Fine structure of helium-like ions and determination of the fine structure constant

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We report a calculation of the fine structure splitting in light helium-like atoms, which accounts for all quantum electrodynamical effects up to order α^5 Ry. For the helium atom, we resolve the previously reported disagreement between theory and experiment and determine the fine structure constant with an accuracy of 31 ppb. The calculational results are extensively checked by comparison with the experimental data for different nuclear charges and by evaluation of the hydrogenic limit of individual corrections.

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Accurate measurements of the fine structure of the 2^3P level of helium and helium-like ions make possible a precise test of quantum electrodynamic (QED) theory of the electron-electron interaction in bound systems. Alternatively, assuming the validity of the theory, the fine structure constant α can be determined with a high accuracy. This fact was first pointed out by Schwartz in 1964 [1]. Fourteen years later, after a series of dedicated studies, Schwartz's program of calculations 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 [2].

Further theoretical progress met serious difficulties. It was only in 1996 that a calculation of the dominant part of the next-order $m\alpha^7$ contribution was reported [3]. To complete the calculation of this contribution turned out to be a challenge. A number of investigations [4–6] reported partial results, yielding significant disagreement with the experimental data. The first complete calculation [7] increased the disagreement even further by reporting differences of more than 10 standard deviations with the experimental results for the $2^3P_0 - 2^3P_1$ $(= \nu_{01})$ and $2^3P_1 - 2^3P_2$ $(= \nu_{12})$ intervals of helium [26].

In our previous investigation [8] we recalculated all effects up to order $m\alpha^7$ to the fine structure of helium with improved numerical precision, and significantly reduced the deviation of theory from experiment. In this Letter we eliminate a small inconsistency in our previous evaluation of Bethe logarithms and obtain agreement with the latest experimental results for helium. We also calculate the fine structure of helium-like ions with nuclear charges Z up to 10 and observe good agreement with most of the experimental data. As an independent check of our calculations, we study the hydrogenic ($Z \to \infty$) limit of individual corrections and demonstrate the consistency of the obtained results with the hydrogen theory.

The agreement observed for helium-like ions and the confirmed hydrogenic limit are substantial evidences of the reliability of our helium results. We are thus in a position to make an independent determination of the fine structure constant. The comparison of our theoretical prediction for the ν_{01} interval in helium (accurate to 57 ppb) with the experimental result [9] (accurate to 24 ppb) determines the value of α with an accuracy of 31 ppb, see Eq. (9) below. This is currently the third-precise method of determination of α, after the electron g factor [10] and the atomic recoil effect [11]. Measurements of α by different methods provide a sensitive test of consistency of theory across a range of energy scales and physical phenomena.

The energy levels of light atoms are addressed here within a rigorous QED approach based on an expansion of both relativistic and radiative effects in powers of α [12]. This approach allows one to consistently improve the accuracy of calculations by accounting for various effects order by order. The helium fine-structure splitting is thus represented as

$$E = m\left[\alpha^4\mathcal{E}^{(4)} + \alpha^5\mathcal{E}^{(5)} + \alpha^6\mathcal{E}^{(6)} + \alpha^7\mathcal{E}^{(7)} + \ldots\right], \quad (1)$$

where the expansion terms $\mathcal{E}^{(n)}$ may include $\ln\alpha$. The summary of results for energy levels up to order of $m\alpha^6$ is given in our previous investigation [13]. In the present Letter we evaluate corrections of order $m\alpha^7$ and $m^2\alpha^6/M$, where M is the nuclear mass. The $m\alpha^7$ correction can be represented as a sum of four parts,

$$\mathcal{E}^{(7)} = \mathcal{E}^{(7)}_{\rm log} + \mathcal{E}^{(7)}_{\rm first} + \mathcal{E}^{(7)}_{\rm sec} + \mathcal{E}^{(7)}_{L}\,. \quad (2)$$

The first part combines all terms with $\ln Z$ and $\ln\alpha$ [3, 14, 15],

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

where $\vec{r} = \vec{r}_1 - \vec{r}_2$, H_0 and E_0 are the Schrödinger Hamiltonian and its eigenvalue, and $H^{(4)}_{\rm fs}$ is the spin-dependent

TABLE I: Contributions of order $m\alpha^7$ and $m^2\alpha^6/M$ to the $2^3P_J - 2^3P_{J'}$ fine-structure intervals of helium-like atoms.

(J,J')	Z	$\mathcal{E}^{(6)}_M/[Z^8\, m/M]$	$\mathcal{E}^{(7)}_{\rm log}/[Z^6\, \ln(Z\alpha)^{-2}]$	$\mathcal{E}^{(7)}_{\rm first}/Z^6$	$\mathcal{E}^{(7)}_{\rm sec}/Z^7$	$\mathcal{E}^{(7)}_L/Z^6$
(0,1)	2	−0.015 21	0.001 105 3	0.002 213 4	0.001 169 3	−0.002 388 1(1)
	3	−0.020 60	−0.001 149 0	0.004 426 9	0.001 581 8	0.005 524 0(1)
	4	−0.023 06	−0.001 846 4	0.005 403 0	0.001 906 7	0.008 307 0(1)
	5	−0.024 39	−0.001 836 2	0.005 842 6	0.002 158 9	0.008 709 1(1)
	6	−0.025 22	−0.001 593 2	0.006 047 0	0.002 357 8	0.008 270 6(1)
	7	−0.025 81	−0.001 287 7	0.006 139 9	0.002 518 6	0.007 560 6(1)
	8	−0.026 24	−0.000 980 6	0.006 176 7	0.002 651 4	0.006 793 0(1)
	9	−0.026 58	−0.000 693 1	0.006 184 0	0.002 763 1	0.006 049 1(1)
	10	−0.026 84	−0.000 431 5	0.006 175 6	0.002 858 2	0.005 357 9(1)
	∞[extrap.]	−0.029 4	0.003 315	0.005 415 7	0.004 045 2	−0.005 095
	∞[exact]		0.003 316	0.005 415 7	0.004 045 2	−0.005 099
(0,2)	2	−0.001 235	0.001 025 6	0.003 016 7	−0.000 393 6	−0.001 716 1(1)
	3	−0.000 418	−0.002 365 8	0.007 084 4	−0.001 857 6	0.010 589 2(1)
	4	−0.000 200	−0.002 947 8	0.009 544 9	−0.002 219 8	0.014 039 4(1)
	5	−0.000 069	−0.002 416 4	0.011 062 7	−0.002 222 6	0.013 743 0(1)
	6	0.000 006	−0.001 587 4	0.012 062 8	−0.002 119 2	0.012 256 1(1)
	7	0.000 045	−0.000 731 5	0.012 760 9	−0.001 988 8	0.010 475 7(1)
	8	0.000 066	0.000 066 1	0.013 271 0	−0.001 858 0	0.008 716 4(1)
	9	0.000 072	0.000 783 4	0.013 657 8	−0.001 735 7	0.007 083 6(1)
	10	0.000 074	0.001 420 7	0.013 959 9	−0.001 624 3	0.005 604 8(1)
	∞[extrap.]	−0.000 03	0.009 945	0.016 2473	0.000 000 8	−0.015 283
	∞[exact]	0	0.009 947	0.016 2471	0	−0.015 296

part of the Breit-Pauli Hamiltonian (see Eq. (3) of Ref. [8]).

The second part of $\mathcal{E}^{(7)}$ is induced by effective Hamiltonians to order $m\alpha^7$, which were derived by one of us (K.P.) in Refs. [7, 8]. (The previous derivation of this correction by Zhang [14] turned out to be not entirely consistent.) The result is

$$\mathcal{E}^{(7)}_{\rm first} = \left\langle H_Q + H_H + H^{(7)}_{\rm fs,amm} \right\rangle , \tag{4}$$

where the Hamiltonian H_Q is induced by the two-photon exchange between the electrons, the electron self-energy, and the vacuum polarization, H_H represents the anomalous magnetic moment (amm) correction to the Douglas-Kroll operators (see Eq. (101) of Ref. [8]), and $H^{(7)}_{\rm fs,amm}$ is the $m\alpha^7$ part of the Breit-Pauli Hamiltonian with inclusion of the amm effect (see Eq. (3) of Ref. [8]). The Hamiltonian H_Q is

$$\begin{aligned} H_Q \; &= Z\,\frac{91}{180}\, i\,\vec p_1 \times \delta^3(r_1)\,\vec p_1\cdot\vec\sigma_1 \\ &- \frac{1}{2}\,(\vec\sigma_1\cdot\vec\nabla)\,(\vec\sigma_2\cdot\vec\nabla)\,\delta^3(r)\,\left[\frac{83}{30}+\ln Z\right] \\ &+ 3\,i\,\vec p_1\times\delta^3(r)\,\vec p_1\cdot\vec\sigma_1\,\left[\frac{23}{10}-\ln Z\right] \\ &- \frac{15}{8\,\pi}\,\frac{1}{r^7}\,(\vec\sigma_1\cdot\vec r)\,(\vec\sigma_2\cdot\vec r) - \frac{3}{4\,\pi}\,i\,\vec p_1\times\frac{1}{r^3}\,\vec p_1\cdot\vec\sigma_1\,. \end{aligned} \tag{5}$$

Here, the terms with $\ln Z$ compensate the logarithmic dependence implicitly present in expectation values of singular operators $1/r^3$ and $1/r^5$.

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

$$\begin{aligned} \mathcal{E}^{(7)}_{\rm sec} &= 2\left\langle H^{(4)}_{\rm fs}\,\frac{1}{(E_0-H_0)'}\,H^{(5)}_{\rm nlog}\right\rangle \\ &+ 2\left\langle H^{(4)}\,\frac{1}{(E_0-H_0)'}\,H^{(5)}_{\rm fs}\right\rangle , \end{aligned} \tag{6}$$

where $H^{(4)} = H^{(4)}_{\rm fs} + H^{(4)}_{\rm nfs}$ is the Breit-Pauli Hamiltonian (see Eq. (6) of Ref. [8]), $H^{(5)}_{\rm fs}$ is the amm correction to $H^{(4)}_{\rm fs}$ and

$$H^{(5)}_{\rm nlog} = -\frac{7}{6\,\pi\,r^3} + \frac{38 Z}{45}\,\left[\delta^3(r_1)+\delta^3(r_2)\right] . \tag{7}$$

The fourth part of $\mathcal{E}^{(7)}$ is the low-energy contribution $\mathcal{E}^{(7)}_L$ that can be interpreted as the relativistic correction to the Bethe logarithm. It is given by [4]

$$\begin{aligned} &\mathcal{E}^{(7)}_L = \\ &-\frac{2}{3\,\pi}\,\delta\left\langle(\vec p_1+\vec p_2)\,(H_0-E_0)\ln\left[\frac{2(H_0-E_0)}{Z^2}\right](\vec p_1+\vec p_2)\right\rangle \\ &+\frac{i\,Z^2}{3\,\pi}\Big\langle\left(\frac{\vec r_1}{r_1^3}+\frac{\vec r_2}{r_2^3}\right)\times\frac{\vec\sigma_1+\vec\sigma_2}{2}\,\ln\left[\frac{2(H_0-E_0)}{Z^2}\right]\left(\frac{\vec r_1}{r_1^3}+\frac{\vec r_2}{r_2^3}\right)\Big\rangle , \end{aligned} \tag{8}$$

where $\delta\,\langle\ldots\rangle$ denotes the first-order perturbation of the matrix element $\langle\ldots\rangle$ by $H^{(4)}_{\rm fs}$.

Our calculational results for the corrections of order $m\alpha^7$ and $m^2\alpha^6/M$ are listed in Table I. For the logarithmic part $\mathcal{E}^{(7)}_{\rm log}$, our results fully confirm the previous

TABLE II: Individual contributions to the $2^3P_J - 2^3P_{J'}$ fine-structure intervals of helium-like atoms, in MHz/Z^4.

(J,J')	Z	$m\alpha^4$	$m\alpha^5$	$m\alpha^6$	$m\alpha^7$(log)	$m\alpha^7$(nlog)	Total
(0,1)	2	1847.73534	3.41900	−0.10109	0.00509	0.00118	1851.05952(11)
	3	1917.79396	3.24978	1.2278	−0.01076	0.01801	1922.27881(59)
	4	1346.96534	1.94384	4.5603	−0.02843	0.04648	1353.4875(39)
	5	765.88557	0.68551	10.360	−0.04139	0.08628	776.976(14)
	6	270.38772	−0.36757	19.239	−0.04886	0.13952	289.349(37)
	7	−139.08557	−1.22955	31.863	−0.05110	0.20903	−108.294(83)
	8	−477.53446	−1.93791	48.920	−0.04855	0.29785	−430.30(17)
	9	−759.77039	−2.52632	71.110	−0.04163	0.40916	−690.82(31)
	10	−997.72326	−3.02103	99.120	−0.03076	0.54619	−901.11(53)
(0,2)	2	1992.75043	2.00994	−0.50717	0.00472	0.00028	1994.25820(11)
	3	1150.27490	−0.94285	−0.86465	−0.02216	0.01483	1148.46007(41)
	4	−384.65915	−4.44824	−1.3897	−0.04539	0.03204	−390.5104(12)
	5	−1739.32853	−7.32066	−2.3939	−0.05446	0.04661	−1749.0509(32)
	6	−2838.55028	−9.58033	−3.9945	−0.04868	0.05688	−2852.1169(77)
	7	−3724.42192	−11.37060	−6.2453	−0.02903	0.06215	−3742.005(16)
	8	−4445.63274	−12.81245	−9.174	0.00327	0.06207	−4467.554(31)
	9	−5041.00923	−13.99389	−12.797	0.04705	0.05647	−5067.697(55)
	10	−5539.33827	−14.97737	−17.124	0.10127	0.04523	−5571.293(91)

calculation [3]. The recoil correction $\mathcal{E}_M^{(6)}$ and a part of the second-order contribution $\mathcal{E}_{\rm sec}^{(7)}$ were calculated for helium by Drake [5]. Our results agree with those of Drake for the second-order part but differ by about 5% for the recoil correction. The difference entails a small shift of about 0.5 kHz for the ν_{01} and ν_{12} intervals. The helium results listed in Table I differ from those reported by us previously [8] only in the Bethe logarithm part $\mathcal{E}_L^{(7)}$. By checking the hydrogenic limit for this correction, we found that our previous evaluation [8] contained a mistake. Its source was a term missing in the final expressions for E_{L1}. More specifically, $\ln K$ and $\ln\kappa$ in Eqs. (168) and (173) of that work should be replaced by $\ln(2K/Z^2)$ and $\ln(2\kappa/Z^2)$, respectively. (To note, the term in question was correctly accounted for in the original calculation [4].) This term increases the theoretical values of the ν_{01} and ν_{12} intervals by 6.1 and 1.6 kHz, respectively.

Table I also presents the results for the high-Z limit of individual $m\alpha^7$ corrections. This limit was evaluated numerically by fitting the $1/Z$ expansion of our numerical data and compared to the analytical results known from the hydrogen theory [16]. A remarkable feature of the $m\alpha^7$ corrections is their strong Z dependence. Table I demonstrates that for the largest Z studied, the values of $\mathcal{E}_{\rm log}^{(7)}$ and $\mathcal{E}_L^{(7)}$ are still very different from their hydrogenic limits (even the sign is often opposite).

Combining the results presented in Table I with the contributions of lower orders from our previous investigation [13], we obtain total theoretical values of the fine-structure intervals in light helium-like atoms summarized in Table II. The uncertainties quoted in the table are due to uncalculated effects to order $m\alpha^8$. These effects were estimated by scaling the $m\alpha^6$ correction by the factor of $(Z\alpha)^2$. For helium, the estimates for the ν_{01} and ν_{12} intervals were obtained by taking the $m\alpha^6$ correction for ν_{02}. In all other instances, the $m\alpha^6$ correction for the corresponding interval was taken. It is remarkable that in all the cases except helium, the theoretical accuracy is significantly (usually by a factor of $1/Z$) better for the ν_{02} interval than for ν_{01} and ν_{12}. This is due to the absence of the leading term in the $1/Z$ expansion of the $m\alpha^6$ correction (and some others) for the ν_{02} interval.

We note that the present calculation is performed for a spinless nucleus. For a nucleus with spin, the hyperfine splitting (hfs) can usually be evaluated separately and employed for an experimental determination of the fine structure. This procedure, however, ignores the mixing between the hfs and the fine structure. So, more accurate calculations should account for both effects simultaneously.

The comparison with experiment is summarized in Table III. The agreement between theory and experiment is usually very good. The only significant discrepancy is for Be^{2+}, where the difference amounts to 1.7 standard deviations (σ) for ν_{12} and $3.5\,\sigma$ for ν_{02}. Our result for the ν_{01} interval of helium agrees well with the experimental values [9, 18, 19]. For the ν_{12} interval, our theory is by about 2σ away from the values obtained in Refs. [9, 24] but in agreement with the latest measurement by Hessels and coworkers [17].

Assuming the validity of the theory, we combine the theoretical prediction for the ν_{01} interval in helium with the experimental result [9] and obtain the following value of the fine structure constant,

$$\alpha^{-1}(\mathrm{He}) = 137.036\,001\,1\,(39)_{\rm theo}\,(16)_{\rm exp}\,, \qquad (9)$$

which is accurate to 31 ppb and agrees with the more precise results of Refs. [10, 11]. The theoretical uncertainty

TABLE III: Comparison of theoretical and experimental results for the fine-structure intervals of helium-like atoms. Units are MHz for He and Li^+ and cm^{-1} for other atoms.

(J,J')	Z	Present work	Experiment	Ref.
(0,1)	2	29 616.952 3(17)	29 616.951 66(70)	[9]
			29 616.952 7(10)	[18]
			29 616.950 9(9)	[19]
	3	155 704.584(48)	155 704.27(66)	[20]
	4	11.557 756(33)	11.558 6(5)	[21]
	5	16.198 21(29)	16.203(18)	[22]
	7	−8.673 1(67)	−8.670 7(7)	[23]
(1,2)	2	2291.178 9(17)	2 291.177 53(35)	[17]
			2 291.175 59(51)	[9]
			2 291.175 9(10)	[24]
	9	−957.886(79)	−957.873 0(12)	[25]
(0,2)	3	93 025.266(34)	93 025.86(61)	[20]
	4	−3.334 663(10)	−3.336 4(5)	[21]
	5	−36.463 787(66)	−36.457(16)	[22]

of the above value of α is more than twice larger than the experimental one. In order to improve the theoretical accuracy, one has to calculate the $m\alpha^8$ correction. Its complete evaluation is extremely difficult. One can hope, however, to identify the dominant part of this effect, since most of $m\alpha^8$ operators should be negligible. This task is simpler to accomplish for the ν_{02} interval, since the effects of the triplet-singlet mixing are absent in this case. It is also possible to estimate the $m\alpha^8$ correction from an independent measurement for a different Z. So, an accurate experimental determination of the ν_{02} interval in a light helium-like ion (preferably, $^{12}C^{4+}$ since it has a spinless nucleus) would yield an estimate for the $m\alpha^8$ term in helium with a 50% accuracy, thus reducing the theoretical uncertainty of this interval by a factor of 2.

In summary, our present study concludes the evaluation of the $m\alpha^7$ correction to the fine structure of light helium-like atoms and resolves the discrepancy between theory and experiment reported in the literature. The theoretical values agree with the latest experimental results for helium, as well as with most of the experimental data for helium-like ions. A combination of the theoretical and experimental results for the $2^3P_1 - 2^3P_0$ interval in helium yields an independent determination of the fine structure constant α accurate to 31 ppb. The precision will be increased further when more accurate estimates of the higher-order effects are obtained from theoretical or experimental studies.

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