Fine structure of helium and light helium-like ions

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Calculational results are presented for the fine-structure splitting of the 2^3P state of helium and helium-like ions with the nuclear charge Z up to 10. Theoretical predictions are in agreement with the latest experimental results for the helium fine-structure intervals as well as with the most of the experimental data available for light helium-like ions. Comparing the theoretical value of the $2^3P_0 - 2^3P_1$ interval in helium with the experimental result [T. Zelevinsky *et al.* Phys. Rev. Lett. **95**, 203001 (2005)], we determine the value of the fine-structure constant α with an accuracy of 31 parts per billion.

PACS numbers: 06.20.Jr, 31.30.jf, 12.20.Ds, 31.15.aj

I. INTRODUCTION

The fine structure splitting of the 2^3P state in helium plays a special role in atomic spectroscopy because it can be used for an accurate determination of the fine structure constant α. This fact was first pointed out by Schwartz in 1964 [1]. The attractive features of the fine structure splitting in helium 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 of the fine structure. Schwartz's suggestion stimulated a sequence of calculations [2–5], 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 [7, 8]. In order to match this level of accuracy in the 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 [9–19]. In 2006, the first complete evaluation of the $m\alpha^7$ correction to the helium fine structure was reported [20]. However, the numerical results presented there disagreed with the experimental values by more than 10 standard deviations.

In our recent investigations [21, 22], we recalculated 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 ($Z \to \infty$) limit of individual corrections and by comparing them with the results known from the hydrogen theory. We found several problems in previous studies. 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. Comparison of our theoretical prediction for the $2^3P_0 - 2^3P_1$ interval in helium (accurate to 57 ppb) with the experimental value [7] (accurate to 24 ppb) determines the value of the fine structure constant α with an accuracy of 31 ppb.

The calculation of the $m\alpha^7$ correction for the fine-structure splitting of light helium-like atoms was reported in our recent Letter [22]. In this paper, we present an extended description of the $m\alpha^7$ correction and a detailed term-by-term comparison of our results with independent calculations by Drake [18] for helium and by Zhang *et al.* [12] for helium-like ions.

II. THE SPIN-DEPENDENT $m\alpha^7$ CORRECTION

The $m\alpha^7$ correction to the fine-structure splitting of a two-electron atom can be conveniently separated into four parts,

$$E^{(7)} \equiv m\alpha^7 \mathcal{E}^{(7)} = m\alpha^7 \left[\mathcal{E}^{(7)}_{\rm log} + \mathcal{E}^{(7)}_{\rm first} + \mathcal{E}^{(7)}_{\rm sec} + \mathcal{E}^{(7)}_{L}\right]. \tag{1}$$

The first term in the brackets above combines all terms with $\ln Z$ and $\ln\alpha$ [10–12, 15, 20],

$$\begin{aligned}\mathcal{E}^{(7)}_{\rm log} &= \ln[(Z\,\alpha)^{-2}]\,\biggl[\biggl\langle\frac{2Z}{3}\,i\,\vec p_1\times\delta^3(r_1)\,\vec p_1\cdot\vec\sigma_1\biggr\rangle \\ &-\biggl\langle\frac{1}{4}(\vec\sigma_1\cdot\vec\nabla)\,(\vec\sigma_2\cdot\vec\nabla)\delta^3(r)\biggr\rangle-\biggl\langle\frac{3}{2}\,i\,\vec p_1\times\delta^3(r)\,\vec p_1\cdot\vec\sigma_1\biggr\rangle \\ &+\frac{8Z}{3}\biggl\langle H^{(4)}_{\rm fs}\frac{1}{(E_0-H_0)'}\,[\delta^3(r_1)+\delta^3(r_2)]\biggr\rangle\biggr]\,,\end{aligned}\tag{2}$$

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 part of the Breit-Pauli Hamiltonian,

$$\begin{aligned}H^{(4)}_{\rm fs} &= \frac{1}{4\,r^3}\Bigl[\bigl(\vec\sigma_2+2\,\vec\sigma_1\bigr)\cdot\vec r\times\vec p_2-\bigl(\vec\sigma_1+2\,\vec\sigma_2\bigr)\cdot\vec r\times\vec p_1\Bigr] \\ &+\frac{Z}{4}\left(\frac{\vec r_1}{r_1^3}\times\vec p_1\cdot\vec\sigma_1+\frac{\vec r_2}{r_2^3}\times\vec p_2\cdot\vec\sigma_2\right) \\ &+\frac{1}{4}\left(\frac{\vec\sigma_1\cdot\vec\sigma_2}{r^3}-3\,\frac{\vec\sigma_1\cdot\vec r\,\vec\sigma_2\cdot\vec r}{r^5}\right)\,.\end{aligned}\tag{3}$$

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 [10, 11] turned out to be not entirely consistent.) The result is

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

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]

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

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

$$\begin{aligned}\int d^3r\frac{1}{r^3}\,f(\vec r)\equiv\lim_{\epsilon\to0}\int d^3r\,\biggl[&\frac{1}{r^3}\,\theta(r-\epsilon) \\ &+4\,\pi\,\delta^3(r)\,(\gamma+\ln\epsilon)\biggr]\,f(\vec r)\,,\end{aligned}\tag{6}$$

and

$$\begin{aligned}&\int d^3r\,\frac{1}{r^7}\left(r^i\,r^j-\frac{\delta^{ij}}{3}\,r^2\right)f(\vec r)\equiv \\ &\quad\lim_{\epsilon\to0}\int d^3r\,\biggl[\frac{1}{r^7}\left(r^i\,r^j-\frac{\delta^{ij}}{3}\,r^2\right)\theta(r-\epsilon) \\ &\quad+\frac{4\,\pi}{15}\,\delta^3(r)\,(\gamma+\ln\epsilon)\left(\partial^i\,\partial^j-\frac{\delta^{ij}}{3}\,\partial^2\right)\biggr]\,f(\vec r)\,,\end{aligned}\tag{7}$$

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]

$$\begin{aligned}
H_H \;&= -\frac{Z}{4}\,p_1^2\,\frac{\vec{r}_1}{r_1^3}\times\vec{p}_1\cdot\vec{\sigma}_1-\frac{3\,Z}{4}\,\frac{\vec{r}_1}{r_1^3}\times\frac{\vec{r}}{r^3}\cdot\vec{\sigma}_1\,(\vec{r}\cdot\vec{p}_2)+\frac{3\,Z}{4}\,\frac{\vec{r}}{r^3}\cdot\vec{\sigma}_1\,\frac{\vec{r}_1}{r_1^3}\cdot\vec{\sigma}_2+\frac{1}{2\,r^4}\,\vec{r}\times\vec{p}_2\cdot\vec{\sigma}_1-\frac{3}{4\,r^6}\,\vec{r}\cdot\vec{\sigma}_1\,\vec{r}\cdot\vec{\sigma}_2\\
&-\frac{1}{4}\,p_1^2\,\frac{\vec{r}}{r^3}\times\vec{p}_1\cdot\vec{\sigma}_1-\frac{1}{4}\,p_1^2\,\frac{\vec{r}}{r^3}\times\vec{p}_2\cdot\vec{\sigma}_1-\frac{Z}{4\,r}\,\frac{\vec{r}_1}{r_1^3}\times\vec{p}_2\cdot\vec{\sigma}_1-\frac{i}{2}\,p_1^2\,\frac{1}{r^3}\,\vec{r}\cdot\vec{p}_2\,\vec{r}\times\vec{p}_1\cdot\vec{\sigma}_1+\frac{3\,i}{4\,r^5}\,\vec{r}\times(\vec{r}\cdot\vec{p}_2)\,\vec{p}_1\cdot\vec{\sigma}_1\\
&-\frac{3}{8\,r^5}\,\vec{r}\times(\vec{r}\times\vec{p}_1\cdot\vec{\sigma}_1)\,\vec{p}_2\cdot\vec{\sigma}_2-\frac{1}{8\,r^3}\,\vec{p}_1\cdot\vec{\sigma}_2\,\vec{p}_2\cdot\vec{\sigma}_1+\frac{21}{16}\,p_1^2\,\frac{1}{r^5}\,\vec{r}\cdot\vec{\sigma}_1\,\vec{r}\cdot\vec{\sigma}_2-\frac{3\,i}{8}\,p_1^2\,\frac{\vec{r}}{r^3}\cdot\vec{\sigma}_1\,\vec{p}_1\cdot\vec{\sigma}_2\\
&+\frac{i}{8}\,p_1^2\,\frac{1}{r^3}\left[\vec{r}\cdot\vec{\sigma}_2\,\vec{p}_2\cdot\vec{\sigma}_1+(\vec{r}\cdot\vec{\sigma}_1)\,(\vec{p}_2\cdot\vec{\sigma}_2)-\frac{3}{r^2}\,\vec{r}\cdot\vec{\sigma}_1\,\vec{r}\cdot\vec{\sigma}_2\,\vec{r}\cdot\vec{p}_2\right]-\frac{1}{4}\,\vec{p}_1\cdot\vec{\sigma}_1\,\vec{p}_1\times\frac{\vec{r}}{r^3}\cdot\vec{p}_2\\
&+\frac{1}{8}\,\vec{p}_1\cdot\vec{\sigma}_1\left[-\vec{p}_1\cdot\vec{\sigma}_2\,\frac{1}{r^3}+3\vec{p}_1\cdot\vec{r}\,\frac{\vec{r}}{r^5}\cdot\vec{\sigma}_2\right]. \qquad (8)
\end{aligned}$$

The Hamiltonian $H^{(7)}_{\rm fs}$ is the $m\alpha^7$ amm correction to the Breit-Pauli Hamiltonian,

$$\begin{aligned}
H^{(7)}_{\rm fs} &= \frac{1}{2\pi^3\,r^3}\,(\vec{\sigma}_1+\vec{\sigma}_2)\cdot\vec{r}\times(\vec{p}_2-\vec{p}_1)\,c_3\\
&+\frac{Z}{2\pi^3}\left(\frac{\vec{r}_1}{r_1^3}\times\vec{p}_1\cdot\vec{\sigma}_1+\frac{\vec{r}_2}{r_2^3}\times\vec{p}_2\cdot\vec{\sigma}_2\right)c_3\\
&+\frac{1}{2\pi^3}\left(\frac{\vec{\sigma}_1\cdot\vec{\sigma}_2}{r^3}-3\,\frac{\vec{\sigma}_1\cdot\vec{r}\,\vec{\sigma}_2\cdot\vec{r}}{r^5}\right)(c_1c_2+c_3)\;, \qquad (9)
\end{aligned}$$

where $c_1=1/2$, $c_2=-0.328\,478\,965$ and $c_3=1.181\,241\,456$ are the expansion coefficients of the free-electron amm in powers of (α/π).

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

$$\begin{aligned}
\mathcal{E}^{(7)}_{\rm sec} &= 2\left\langle H^{(4)}_{\rm fs}\frac{1}{(E_0-H_0)'}H^{(5)}_{\rm nlog}\right\rangle\\
&+2\left\langle\left[H^{(4)}_{\rm fs}+H^{(4)}_{\rm nfs}\right]\frac{1}{(E_0-H_0)'}H^{(5)}_{\rm fs}\right\rangle\;, \qquad (10)
\end{aligned}$$

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

$$H^{(5)}_{\rm nlog} = -\frac{7}{6\,\pi\,r^3}+\frac{38Z}{45}\,\left[\delta^3(r_1)+\delta^3(r_2)\right]\;, \qquad (11)$$

$H^{(4)}_{\rm nfs}$ is the spin-independent part of the Breit-Pauli Hamiltonian (with the term $\propto\delta^3(r)$ omitted since it does not contribute in our case),

$$\begin{aligned}
H^{(4)}_{\rm nfs} \;&=\; -\frac{1}{8}\,(p_1^4+p_2^4)+\frac{Z\,\pi}{2}\,\left[\delta^3(r_1)+\delta^3(r_2)\right]\\
&-\frac{1}{2}\,p_1^i\left(\frac{\delta^{ij}}{r}+\frac{r^i\,r^j}{r^3}\right)p_2^j\,, \qquad (12)
\end{aligned}$$

and $H^{(5)}_{\rm fs}$ is the $m\alpha^5$ amm correction to $H^{(4)}_{\rm fs}$,

$$\begin{aligned}
H^{(5)}_{\rm fs} &= \frac{1}{4\pi\,r^3}\,(\vec{\sigma}_1+\vec{\sigma}_2)\cdot\vec{r}\times(\vec{p}_2-\vec{p}_1)\\
&+\frac{Z}{4\pi}\left(\frac{\vec{r}_1}{r_1^3}\times\vec{p}_1\cdot\vec{\sigma}_1+\frac{\vec{r}_2}{r_2^3}\times\vec{p}_2\cdot\vec{\sigma}_2\right)\\
&+\frac{1}{4\pi}\left(\frac{\vec{\sigma}_1\cdot\vec{\sigma}_2}{r^3}-3\,\frac{\vec{\sigma}_1\cdot\vec{r}\,\vec{\sigma}_2\cdot\vec{r}}{r^5}\right)\;. \qquad (13)
\end{aligned}$$

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 $\mathcal{E}^{(7)}_L$ and interpreted as the relativistic correction to the Bethe logarithm. The expression for

TABLE I: Summary of individual contributions to the fine-structure intervals in helium, in kHz. The parameters [23] 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 values by Drake are taken from Table 3 of Ref. [18]. The label $(+m/M)$ indicates that the corresponding entry comprises both the non-recoil and recoil contributions of the specified order in α. The uncertainty due to the value of α is not shown.

Term	ν_{01}	ν_{12}	Ref.
$m\alpha^4(+m/M)$	29 563 765.45	2 320 241.43	
	29 563 765.23^a	2 320 241.42^a	[18]
$m\alpha^5(+m/M)$	54 704.04	−22 544.00	
	54 704.04	−22 545.01	[18]
$m\alpha^6$	−1 607.52(2)	−6 506.43	
	−1 607.61(4)	−6 506.45(7)	[18]
$m\alpha^6 m/M$	−9.96	9.15	
	−10.37(5)	9.80(11)	[18]
$m\alpha^7\log(Z\alpha)$	81.43	−5.87	
	81.42^b	−5.87^b	[18]
$m\alpha^7$, nlog	18.86	−14.38	
$m\alpha^8$	±1.7	±1.7	
Total theory	29 616 952.29 ± 1.7	2 291 178.91 ± 1.7	
Experiment	29 616 951.66(70)^c	2 291 177.53(35)^f	
	29 616 952.7(10)^d	2 291 175.59(51)^c	
	29 616 950.9(9)^e	2 291 175.9(10)^g	

^{a} the original result was scaled to the present value of α.
^{b} the original result was altered by the substitution $\ln(\alpha) \to \ln(Z\alpha)$ in the terms proportional to $\ln(\alpha)$, in order to comply with the present result for the logarithmic $m\alpha^7$ contribution.
^{c} Ref. [7]. ^{d} Ref. [24]. ^{e} Ref. [25]. ^{f} Ref. [8]. ^{g} Ref. [26].

$\mathcal{E}_L^{(7)}$ reads [16]

$$\mathcal{E}_L^{(7)} = -\frac{2}{3\,\pi}\,\delta\left\langle (\vec{p}_1+\vec{p}_2)\,\cdot (H_0-E_0)\ln\left[\frac{2(H_0-E_0)}{Z^2}\right](\vec{p}_1+\vec{p}_2)\right\rangle + \frac{i\,Z^2}{3\,\pi}\left\langle\left(\frac{\vec{r}_1}{r_1^3}+\frac{\vec{r}_2}{r_2^3}\right)\times\frac{\vec{\sigma}_1+\vec{\sigma}_2}{2}\ln\left[\frac{2(H_0-E_0)}{Z^2}\right]\left(\frac{\vec{r}_1}{r_1^3}+\frac{\vec{r}_2}{r_2^3}\right)\right\rangle, \tag{14}$$

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

III. RESULTS: HELIUM

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

$$\nu_{01} = \big[E(2^3P_0) - E(2^3P_1)\big]/h\,, \tag{15}$$
$$\nu_{12} = \big[E(2^3P_1) - E(2^3P_2)\big]/h\,. \tag{16}$$

We note that the style of breaking the total result into separate entries used in Table I differs from that used in the summary tables of the previous papers by K.P. *et al.* [20, 21]. Particulary, 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 I contain only the contributions of the order specified.

A term-by-term comparison with the independent calculation by Drake [18] is made whenever possible. We observe good agreement between the two calculations for the lower-order terms, 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

TABLE II: Individual contributions to the fine-structure intervals of helium-like atoms, in MHz/Z^4. The label $(+m/M)$ indicates that the corresponding entry comprises both the non-recoil and recoil contributions of the specified order in α. For Z = 3, 7, and 10, a term-by-term comparison is made with the previous calculation by Zhang *et. al.* [12]. The results of Ref. [12] for the leading $m\alpha^4$ correction were scaled to the present value of α. The deviation for the $m\alpha^7$(log) contribution is due to the difference in the expressions for this term.

Z	$m\alpha^4(+m/M)$	$m\alpha^5(+m/M)$	$m\alpha^6$	$m\alpha^6 m/M$	$m\alpha^7$(log)	$m\alpha^7$(nlog)	Total	Ref.
ν_{01}								
2	1847.735 34	3.419 00	−0.100 47	−0.000 62	0.005 09	0.001 18	1851.059 52 (11)	
3	1917.793 96	3.249 78	1.230 26	−0.002 43	−0.010 76	0.018 01	1922.278 81 (59)	
	1917.793 97	3.249 78	1.230 25		−0.010 27		1922.26 (2)	[12]
4	1346.965 34	1.943 84	4.566 98	−0.006 70	−0.028 43	0.046 48	1353.4875 (39)	
5	765.885 57	0.685 51	10.374 47	−0.014 17	−0.041 39	0.086 28	776.976 (14)	
6	270.387 72	−0.367 57	19.266 47	−0.027 89	−0.048 86	0.139 52	289.349 (37)	
7	−139.085 57	−1.229 55	31.908 79	−0.045 30	−0.051 10	0.209 03	−108.294 (83)	
	−139.085 58	−1.229 55	31.908 82		−0.046 33		−108.5 (3)	[12]
8	−477.534 46	−1.937 91	48.988 80	−0.068 79	−0.048 55	0.297 85	−430.30 (17)	
9	−759.770 39	−2.526 32	71.203 90	−0.093 96	−0.041 63	0.409 16	−690.82 (31)	
10	−997.723 26	−3.021 03	99.257 05	−0.137 44	−0.030 76	0.546 19	−901.11 (53)	
	−997.723 25	−3.021 03	99.257 05		−0.021 29		−901.5	[12]
ν_{02}								
2	1992.750 43	2.009 94	−0.507 12	−0.000 05	0.004 72	0.000 28	1994.258 20 (11)	
3	1150.274 90	−0.942 85	−0.864 60	−0.000 05	−0.022 16	0.014 83	1148.460 07 (41)	
	1150.274 91	−0.942 85	−0.864 60		−0.023 48		1148.44 (2)	[12]
4	−384.659 15	−4.448 24	−1.389 63	−0.000 06	−0.045 39	0.032 04	−390.5104 (12)	
5	−1739.328 53	−7.320 66	−2.393 83	−0.000 04	−0.054 46	0.046 61	−1749.0509 (32)	
6	−2838.550 28	−9.580 33	−3.994 54	0.000 01	−0.048 68	0.056 88	−2852.1169 (77)	
7	−3724.421 92	−11.370 60	−6.245 32	0.000 08	−0.029 03	0.062 15	−3742.005 (16)	
	−3724.421 93	−11.370 60	−6.263 64		−0.041 90		−3742.1 (3)	[12]
8	−4445.632 74	−12.812 45	−9.174 16	0.000 17	0.003 27	0.062 07	−4467.554 (31)	
9	−5041.009 23	−13.993 89	−12.797 23	0.000 25	0.047 05	0.056 47	−5067.697 (55)	
10	−5539.338 27	−14.977 37	−17.124 41	0.000 38	0.101 27	0.045 23	−5571.293 (91)	
	−5539.338 27	−14.977 38	−17.145 16		0.075 67		−5571.4	[12]

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 estimates of the uncalculated higher-order effects for helium are much larger than those in the previous studies [17, 18]. The previous estimates amounted to significantly less than 1 kHz for both intervals and were based on some logarithmic contributions to order $m\alpha^8$ that were identified by analogy with the hydrogen fine structure. We now believe that the dominant $m\alpha^8$ contribution might be of relativistic origin. Our estimates of ±1.7 kHz for both intervals were obtained by multiplying the $m\alpha^6$ contribution for the sum of $\nu_{01} + \nu_{12}$ by the factor of $(Z\alpha)^2$.

Our result for the ν_{01} interval of helium agrees well with the experimental values [7, 24, 25]. For the ν_{12} interval, our theory is by about 2σ away from the values obtained in Refs. [7, 26] but in agreement with the latest measurement by Hessels and coworkers [8]. Assuming the validity of the theory, we combine the theoretical prediction for the ν_{01} interval in helium with the experimental result [7] and obtain the following value of the fine structure constant,

$$\alpha^{-1}(\text{He}) = 137.036\,001\,1\,(39)_{\text{theo}}\,(16)_{\text{exp}}\,, \tag{17}$$

which is accurate to 31 ppb and agrees with the more precise results of Refs. [27–29].

IV. RESULTS: HELIUM-LIKE IONS

Table II gives the summary of individual contributions to the fine-structure intervals of helium-like atoms with the nuclear charge number Z up to 10. We choose to present results for the intervals ν_{01} and $\nu_{02} \equiv \nu_{01} + \nu_{12}$, and not for ν_{01} and ν_{12}, as is customary. The reason to consider ν_{02} is that this interval is free from effects of the $2^3P_1 - 2^1P_1$ mixing, which strongly affect the ν_{01} and ν_{12} intervals. As a result of the absence of the mixing effects, all corrections to ν_{02} starting with the order of $m\alpha^6$ demonstrate a weaker Z dependence as compared to those to ν_{01} and ν_{12}. The most drastic difference occurs for the $\alpha^6 m^2/M$ correction: for $Z = 10$, this correction for ν_{02} is by 3 orders of magnitude smaller than that for ν_{01}.

The uncertainty of the theoretical values specified in Table II is solely due to uncalculated higher-order effects. Its estimation for helium was already discussed. For helium-like ions, we obtain the uncertainty by multiplying the $m\alpha^6$ contribution for the corresponding interval by the factor of $(Z\alpha)^2$. So, our error estimates are typically by a factor of $1/Z$ smaller for the ν_{02} interval than for the ν_{01} (or, equivalently, ν_{12}) interval.

For $Z = 3$, 7, and 10, Table II presents a term-by-term comparison with the previous calculation by Zhang *et. al.* [12]. We observe excellent agreement for the $m\alpha^4$ and $m\alpha^5$ corrections. For the $m\alpha^6$ correction, the agreement is excellent in all cases except for the ν_{02} interval and $Z = 7$ and 10, where a small deviation is present. The results of the two calculations for the $m\alpha^7$(log) correction are different, but this is explained by the difference in the expressions for this term. If we use the same expression as in Ref. [12], excellent agreement is found again.

In Fig. 1 we plot our numerical results for the $m\alpha^7$ correction as a function of the nuclear charge number Z, together with the fit of the $1/Z$ expansion and with the asymptotical high-Z limit of this correction. The form of the $1/Z$ expansion and the values of the first coefficient(s) are known. For the ν_{02} interval, the leading term scales as Z^6 and is calculated for hydrogen in Ref. [30]. For the ν_{12} interval, there are additional Z^7 and Z^6 contributions due to the triplet-singlet mixing, which are obtained by expanding the following expression in $1/Z$,

$$\delta E_{\rm mix} = \frac{\left|\langle 2^1P_1|H^{(4)}_{\rm fs}|2^3P_1\rangle\right|^2}{E_0(2^3P_1) - E_0(2^1P_1)}\,.$$

The resulting asymptotic form of the nonlogarithmic $m\alpha^7$ correction is

$$\mathcal{E}^{(7,\rm nlog)}(\nu_{01})/Z^7 = 0.004045 - 0.015524/Z + O(1/Z^2)\,, \tag{18}$$

$$\mathcal{E}^{(7,\rm nlog)}(\nu_{02})/Z^6 = -0.021706 + O(1/Z)\,. \tag{19}$$

By fitting the $1/Z$ expansion of our numerical data for $\mathcal{E}^{(7,\rm nlog)}$, we were able to reproduce well the values of the coefficients given above, which served as an important check of our calculations.

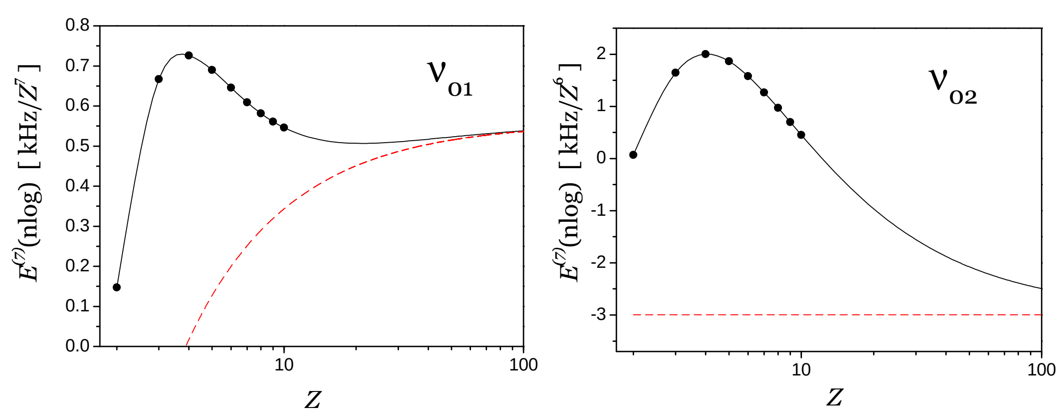

FIG. 1: Nonlogarithmic $m\alpha^7$ correction to the fine-structure intervals of helium-like atoms, for the ν_{01} interval (left) and for the ν_{02} interval (right). Black dots denote the numerical results, solid line stands for the fit of the $1/Z$ expansion, and the dashed (red) line indicates the asymptotic high-Z results. Note that the results in different graphs are scaled by different factors. It is Z^7 for the ν_{01} interval and Z^6, for ν_{02}. The different Z scaling is the consequence of the triplet-singlet mixing effects.

The comparison of the present theoretical predictions with experiment data is summarized in Table III. The agreement is very good in most cases. The only significant discrepancy is for Be^{2+}, where the difference of 1.7 standard deviations (σ) is observed for ν_{12} and that of $3.5\,\sigma$, for ν_{02}. It is important that for both the ν_{01} and ν_{12} intervals there are experimental results available for helium-like ions, whose accuracy significantly exceeds the theoretical errors. These are the measurement of ν_{01} in helium-like nitrogen by Thompson *at al.* [31] and that of ν_{12} in helium-like fluorine by Myers *et al.* [32]. Good agreement of the present theory with these experimental results suggests that the theoretical errors (i.e., the uncalculated higher-order effects) were reasonably estimated. It is

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

Z	Present theory	Experiment	Ref.
ν_{01}			
3	155 704.584(48)	155 704.27(66)	[33]
4	11.557 756(33)	11.558 6(5)	[34]
5	16.198 21(29)	16.203(18)	[35]
7	−8.673 1(67)	−8.670 7(7)	[31]
8	−58.791 (23)	−59.2 (1.1)	[36]
10	−300.58(18)	−300.7(2.2)	[36]
ν_{12}			
9	−957.886(79)	−957.873 0(12)	[32]
ν_{02}			
3	93 025.266(34)	93 025.86(61)	[33]
4	−3.334 663(10)	−3.336 4(5)	[34]
5	−36.463 787(66)	−36.457(16)	[35]
8	−610.392 3(42)	−611.3(7)	[36]
10	−1858.383 (30)	−1858.3(1.5)	[36]

unfortunate that there are no experimental results with comparable accuracy available for the ν_{02} interval. Since ν_{02} is not affected by the triplet-singlet mixing effects, accurate experimental results for this interval in light helium-like ions would yield an improved estimate for the uncalculated higher-order effects in helium, thus increasing accuracy of determination of α from the helium fine structure.

Comparing theoretical and experimental results for the fine structure of helium-like ions, one should keep in mind that the present calculation is carried out for a spinless nucleus, whereas the experimental results listed in Table III were performed for non-zero nuclear spin isotopes. For a nucleus with spin, the hyperfine splitting can usually be evaluated separately and employed for an experimental determination of the fine structure. This procedure, however, ignores the mixing between the hyperfine and the fine splittings. So, more accurate calculations should account for both effects simultaneously.

In summary, the 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 for the $2^3P_0 - 2^3P_1$ interval in helium yields an independent determination of the fine structure constant α accurate to 31 ppb.

Support by NIST through Precision Measurement Grant PMG 60NANB7D6153 and by the Helmholtz Gemeinschaft (Nachwuchsgruppe VH-NG-421) is gratefully acknowledged.

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