \vec{\sigma}_1) \vec{p}_2 \cdot \vec{\sigma}_2$	$H_{11} = -\frac{3}{8r^5} \vec{r} \times (\vec{r} \times \vec{p}_1 \cdot \vec{\sigma}_1) \vec{p}_2 \cdot \vec{\sigma}_2$
$B_{12} = -\frac{1}{16r^3} \vec{p}_1 \cdot \vec{\sigma}_2 \vec{p}_2 \cdot \vec{\sigma}_1$	$H_{12} = -\frac{1}{8r^3} \vec{p}_1 \cdot \vec{\sigma}_2 \vec{p}_2 \cdot \vec{\sigma}_1$
$B_{13} = \frac{3}{2} p_1^2 \frac{1}{r^5} \vec{r} \cdot \vec{\sigma}_1 \vec{r} \cdot \vec{\sigma}_2$	$H_{13} = \frac{21}{16} p_1^2 \frac{1}{r^5} \vec{r} \cdot \vec{\sigma}_1 \vec{r} \cdot \vec{\sigma}_2$
$B_{14} = -\frac{i}{4} p_1^2 \frac{\vec{r}}{r^3} \cdot \vec{\sigma}_1 \vec{p}_1 \cdot \vec{\sigma}_2$	$H_{14} = -\frac{3i}{8} p_1^2 \frac{\vec{r}}{r^3} \cdot \vec{\sigma}_1 \vec{p}_1 \cdot \vec{\sigma}_2$
$B_{15} = \frac{i}{8} p_1^2 \frac{\vec{r}}{r^3} \cdot \vec{\sigma}_1 \vec{p}_2 \cdot \vec{\sigma}_2$	$H_{15} = \frac{i}{8} p_1^2 \frac{1}{r^3} (\vec{r} \cdot \vec{\sigma}_2 \vec{p}_2 \cdot \vec{\sigma}_1 + (\vec{r} \cdot \vec{\sigma}_1)$ $\times (\vec{p}_2 \cdot \vec{\sigma}_2) - \frac{3}{r^2} \vec{r} \cdot \vec{\sigma}_1 \vec{r} \cdot \vec{\sigma}_2 \vec{r} \cdot \vec{p}_2)$
	$H_{16} = -\frac{1}{4} \vec{p}_1 \cdot \vec{\sigma}_1 \vec{p}_1 \times \frac{\vec{r}}{r^3} \cdot \vec{p}_2$
	$H_{17} = \frac{1}{8} \vec{p}_1 \cdot \vec{\sigma}_1 (-\vec{p}_1 \cdot \vec{\sigma}_2 \frac{1}{r^3} + 3\vec{p}_1 \cdot \vec{r} \frac{\vec{r}}{r^5} \cdot \vec{\sigma}_2)$

The finite nuclear mass corrections to the $m \alpha^6$ contribution can be divided into the mass scaling, the mass polarization, and the operator parts. The mass scaling prefactor is $(m_r/M)^4$ for the B_2 , B_3 , B_4 , and B_5 , $(m_r/M)^5$ for the other B_i operators, $(m_r/M)^6$ for the second-order corrections involving the first term in Eq. (10), and $(m_r/M)^5$ for all other second-order corrections. The mass polarization effect is most easily accounted for by including the mass polarization operator into the zeroth-order Hamiltonian. The operator part comes from recoil corrections to $H_{\text{fs}}^{(4)}$, $H_{\text{nf s}}^{(4)}$, and $H_{\text{fs}}^{(6)}$. The recoil part of $H_{\text{fs}}^{(4)}$ is given by Eq. (8). The spin-independent recoil part of the Breit-Pauli Hamiltonian is

$$H_{\text{nf s,rec}}^{(4)} = -\frac{Z}{2} \frac{m}{M} \sum_{a=1,2} p_a^i \left(\frac{\delta^{ij}}{r_a} + \frac{r_a^i r_a^j}{r_a^3} \right) (p_1^j + p_2^j). \quad (12)$$

Recoil corrections to the DK operators were studied by Zhang [14] and by K.P. and

Sapirstein [19]. The result is given by the effective Hamiltonian

$$\begin{aligned}
H_{\text{fs,rec}}^{(6)} = & \frac{m}{M} \left[\frac{iZ}{4} p_1^2 \frac{1}{r_1} \vec{\sigma}_1 \cdot (\vec{p}_1 \times \vec{p}_2) - \frac{iZ}{4} p_1^2 \frac{\vec{r}_1}{r_1^3} (\vec{\sigma}_1 \cdot \vec{r}_1 \times \vec{p}_1) \cdot (\vec{p}_1 + \vec{p}_2) \right. \\
& - \frac{3Z}{4} p_1^2 \vec{\sigma}_1 \cdot \frac{\vec{r}_1}{r_1^3} \times (\vec{p}_1 + \vec{p}_2) + Z \vec{\sigma}_1 \cdot \frac{\vec{r}}{r_1 r^3} \times (\vec{p}_1 + \vec{p}_2) + Z \vec{\sigma}_1 \cdot \frac{\vec{r}}{r^3} \times \frac{\vec{r}_1}{r_1^3} (\vec{r}_1 \cdot (\vec{p}_1 + \vec{p}_2)) \\
& \left. + Z^2 \vec{\sigma}_1 \cdot \frac{\vec{r}_1}{r_1^3} \times \frac{\vec{r}_2}{r_2^3} (\vec{r}_1 \cdot \vec{p}_1) - \frac{Z^2}{2} \vec{\sigma}_1 \cdot \frac{\vec{r}_1}{r_1^4} \times (\vec{p}_1 + \vec{p}_2) - \frac{Z^2}{4} \vec{\sigma}_1 \cdot \frac{\vec{r}_2}{r_2^3} \vec{\sigma}_2 \cdot \frac{\vec{r}_1}{r_1^3} \right]. \quad (13)
\end{aligned}$$

4. The spin-dependent $m\alpha^7$ correction

The $m\alpha^7$ correction to the helium fine structure can be conveniently separated into four parts,

$$\mathcal{E}^{(7)} = \mathcal{E}_{\text{log}}^{(7)} + \mathcal{E}_{\text{first}}^{(7)} + \mathcal{E}_{\text{sec}}^{(7)} + \mathcal{E}_L^{(7)}. \quad (14)$$

The first term in the brackets above combines all terms with $\ln Z$ and $\ln \alpha$ [11, 12, 13, 15, 20],

$$\begin{aligned}
\mathcal{E}_{\text{log}}^{(7)} = & \ln[(Z\alpha)^{-2}] \left[\left\langle \frac{2Z}{3} i \vec{p}_1 \times \delta^3(r_1) \vec{p}_1 \cdot \vec{\sigma}_1 \right\rangle - \left\langle \frac{1}{4} (\vec{\sigma}_1 \cdot \vec{\nabla}) (\vec{\sigma}_2 \cdot \vec{\nabla}) \delta^3(r) \right\rangle \right. \\
& \left. - \left\langle \frac{3}{2} i \vec{p}_1 \times \delta^3(r) \vec{p}_1 \cdot \vec{\sigma}_1 \right\rangle + \frac{8Z}{3} \left\langle H_{\text{fs}}^{(4)} \frac{1}{(E_0 - H_0)'} [\delta^3(r_1) + \delta^3(r_2)] \right\rangle \right]. \quad (15)
\end{aligned}$$

The second part of $\mathcal{E}^{(7)}$ is induced by effective Hamiltonians to order $m\alpha^7$. They were derived by one of us (K.P.) in Refs. [20, 21]. (The previous derivation of this correction by Zhang [11, 12] turned out to be not entirely consistent.) The result is

$$\mathcal{E}_{\text{first}}^{(7)} = \left\langle H_Q + H_H + H_{\text{fs,amm}}^{(7)} \right\rangle. \quad (16)$$

The Hamiltonian H_Q is induced by the two-photon exchange between the electrons, the electron self-energy and the vacuum polarization. It is given by [20]

$$\begin{aligned}
H_Q = & Z \frac{91}{180} i \vec{p}_1 \times \delta^3(r_1) \vec{p}_1 \cdot \vec{\sigma}_1 - \frac{1}{2} (\vec{\sigma}_1 \cdot \vec{\nabla}) (\vec{\sigma}_2 \cdot \vec{\nabla}) \delta^3(r) \left[\frac{83}{30} + \ln Z \right] \\
& + 3 i \vec{p}_1 \times \delta^3(r) \vec{p}_1 \cdot \vec{\sigma}_1 \left[\frac{23}{10} - \ln Z \right] - \frac{15}{8\pi} \frac{1}{r^7} (\vec{\sigma}_1 \cdot \vec{r}) (\vec{\sigma}_2 \cdot \vec{r}) - \frac{3}{4\pi} i \vec{p}_1 \times \frac{1}{r^3} \vec{p}_1 \cdot \vec{\sigma}_1. \quad (17)
\end{aligned}$$

Here, the terms with $\ln Z$ compensate the logarithmic dependence implicitly present in expectation values of singular operators $1/r^3$ and $1/r^5$, so that matrix elements of H_Q do not have any logarithms in their $1/Z$ expansion. The singular operators are defined through their integrals with the arbitrary smooth function f ,

$$\int d^3r \frac{1}{r^3} f(\vec{r}) \equiv \lim_{\epsilon \rightarrow 0} \int d^3r \left[\frac{1}{r^3} \theta(r - \epsilon) + 4\pi \delta^3(r) (\gamma + \ln \epsilon) \right] f(\vec{r}), \quad (18)$$

and

$$\begin{aligned}
\int d^3r \frac{1}{r^7} \left(r^i r^j - \frac{\delta^{ij}}{3} r^2 \right) f(\vec{r}) \equiv & \quad (19) \\
\lim_{\epsilon \rightarrow 0} \int d^3r \left[\frac{1}{r^7} \left(r^i r^j - \frac{\delta^{ij}}{3} r^2 \right) \theta(r - \epsilon) + \frac{4\pi}{15} \delta^3(r) (\gamma + \ln \epsilon) \left(\partial^i \partial^j - \frac{\delta^{ij}}{3} \partial^2 \right) \right] f(\vec{r}), &
\end{aligned}$$

where γ is the Euler constant. The effective Hamiltonian H_H represents the anomalous magnetic moment (amm) correction to the Douglas-Kroll $m\alpha^6$ operators and is given by [20]

$$H_H = \sum_{i=1}^{17} H_i, \quad (20)$$

where H_i are presented in Table 1. The last term of $\mathcal{E}_{\text{first}}^{(7)}$ in Eq. (16), the Hamiltonian $H_{\text{fs,amm}}^{(7)}$ is the $m\alpha^7$ amm correction to the Breit-Pauli Hamiltonian, see Eq. (2).

The third part of $\mathcal{E}^{(7)}$ is given by the second-order matrix elements of the form [20]

$$\mathcal{E}_{\text{sec}}^{(7)} = 2 \left\langle H_{\text{fs}}^{(4)} \frac{1}{(E_0 - H_0)'} H_{\text{nlog}}^{(5)} \right\rangle + 2 \left\langle \left[H_{\text{fs}}^{(4)} + H_{\text{nfs}}^{(4)} \right] \frac{1}{(E_0 - H_0)'} H_{\text{fs}}^{(5)} \right\rangle, \quad (21)$$

where $H_{\text{nlog}}^{(5)}$ is the effective Hamiltonian responsible for the nonlogarithmic $m\alpha^5$ correction to the energy,

$$H_{\text{nlog}}^{(5)} = -\frac{7}{6\pi r^3} + \frac{38Z}{45} [\delta^3(r_1) + \delta^3(r_2)], \quad (22)$$

$H_{\text{nfs}}^{(4)}$ is the spin-independent part of the Breit-Pauli Hamiltonian given by Eq. (10), and $H_{\text{fs}}^{(5)}$ is the $m\alpha^5$ amm correction to $H_{\text{fs}}^{(4)}$, see Eq. (2).

The fourth part of $\mathcal{E}^{(7)}$ is the contribution induced by the emission and reabsorption of virtual photons of low energy. It is denoted as $\mathcal{E}_L^{(7)}$ and interpreted as the relativistic correction to the Bethe logarithm. The expression for $\mathcal{E}_L^{(7)}$ reads [16]

$$\begin{aligned} \mathcal{E}_L^{(7)} = & -\frac{2}{3\pi} \delta \left\langle (\vec{p}_1 + \vec{p}_2) \cdot (H_0 - E_0) \ln \left[\frac{2(H_0 - E_0)}{Z^2} \right] (\vec{p}_1 + \vec{p}_2) \right\rangle \\ & + \frac{iZ^2}{3\pi} \left\langle \left(\frac{\vec{r}_1}{r_1^3} + \frac{\vec{r}_2}{r_2^3} \right) \times \frac{\vec{\sigma}_1 + \vec{\sigma}_2}{2} \ln \left[\frac{2(H_0 - E_0)}{Z^2} \right] \left(\frac{\vec{r}_1}{r_1^3} + \frac{\vec{r}_2}{r_2^3} \right) \right\rangle, \end{aligned} \quad (23)$$

where $\delta \langle \dots \rangle$ denotes the first-order perturbation of the matrix element $\langle \dots \rangle$ by $H_{\text{fs}}^{(4)}$, implying perturbations of the reference-state wave function, the reference-state energy, and the electron Hamiltonian.

5. Results for helium fine-structure

The summary of individual contributions to the fine-structure intervals of helium is given in Table 2. Numerical results are presented for the large ν_{01} and the small ν_{12} intervals, defined by

$$\nu_{01} = [E(2^3P_0) - E(2^3P_1)]/h, \quad (24)$$

$$\nu_{12} = [E(2^3P_1) - E(2^3P_2)]/h. \quad (25)$$

We note that the style of breaking the total result into separate entries used in Table 2 differs from that used in the summary tables of the previous papers by K.P. *et al.* [20, 21]. Particularly, the lower-order terms listed in Table III of Ref. [20] and in Table II of Ref. [21] contained contributions of higher orders, whereas in the present work, the entries in Table 2 contain only the contributions of the order specified.

A term-by-term comparison with the independent calculation by Drake [18] was performed in Ref. [23]. We observe good agreement between the two calculations for the lower-order terms,

Table 2. Summary of individual contributions to the fine-structure intervals in helium, in kHz. The parameters [25] are $\alpha^{-1} = 137.035\,999\,679(94)$, $cR_\infty = 3\,289\,841\,960\,361(22)$ kHz, and $m/M = 1.370\,933\,555\,70 \times 10^{-4}$. The label (+ m/M) indicates that the corresponding entry comprises both the non-recoil and recoil contributions of the specified order in α .

Term	ν_{01}	ν_{12}	ν_{02}
$m\alpha^4(+m/M)$	29 563 765.45	2 320 241.43	
$m\alpha^5(+m/M)$	54 704.04	-22 544.00	
$m\alpha^6$	-1 607.52(2)	-6 506.43	
$m\alpha^6 m/M$	-9.96	9.15	
$m\alpha^7 \log(Z\alpha)$	81.43	-5.87	
$m\alpha^7, \text{nlog}$	18.86	-14.38	
$m\alpha^8$	± 1.7	± 1.7	
Total theory	$29\,616\,952.29 \pm 1.7$	$2\,291\,178.91 \pm 1.7$	$31\,908\,131.20 \pm 1.7$
Experiment	$29\,616\,951.66(70)^a$	$2\,291\,177.53(35)^d$	$31\,908\,131.25(30)^f$
	$29\,616\,952.7(10)^b$	$2\,291\,175.59(51)^a$	$31\,908\,126.78(94)^a$
	$29\,616\,950.9(9)^c$	$2\,291\,175.9(10)^e$	

^a Ref. [7], ^b Ref. [26], ^c Ref. [27], ^d Ref. [8], ^e Ref. [28], ^f Ref. [9].

namely, for the $m\alpha^4$, $m\alpha^5$, and $m\alpha^6$ corrections. However, for the recoil correction to order $m\alpha^6$, our results differ from Drake's ones by about 0.5 kHz for both intervals. The reason for this disagreement seems to be different for the large and the small intervals. For the large interval, the deviation is due to the recoil operator part, whereas for the small interval, it is mainly due to the mass polarization part (see discussion in Ref. [21]).

Our present estimates of the uncalculated higher-order effects for helium are larger than those in the previous studies [17, 18]. The previous estimates were significantly less than 1 kHz. They were based on logarithmic contributions to order $m\alpha^8$ corresponding to the hydrogen fine structure. However, a larger contribution might originate from the nonlogarithmic relativistic corrections. So our present estimate is obtained by multiplying the $m\alpha^6$ contribution for the $\nu_{02} = \nu_{01} + \nu_{12}$ interval by the factor of $(Z\alpha)^2$, which yields a conservative estimate of ± 1.7 kHz for all ν_{01} , ν_{12} , and ν_{02} intervals. All nuclear structure effects are completely negligible at the current precision level. The finite nuclear size correction is estimated to yield 18 Hz for ν_{01} and 6 Hz for ν_{12} .

Our result for the ν_{01} interval of helium agrees well with all recent experimental values [7, 26, 27]. For the ν_{12} interval, our theory is by about 2σ away from the values obtained in Refs. [7, 28] but in agreement with the latest measurement by Hessels and coworkers [8]. Our theoretical prediction for the ν_{02} interval is in an excellent agreement with the very recent measurement of Smiciklas and Shiner [9]. Comparison with this experimental result suggests that the higher-order contribution might be in fact much smaller than our conservative estimate. This means that, if an independent measurement on Li^+ or Be^{2+} confirms the smallness of the $m\alpha^8$ terms, the helium determination of α will be significantly improved. The measurement should be performed for the $2^3P_0 - 2^3P_2$ transition, since it is not affected by the significantly varying with Z singlet-triplet mixing correction.

In summary, theory of the fine structure of helium and light helium-like ions is now complete up to orders $m\alpha^7$ and $\alpha^6 m^2/M$. Theoretical predictions agree with the latest experimental

results for helium, as well as with most of the experimental data for light helium-like ions. A combination of the theoretical and experimental results [9] for the $2^3P_0 - 2^3P_2$ interval in helium yields an independent determination of the fine structure constant α ,

$$\alpha^{-1} = 137.035\,999\,55(64)(4)(368), \quad (26)$$

where the first error is the experimental uncertainty, the second one is the numerical uncertainty, and the third one comes from the estimate of $m\alpha^8$ term (± 1.7 kHz). The result (26) is accurate to 27 ppb and in agreement with the value obtained from the electron g factor [29].

Acknowledgments

Support by NIST through Precision Measurement Grant PMG 60NANB7D6153 is gratefully acknowledged.

References

- [1] Schwartz C 1964 Phys. Rev. **134** A1181
- [2] Douglas M and Kroll N 1974 Ann. Phys. (NY) **82** 89
- [3] Hambro L 1972 Phys. Rev. A **5** 2027
- [4] Hambro L 1972 Phys. Rev. A **6** 865
- [5] Hambro L 1973 Phys. Rev. A **7** 479
- [6] Lewis M L and Serafino P H 1978 Phys. Rev. A **18** 867
- [7] Zelevinsky T, Farkas D and Gabrielse G 2005 Phys. Rev. Lett. **95** 203001
- [8] Borbely J S, George M C, Lombardi L D, Weel M, Fitzakerley D W and Hessels E A 2009 Phys. Rev. A **79** 0605030(R)
- [9] Smiciklas M and Shiner D 2010 Phys. Rev. Lett. *in print*
- [10] Yan Z -C and Drake G W F 1995 Phys. Rev. Lett. **74** 4791
- [11] Zhang T 1996 Phys. Rev. A **54** 1252
- [12] Zhang T 1996 Phys. Rev. A **53** 3896
- [13] Zhang T, Yan Z -C and Drake G W F 1996 Phys. Rev. Lett. **77** 1715
- [14] Zhang T 1997 Phys. Rev. A **56** 270
- [15] Pachucki K 1999 J. Phys. B **32** 137
- [16] Pachucki K and Sapirstein J 2000 J. Phys. B **33** 5297
- [17] Pachucki K and Sapirstein J 2002 J. Phys. B **35** 1783
- [18] Drake G W F 2002 Can. J. Phys. **80** 1195
- [19] Pachucki K and Sapirstein J 2003 J. Phys. B **36** 803
- [20] Pachucki K 2006 Phys. Rev. Lett. **97** 013002
- [21] Pachucki K and Yerokhin V A 2009 Phys. Rev. A **79** 062516; *ibid.* 2009 **80** 019902(E); *ibid.* 2010 **81** 039903(E)
- [22] Pachucki K and Yerokhin V A 2010 Phys. Rev. Lett. **104** 070403
- [23] Pachucki K and Yerokhin V A 2010 Can. J. Phys. *in print*
- [24] Aoyama T, Hayakawa M, Kinoshita T and Nio M 2007 Phys. Rev. Lett. **99** 110406
- [25] Mohr P J, Taylor B N and Newell D B 2008 Rev. Mod. Phys. **80** 633
- [26] Giusfredi G, Pastor P C, Natale P D, Mazzotti D, de Mauro C, Fallani L, Hagel G, Krachmalnicoff V and Inguscio M 2005 Can. J. Phys. **83** 301
- [27] George M C, Lombardi L D and Hessels E A 2001 Phys. Rev. Lett. **87** 173002
- [28] Castilleja J, Livingston D, Sanders A and Shiner D 2000 Phys. Rev. Lett. **84** 4321
- [29] Hanneke D, Fogwell S and Gabrielse G 2008 Phys. Rev. Lett. **100** 120801