

QED calculation of ionization energies of $1snd$ states in helium

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Quantum electrodynamical (QED) calculations of ionization energies of the $1sndD$ states are performed for the helium atom. We reproduce the previously known relativistic and QED effects up to order $m\alpha^5$ and extend the theory by calculating the complete $m\alpha^6$ correction. The total contribution of the $m\alpha^6$ effects is shown to be much smaller than previously estimated, due to a large cancelation between the radiative and non-radiative parts of this correction. As a result of our calculations, we confirm the previously reported deviations between measured transition energies and theoretical predictions for the $nD-2S$ and $nD-2P$ transitions. Possible reasons for this discrepancy are analyzed.

I. INTRODUCTION

Helium is the simplest few-electron atom, and it has played a special role in physics since the early days of quantum mechanics. The relativistic effects in helium are smaller than the nonrelativistic energy roughly by a factor of $(Z\alpha)^2$ (where $Z = 2$ is the helium nuclear charge number and α is the fine-structure constant) and thus can be accounted for by perturbation theory, yielding a convenient approach for an accurate theoretical description of helium spectra. Being a monatomic gas, helium is easy to work with and can be studied experimentally to great accuracy due to the presence of narrow spectral lines in the spectrum. A large body of experimental results exists for helium spectra, many of them reaching the relative precision of a few parts in 10^{-12} [1–10].

Motivated by the experimental success, numerous theoretical calculations have been performed for transition energies of the helium atom. In particular, extensive calculations by Drake *et al.* [11–13] covered all states with angular momentum up to $L = 8$ and principal quantum number up to $n = 10$. These calculations accounted for all QED effects up to order $m\alpha^5$ and partly included some higher-order QED effects. The first complete calculation of the next-order $m\alpha^6$ effects was accomplished by one of us for the $n = 1$ and $n = 2$ states of helium [14–16] and later extended to light helium-like ions [17].

The present status of the theory of the $n = 1$ and $n = 2$ states of helium was summarized in a recent review [18]. The comparison with available experimental data presented in that work showed good agreement for the intrashell $n = 2$ transitions. However, recent experiments [4, 6, 10] have reported deviations from theoretical predictions for transitions involving D states. In order to clarify this, we have performed in Ref. [19] an independent calculation of the helium $3D$ ionization energies, including the complete $m\alpha^6$ correction. As a result, we confirmed the systematic deviation between the theoretical and experimental $3D-2S, 2P$ transition energies on the level of 1.5–3 standard deviations.

In the present work we aim to gain further insight into the reported discrepancy between theory and experiment, by calculating the ionization energies of the higher excited nD states of helium, for which theoretical predictions can be much more accurate in terms of the absolute uncertainty. We will reproduce the previously known QED effects up to order $m\alpha^5$ and extend the previous theory by calculating the complete $m\alpha^6$ correction.

II. CALCULATION

In the general spirit of the Nonrelativistic QED approach, the energies of the helium atom are represented as a double expansion in small parameters α and m/M , where α is the fine-structure constant and m/M is the electron-to-nucleus mass ratio. Specifically, we express the energy E of a $1sndD$ state as

$$E = m \left\{ \alpha^2 \left[E^{(2,0)} + \frac{m}{M} E^{(2,1)} + \frac{m^2}{M^2} E^{(2,2+)} \right] + \alpha^4 \left[E^{(4,0)} + \frac{m}{M} E^{(4,1)} \right] + \alpha^5 \left[E^{(5,0)} + \frac{m}{M} E^{(5,1)} \right] + \alpha^6 E^{(6,0)} + \alpha^7 E^{(7,0)} + E_{\text{MIX}} + E_{\text{FNS}} \right\}, \quad (1)$$

where the superscripts i and j in $E^{(i,j)}$ specify the order in α and m/M , respectively.

The individual contributions to energies of the D states were examined in detail in our previous investigation [19]. The leading contribution $E^{(2,0)}$ is the nonrelativistic energy for the infinitely heavy nucleus. $E^{(2,1)}$ and $E^{(2,2+)}$ are the first-order and higher-order finite-nuclear-mass corrections to the nonrelativistic energy. The latter contains nuclear mass contributions $\propto (m/M)^2$ and higher. $E^{(4,0)}$ and $E^{(4,1)}$ are the leading relativistic (Breit) correction in the nonrecoil limit and the corresponding first-order recoil correction, respectively. $E^{(5,0)}$ and $E^{(5,1)}$ are the leading QED correction in the nonrecoil limit and the

corresponding first-order recoil correction, respectively. $E^{(6,0)}$ and $E^{(7,0)}$ are the higher-order QED corrections. E_{MIX} is the correction due to mixing between the triplet n^3D_2 and singlet n^1D_2 states. This contribution is enhanced due to a small energy difference of these states and thus requires a separate treatment, see Ref. [19] for details. Finally, E_{FNS} is the correction induced by the finite nuclear size.

The main part of the present investigation is the complete calculation of the QED effects of order $m\alpha^6$, i.e. $E^{(6,0)}$. It is convenient to split this correction into the radiative and non-radiative parts,

$$E^{(6,0)} = E_{\text{rad}}^{(6,0)} + E_{\text{nrad}}^{(6,0)}. \quad (2)$$

The radiative part is the sum of the one-loop and two-loop radiative contributions, $E_{\text{rad}}^{(6,0)} = E_{R1} + E_{R2}$,

$$E_{R1} = Z^2 \left[\frac{427}{96} - 2 \ln 2 \right] 2\pi \langle \delta^3(r_1) \rangle + \left[\frac{6\zeta(3)}{\pi^2} - \frac{697}{27\pi^2} - 8 \ln 2 + \frac{1099}{72} \right] \pi \langle \delta^3(r) \rangle, \quad (3)$$

$$E_{R2} = Z \left[-\frac{9\zeta(3)}{4\pi^2} - \frac{2179}{648\pi^2} + \frac{3 \ln 2}{2} - \frac{10}{27} \right] 2\pi \langle \delta^3(r_1) \rangle + \left[\frac{15\zeta(3)}{2\pi^2} + \frac{631}{54\pi^2} - 5 \ln 2 + \frac{29}{27} \right] \pi \langle \delta^3(r) \rangle, \quad (4)$$

which were obtained from Ref. [20]. The nonradiative contribution is the remaining part of the $m\alpha^6$ correction. The corresponding formulas are long and cumbersome; they are presented in Ref. [19] and will not be repeated here.

The dominant contribution to the radiative correction $E_{\text{rad}}^{(6,0)}$ comes from the part proportional to $\langle \delta^3(r_1) \rangle$. This part has been known for a long time and was included in previous calculations, in particular those in Ref. [13]. Conversely, the nonradiative $m\alpha^6$ correction was not known until recently and thus defined the uncertainty of theoretical predictions in the helium atom and in light helium-like ions.

The first complete calculation of the $m\alpha^6$ effects was accomplished for the $n = 1$ and $n = 2$ states of helium by one of us in Refs. [14–16]. This calculation was later extended to light helium-like ions [17] and to the hydrogen molecule [21]. In our previous investigation we performed a calculation of the $m\alpha^6$ effects for the helium $3D$ states [19], and the main part of the present investigation is to extend this calculation to the higher excited nD states with $n = 4, 5$, and 6 .

The numerical approach of the evaluation is described in detail in Ref. [19]. In the present work we employed increased computer resources in order to improve the numerical accuracy for the $n = 3$ state and to ensure the controllable convergence of the results for the higher excited states. Numerical results of our calculations of the $m\alpha^6$ corrections for ionization energies of $1snd$ states of ^4He are presented in Table I.

We find that both the radiative and nonradiative $m\alpha^6$ corrections to the ionization energy for higher excited n states decrease as $1/n^3$, which is the typical scaling for most of the QED effects. Much less typical is the fact that the radiative and nonradiative contributions for the D states are of the same order of magnitude. In most calculations performed so far, the radiative effects were found to yield the dominant contribution, whereas the nonradiative QED effects originating from the electron-electron interaction were rather small. In particular, Morton *et al.* [13] estimated the omitted nonradiative $m\alpha^6$ effects as 10% of the $m\alpha^6$ radiative contribution. Our numerical calculations summarized in Table I show that the typical pattern of magnitudes of the radiative versus nonradiative effects is broken for the helium D states, the nonradiative part being as large as the radiative one and of the opposite sign.

Having calculated the $m\alpha^6$ effects for a series of nD states, we are able to analyse the n dependence of the corresponding corrections. Specifically, we fit the numerical results listed in Table I to the $1/n$ asymptotic expansion of the following form

$$E^{(6)} = \frac{1}{n^3} \sum_{i=0}^2 \frac{c_i}{n^i}. \quad (5)$$

The obtained coefficients c_i are presented in Table II. Using these results, we can compute the $m\alpha^6$ correction for the nD states with $n > 6$.

Table III summarizes our calculations of the ionization energies of the $4D$, $5D$, and $6D$ states in helium. Results include QED effects of order $m\alpha^5$ and $m\alpha^6$. In particular, we performed computations of the Bethe logarithms for the $4D$, $5D$, and $6D$ states, and our results agree with previous Bethe-logarithm calculations [22, 23]. Our calculations of the ionization energies are complete up to order $m\alpha^6$, while the QED effects of order $m\alpha^7$ were estimated by scaling the hydrogenic results for the one-, two-, and three-loop QED effects, as described in Ref. [19]. The uncertainty of these estimations was taken as 100%.

The comparison of our total results with the previous theoretical predictions by Morton *et al.* [13] demonstrates that the difference comes exclusively from the non-radiative $m\alpha^6$ QED effects not included in the previous calculation. Apart from this addition, the consistency between two independent calculations is nearly perfect, the residual differences being on the level of just 1-3 kHz. However, as already mentioned, the magnitude of the nonradiative $m\alpha^6$ effects calculated in this work turned out to be much larger than previously expected, which resulted in a shift of the theoretical values of Ref. [13] by about 10 times their estimated uncertainty.

In the present work we performed explicit numerical calculations for the nD states with n up to $n = 6$. With the help of the approximate formula (5), we can obtain the $m\alpha^6$ effects also for the higher- n states. In view of the great consistency between our present calculation and

the one by Morton *et al.* [13], we update their results for the nD states with $n = 7-10$, by adding the nonradiative $m\alpha^6$ correction as obtained from Eq. (5) and rescaling their results with the latest value of the Rydberg constant [24].

The list of the final theoretical ionization energies of nD states of ${}^4\text{He}$ for $n \leq 10$ is presented in Table IV. The small difference of the $3D$ energies from those reported in our previous work [19] is due to the updated value of the Rydberg constant. The actual Rydberg constant [24] differs from the previous CODATA 2014 value [25] by about 5 standard deviations, as a result of recent measurements of the Lamb shift in hydrogen [26, 27] and the electron-proton scattering [28]. The change of the Rydberg constant induced a shift of the $3D$ ionization energies of about 10 kHz, about half of the theoretical uncertainty.

Table V compares the present theoretical values with the available experimental results for various transitions involving nD states. We observe that the theoretical predictions for the $nD-2S$ and $nD-2P$ transitions are systematically larger than the measured values, the difference varying from 1.5 to 3σ . This is in contrast to the situation for the intrashell $n = 2$ transitions, where theoretical predictions are in good agreement with experimental observations [18].

Analyzing possible reasons for the deviations between theory and experiment summarized in Table V, we first observe that the theoretical energies of the nD states should be considered as well established on the 1 MHz level. Indeed, the nonradiative $m\alpha^6$ effects calculated only in this work and not confirmed independently contribute only 0.3 MHz for the $3D$ states and much less (decreasing as $1/n^3$) for the higher- n D states. All other theoretical contributions for the nD states are cross-checked by two independent calculations and agree up to a few kHz. Therefore, we must assume that the reason for the deviations comes from the theoretical energies of the $n = 2$ states. Bearing in mind the good agreement between theory and experiment for the intrashell $n = 2$ transitions [18], we might expect an unaccounted-for contribution of the order of 1 MHz that is nearly the same for the S and P states and, even more unusually, for the triplet and singlet states.

Theoretical energies of the $n = 2$ states are independently checked up to order $m\alpha^5$. Therefore, possible

unaccounted-for contributions could come either from the $m\alpha^6$ effects (whose calculations [15, 16] have not been confirmed independently yet) or from the unknown $m\alpha^7$ effects. The latter possibility is likely to be tested soon, when the project of calculations of all $m\alpha^7$ QED effects for the triplet states of helium is completed [29, 30].

III. SUMMARY

We performed calculations of relativistic and QED effects to the ionization energies of $1sndD$ states in helium. Consequently, we reproduced the previously known relativistic and QED effects up to order $m\alpha^5$ and extended the previous theory by evaluating the complete $m\alpha^6$ correction. We found that the radiative and non-radiative $m\alpha^6$ contributions for the $1sndD$ states are of the same magnitude and of different sign, thus cancelling each other to a large extent. This is very different from the situation for the S and P states, where the radiative part is by far the dominant one.

As a consequence of our calculations, we confirm the previously reported deviations between measured transition energies and theoretical predictions for the $nD-2S$ and $nD-2P$ transitions on the level of 1.5–3 standard deviations. The reason for this disagreement is not known. The most plausible explanation would involve a missing contribution in the theoretical prediction for the $n = 2$ states, a part of which is not cross-checked by independent calculations (the $m\alpha^6$ effects) or not yet calculated (the $m\alpha^7$ effects). We conclude that further theoretical investigations of higher-order QED effects in helium are needed in order to find out the exact reason for the observed discrepancy.

ACKNOWLEDGEMENT

V.A.Y. acknowledges support from the Russian Science Foundation (Grant No. 20-62-46006). The work of K.P., M.P., and V.P was supported from the National Science Center (Poland) Grant No. 2017/27/B/ST2/02459. Additionally, V.P. acknowledges support from the Czech Science Foundation - GACR (Grant No. P209/18-00918S)

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TABLE I. Radiative (rad) and non-radiative (nrad) $m\alpha^6$ corrections for ionization energies of $1snd$ states of ${}^4\text{He}$, in units of $10^{-3}m\alpha^6$. Conversion factor to MHz is 0.018658054.

n	Term	n^1D	n^3D_1	n^3D_2	n^3D_3
3	rad	-10.7644	-13.3384	-13.3384	-13.3384
	nrad	18.3532 (8)	14.2110 (40)	19.1548 (12)	22.5100 (42)
	sum	7.5888 (8)	0.8727 (40)	5.8164 (12)	9.1717 (42)
4	rad	-4.9107	-6.3733	-6.3733	-6.3733
	nrad	7.6737 (12)	6.2152 (50)	8.1596 (17)	9.5068 (33)
	sum	2.7629 (12)	-0.1581 (50)	1.7863 (17)	3.1335 (33)
5	rad	-2.6027	-3.4394	-3.4394	-3.4394
	nrad	3.9135 (63)	3.2304 (64)	4.1985 (23)	4.8699 (40)
	sum	1.3109 (63)	-0.2090 (64)	0.7591 (23)	1.4306 (40)
6	rad	-1.5340	-2.0456	-2.0456	-2.0456
	nrad	2.2606 (43)	1.8855 (80)	2.4381 (50)	2.8206 (43)
	sum	0.7265 (43)	-0.1601 (80)	0.3925 (50)	0.7751 (43)

TABLE II. Coefficients of the asymptotic $1/n$ expansion (5) for the radiative (rad) and non-radiative (nrad) $m\alpha^6$ corrections of $1snd$ states of ${}^4\text{He}$, in units of $m\alpha^6$.

Coefficient	n^1D		n^3D_1		n^3D_2		n^3D_3	
	rad	nrad	rad	nrad	rad	nrad	rad	nrad
c_0	-0.3457	0.4874	-0.4684	0.4098	-0.4684	0.5320	-0.4684	0.6093
c_1	0.0071	-0.0144	-0.0062	0.0427	-0.0062	-0.0233	-0.0062	-0.0002
c_2	0.4745	0.1159	0.9930	-0.3627	0.9930	-0.0637	0.9930	-0.0134

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TABLE III. Individual contributions to theoretical ionization energies of the $1snd$ states of ^4He , in MHz. Fundamental constants are [24] $R_\infty c = 3\,289\,841\,960.250\,8(64)$ MHz, $\alpha^{-1} = 137.035\,999\,084(21)$, $M/m = 7\,294.299\,541\,36$. Theoretical energies of Morton *et al.* [13] are rescaled for the updated value of the Rydberg constant.

	4^1D_2	4^3D_1	4^3D_2	4^3D_3
$E^{(2,0)}$	-205811500.938	-205870726.799	-205870726.799	-205870726.799
$E^{(2,1)}$	28098.869	28250.067	28250.067	28250.067
$E^{(2,2+)}$	-7.810	-7.677	-7.677	-7.677
$E^{(4,0)}$	-527.343	-55.787	-602.728	-647.005
$E^{(4,1)}$	0.108	-0.179	0.053	0.083
$E^{(5,0)}$	-6.289	-7.426	-8.266	-7.722
$E^{(5,1)}$	-0.002	0.002	0.003	0.002
E_{MIX}	7.684	0.	-7.684	0.
$E_{\text{rad}}^{(6,0)}$	-0.092	-0.119	-0.119	-0.119
$E_{\text{nrad}}^{(6,0)}$	0.143	0.116	0.152	0.177
$E^{(7,0)}$	0.009 (9)	0.011 (11)	0.011 (11)	0.011 (11)
E_{FNS}	-0.004	-0.005	-0.005	-0.005
Total	-205783935.664 (9)	-205842547.795 (11)	-205843102.990 (11)	-205843138.986 (11)
Morton 2006	-205783935.809 (9)	-205842547.913 (10)	-205843103.143 (10)	-205843139.163 (10)
Difference	0.145 (12)	0.119 (15)	0.153 (15)	0.178 (15)
	5^1D_2	5^3D_1	5^3D_2	5^3D_3
$E^{(2,0)}$	-131697875.337	-131732032.364	-131732032.364	-131732032.364
$E^{(2,1)}$	17990.063	18077.238	18077.238	18077.238
$E^{(2,2+)}$	-4.992	-4.916	-4.916	-4.916
$E^{(4,0)}$	-321.862	-79.757	-359.518	-382.521
$E^{(4,1)}$	0.068	-0.085	0.034	0.050
$E^{(5,0)}$	-3.314	-3.989	-4.418	-4.140
$E^{(5,1)}$	-0.001	0.001	0.001	0.001
E_{MIX}	3.490	0.	-3.490	0.
$E_{\text{rad}}^{(6,0)}$	-0.049	-0.064	-0.064	-0.064
$E_{\text{nrad}}^{(6,0)}$	0.073	0.060	0.078	0.091
$E^{(7,0)}$	0.005 (5)	0.006 (6)	0.006 (6)	0.006 (6)
E_{FNS}	-0.002	-0.002	-0.002	-0.002
Total	-131680211.860 (5)	-131714043.872 (6)	-131714327.415 (6)	-131714346.623 (6)
Morton 2006	-131680211.934 (5)	-131714043.934 (6)	-131714327.494 (6)	-131714346.715 (6)
Difference	0.074 (7)	0.061 (8)	0.079 (8)	0.092 (8)
	6^1D_2	6^3D_1	6^3D_2	6^3D_3
$E^{(2,0)}$	-91445943.507	-91466919.734	-91466919.734	-91466919.734
$E^{(2,1)}$	12497.472	12551.001	12551.001	12551.001
$E^{(2,2+)}$	-3.463	-3.416	-3.416	-3.416
$E^{(4,0)}$	-206.310	-66.005	-227.805	-241.222
$E^{(4,1)}$	0.044 (1)	-0.046	0.023	0.032
$E^{(5,0)}$	-1.947	-2.366	-2.614	-2.454
$E^{(5,1)}$	-0.001	0.001	0.001	0.001
E_{MIX}	1.902	0.	-1.902	0.
$E_{\text{rad}}^{(6,0)}$	-0.029	-0.038	-0.038	-0.038
$E_{\text{nrad}}^{(6,0)}$	0.042	0.035	0.045	0.053
$E^{(7,0)}$	0.003 (3)	0.004 (4)	0.004 (4)	0.004 (4)
E_{FNS}	-0.001	-0.001	-0.001	-0.001
Total	-91433655.795 (3)	-91454440.567 (4)	-91454604.437 (4)	-91454615.775 (4)
Morton 2006	-91433655.838 (3)	-91454440.602 (4)	-91454604.483 (4)	-91454615.829 (4)
Difference	0.043 (4)	0.035 (5)	0.046 (5)	0.054 (5)

TABLE IV. Theoretical ionization energies of the $1snd$ states of ${}^4\text{He}$, in MHz.

n	n^1D_2	n^3D_1	n^3D_2	n^3D_3
3	-365 917 748.661 (19)	-366 018 892.691 (23)	-366 020 217.716 (23)	-366 020 292.981 (23)
4	-205 783 935.6645 (86)	-205 842 547.795 (11)	-205 843 102.990 (11)	-205 843 138.986 (11)
5	-131 680 211.8599 (46)	-131 714 043.8724 (60)	-131 714 327.4151 (60)	-131 714 346.6227 (60)
6	-91 433 655.7952 (30)	-91 454 440.5666 (36)	-91 454 604.4375 (36)	-91 454 615.7752 (36)
7	-67 169 717.1272 (20)	-67 183 264.5655 (20)	-67 183 367.6781 (20)	-67 183 374.8986 (20)
8	-51 423 248.1215 (10)	-51 432 523.2304 (20)	-51 432 592.2710 (20)	-51 432 597.1421 (20)
9	-40 628 480.2532 (9)	-40 635 090.4352 (10)	-40 635 138.9071 (10)	-40 635 142.3441 (10)
10	-32 907 601.9048 (6)	-32 912 470.7471 (9)	-32 912 506.0729 (9)	-32 912 508.5867 (9)

TABLE V. Comparison of different theoretical predictions with experimental results for transition energies involving nD states in ${}^4\text{He}$, in MHz. The experimental value for the $3^1D - 3^3D_1$ transition energy was obtained by combining several measurements for different transitions [6–8, 10].

Transition	Experiment	Ref.	Present theory	Difference from experiment	Morton 2006 [13]	Difference from experiment
$3^1D - 2^1S$	594 414 291.803 (13)	[10]	594 414 289.3 (1.9)	2.5 (1.9)	594 414 292. (5.)	0. (5.)
$3^3D_1 - 2^3S$	786 823 850.002 (56)	[31]	786 823 848.7 (1.3)	1.3 (1.3)	786 823 845. (7.)	4. (7.)
$3^3D_1 - 2^3P_0$	510 059 755.352 (28)	[6]	510 059 754.2 (0.7)	1.2 (0.7)	510 059 749. (2.)	6. (2.)
$3^1D - 2^1P$	448 791 399.11 (27)	[4]	448 791 397.8 (0.4)	1.3 (0.5)	448 791 400.5 (2)	-1.4 (2)
$7^1D - 2^1S$	893 162 323.88 (12)	[32]	893 162 320.9 (1.9)	3.0 (1.9)	893 162 324. (5.)	0. (5.)
$8^1D - 2^1S$	908 908 792.76 (7)	[32]	908 908 789.9 (1.9)	2.9 (1.9)	908 908 793. (5.)	0. (5.)
$9^1D - 2^1S$	919 703 560.56 (11)	[32]	919 703 557.7 (1.9)	2.9 (1.9)	919 703 561. (5.)	0. (5.)
$10^1D - 2^1S$	927 424 439.05 (10)	[32]	927 424 436.1 (1.9)	3.0 (1.9)	927 424 439. (5.)	0. (5.)
$5^3D_2 - 2^3P_2$	744 396 218.(7.)	[33]	744 396 227.7 (0.7)	10.(7.)	744 396 231.(2.)	13.(7.)
$3^1D - 3^3D_1$	101 143.943 (31)	[6–8, 10]	101 144.029 (23)	0.086 (37)	101 143.95 (3)	0.01 (4)
$5^1D - 5^3D_1$	33 850.(10.)	[33]	33 832.013 (8)	18.(10.)	33 832.000 (8)	18.(10.)
$5^3D_1 - 5^3D_2$	279.(10.)	[33]	283.543 (8)	5.(10.)	283.560 (8)	5.(10.)
$5^3D_1 - 5^3D_3$	297.(10.)	[33]	302.750 (8)	6.(10.)	302.781 (8)	6.(10.)