PHYSICAL REVIEW A VOLUME 48, NUMBER 1 JULY 1993

Energy corrections of order $mc^2\alpha^6 \ln \alpha$ in helium

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(5 April 1993)

Quantum-electrodynamic corrections of $O(mc^2\alpha^6 \ln \alpha)$ to the electron-electron interaction in helium are evaluated for several states. The additional energy shift, which is an order of α smaller than the leading Araki-Sucher terms, raises the predicted energy of the $1s2s\ ^1S_0$ state by 2.49 MHz to $-960\,332\,039.43(18)$ MHz relative to $He^+(1s)$. The new value significantly alters the comparison with recent high-precision experiments.

PACS numbers: 31.20.Di, 31.30.Jv

I. INTRODUCTION

The study of two-electron quantum-electrodynamic (QED) effects in the energy levels of helium has recently become feasible due to the availability of high-precision variational calculations for the lower-order nonrelativistic and relativistic contributions to the energy of $O(\alpha^2 mc^2)$ and $O(\alpha^4 mc^2)$, respectively [1–5]. The procedure [6] is to combine the calculations with transition frequency measurements from, say, the $1s2s\ ^1S_0$ state to higher-lying $1snp\ ^1P_1$ [7] and $1snd\ ^1D_2$ [8] states. After the calculated lower-order terms have been subtracted, there remains an experimental value for the QED shift in the (negative) ionization energy of the $1s2s\ ^1S_0$ state accurate to about ± 0.3 MHz, out of a total QED shift of about 2807 MHz. The agreement between theory and experiment is at present better than ± 0.7 MHz, even though uncalculated terms of $O(\alpha^6 mc^2)$ might well be expected to contribute at this level. The purpose of this paper is to evaluate the contributions of order $mc^2\alpha^6 \ln \alpha$ and show that they do indeed affect the comparison between theory and experiment.

II. THEORY

The required terms of order $mc^2\alpha^6 \ln \alpha$ (i.e., $\alpha^4 \ln \alpha$ a.u.) can be extracted from related derivations already done for positronium and other two-body QED systems. A complete result through terms of this order for the positronium case was first obtained by Fell [9]. His results correspond to the expression (in units with $\hbar = c = 1$)

$$\delta E(n,l) = \frac{1}{24} m\alpha^6 \ln \alpha^{-1} \left(\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 + \frac{1}{4}(3 + \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2) \right) \frac{\delta_{l,0}}{n^3} , \tag{1}$$

where $\boldsymbol{\sigma}_1$ and $\boldsymbol{\sigma}_2$ are Pauli spin operators. The term in inner parentheses comes from the one-photon annihilation diagram, which had been previously calculated by Caswell and Lepage [10]. The more general case of attracting particles with different masses m and M was considered by Khriplovich, Milstein, and Yelkhovsky [11] with the result

$$\delta E(n,l) = \frac{4}{3} \frac{\mu^5}{M^2 m^2} \alpha^6 \ln \alpha^{-1} \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 \frac{\delta_{l,0}}{n^3} , \tag{2}$$

where $\mu = mM/(m+M)$ is the reduced mass, and the annihilation term no longer contributes. The effective perturbation operator responsible for this energy shift for equal masses can be written to logarithmic accuracy in the form

$$V = \frac{\pi\alpha^3}{3m^2} \ln \alpha^{-1} \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 \delta(\mathbf{r}_{12}). \tag{3}$$

For the case of the electron-electron interaction in atoms, the repulsive instead of attractive force between the particles leads to a change in overall sign of the energy correction. This prescription becomes especially obvious in the approach used in Ref. [12], where the effective operator arises from three-photon-exchange Feynman diagrams. Then, with logarithmic accuracy, the e-e interaction is not influenced by the interaction of the electrons with the nucleus since it originates at interelectron distances $(a_0/\alpha) \ll r_{12} \ll a_0$ (a_0 is the Bohr radius). At these distances, the electron-electron interaction responsible for the effect is much stronger than the interaction with the nucleus if Z is not too large. The same result can also be obtained by a direct analysis of the Feynman diagrams. In this way we come finally to the following electron-electron effective operator:

$$V_{e\text{-}e} = -\frac{\pi\alpha^3}{3m^2} \ln \alpha^{-1} \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 \delta(\mathbf{r}_{12}). \tag{4}$$

The above is an order of α smaller than the leading Araki-Sucher terms $\Delta E_{\mathrm{L},2}$ [13,14] previously evaluated to high precision [1–3].

In LS coupling, the spatial part of the two-electron wave function is purely symmetric for singlet states, and purely antisymmetric for triplet states. Thus for triplet states, the wave function vanishes at $\mathbf{r}_{12} = 0$, and so

$\langle\delta(\mathbf{r}_{12})\rangle = 0$. There is therefore no energy correction for triplet states. For singlet states the perturbation (4) simplifies to (in atomic units)

$$V^{\rm s}_{e\text{-}e} = \pi\alpha^4 \ln\alpha^{-1}\delta(\mathbf{r}_{12}). \tag{5}$$

Deviations from LS coupling come from the spin-dependent terms in the Breit interaction, leading to singlet-triplet mixing. For $L > 0$, this can be taken into account to a good degree of approximation by diagonalizing the Breit interaction in the subspace of singlet-triplet states with the same nL quantum numbers. If $\theta_{n,L}$ is the singlet-triplet mixing angle, and

$$\langle V^{\rm s}_{e\text{-}e}\rangle_{n,L} = \langle 1snl\ ^1L|V^{\rm s}_{e\text{-}e}|1snl\ ^1L\rangle \tag{6}$$

is the expectation value of $V^{\rm s}_{e\text{-}e}$ for the singlet state in pure LS coupling, then the energy shifts for the mixed states are

$$\Delta E'_{\rm L,2}({\rm singlet}) = \langle V^{\rm s}_{e\text{-}e}\rangle_{n,L}\cos^2\theta_{n,L}, \tag{7}$$

$$\Delta E'_{\rm L,2}({\rm triplet}) = \langle V^{\rm s}_{e\text{-}e}\rangle_{n,L}\sin^2\theta_{n,L}. \tag{8}$$

For $L = 1$ and 2, $\sin^2\theta_{n,L}$ is so small that singlet-triplet splitting is not significant. Although $\sin^2\theta_{n,L}$ rapidly increases with increasing L, the matrix elements of $\delta(\mathbf{r}_{12})$ decrease even more rapidly, making $\langle V^{\rm s}_{e\text{-}e}\rangle_{n,L}$ negligible for high L. [An asymptotic expression for matrix elements of $\delta(\mathbf{r}_{12})$, which becomes exact in the limit of high L, is given by Eqs. (111) and (112) of Ref. [1].] Thus, singlet-triplet mixing is never an important consideration. This is illustrated by the numerical results in the following section.

III. CALCULATIONS AND RESULTS

High-precision matrix elements of $\delta(\mathbf{r}_{12})$ obtained with correlated variational wave functions calculated from doubled Hylleraas basis sets have been tabulated by Drake and Yan [1] for all states with $L > 0$ up to $n = 10$ and $L = 7$. For the S states, results for $n = 1$ and 2 are given by Drake [6]. Values for the higher-lying S states obtained by the same methods, and improved values for $n = 1$ and 2, are given in Table I.

The calculated energy shifts, including the singlet-triplet mixing correction for $L \geq 1$, are listed in Table II. The shift is of course largest (30.666 MHz) for the ground state, but it is much less than the ± 4.5 GHz uncertainty in the location of the $1s^2\ ^1S_0$ state relative to the excited states [15]. The one case where the additional shift significantly affects the comparison between theory and experiment is the $1s2s\ ^1S_0$ state. The theoretical contributions to its (negative) ionization energy are summarized in Table III. The electron-nucleus QED term $\Delta E_{\rm L,1}$ includes a recent high-precision calculation of the two-electron Bethe logarithm by Baker *et al.* [16]. This produces an upward shift of 93.54(18) MHz relative to the $1/Z$ expansion calculation of the Bethe logarithm by Goldman and Drake [17], thereby removing what would otherwise be a significant discrepancy between theory and experiment. The $\Delta E_{\rm L,2}$ term in Table III is the contribution from the lowest-order Araki-Sucher correction to the electron-electron interaction.

The transition frequency measurements from the

TABLE I. Calculated values of $\pi\langle\delta(\mathbf{r}_{12})\rangle$ for the $1sns\ ^1S_0$ states of helium (in atomic units). Numbers in parentheses denote the uncertainties in the final figure(s) quoted.

n	$\pi\langle\delta(\mathbf{r}_{12})\rangle$
1	0.334 093 840(4)
2	0.027 169 868(4)
3	0.007 644 317(5)
4	0.003 136 293(5)
5	0.001 577 861 6(17)
6	0.000 902 167 98(7)
7	0.000 563 147 72(12)
8	0.000 374 740 6(11)
9	0.000 261 804 9(12)
10	0.000 190 042 7(15)

TABLE II. Energy shifts $\Delta E'_{\rm L,2}$ of $O(mc^2\alpha^6\ln\alpha)$ for various states of helium, including singlet-triplet mixing (in units of kHz).

State	$\Delta E'_{\rm L,2}$(singlet)	$\Delta E'_{\rm L,2}$(triplet)	$\sin\theta_{n,L}$
$1S$	30 666.344		
$2S$	2 493.911		
$3S$	701.669		
$4S$	287.879		
$5S$	144.831		
$6S$	82.810		
$7S$	51.691		
$8S$	34.397		
$9S$	24.031		
$10S$	17.444		
$2P$	211.997	0.000 0164	0.000 278
$3P$	72.672	0.000 0048	0.000 256
$4P$	32.143	0.000 0020	0.000 250
$5P$	16.817	0.000 0010	0.000 247
$6P$	9.847	0.000 0006	0.000 246
$7P$	6.246	0.000 0004	0.000 245
$8P$	4.204	0.000 0003	0.000 245
$9P$	2.963	0.000 0002	0.000 244
$10P$	2.165	0.000 0001	0.000 244
$3D$	0.659	0.000 1607	0.015 610
$4D$	0.388	0.000 0504	0.011 396
$5D$	0.226	0.000 0231	0.010 114
$6D$	0.139	0.000 0127	0.009 529
$7D$	0.091	0.000 0077	0.009 207
$8D$	0.062	0.000 0051	0.009 009
$9D$	0.045	0.000 0035	0.008 878
$10D$	0.033	0.000 0025	0.008 786
$4F$	0.000 76	0.000 44	0.604 102
$5F$	0.000 71	0.000 31	0.549 929
$6F$	0.000 54	0.000 20	0.518 074
$7F$	0.000 39	0.000 13	0.498 418
$8F$	0.000 29	0.000 09	0.485 577
$9F$	0.000 21	0.000 06	0.476 762
$10F$	0.000 16	0.000 05	0.470 459

$1s2s\ ^1S_0$ state to the $1snp\ ^1P_1$ states [7] and $1snd\ ^1D_2$ states [8] can be used to extract an experimental value for the $1s2s\ ^1S_0$ ionization energy either by a direct quantum-defect extrapolation to the series limit, or by taking the calculated positions of the higher-lying Rydberg states [1] as known points of reference and subtracting. As discussed in detail by Drake [4], the two methods agree, although the latter is slightly more accurate. It gives the results

$-960\,332\,041.52(21)$ MHz from the P states,
$-960\,332\,040.87(15)$ MHz from the D states.

The reason for the difference of 0.65 ± 0.26 MHz between the two measurements is not clear since it is largely independent of the method of analysis. With the additional shift of 2.49 MHz evaluated here included, the differences, theory minus experiment for the energy of the $1s2s\ ^1S_0$ state, are

1.42 ± 0.28 MHz from the P states,
2.17 ± 0.24 MHz from the D states.

IV. DISCUSSION

The results of the previous section show that the additional shift of $O(\alpha^4 \ln \alpha)$ a.u. evaluated here worsens the agreement between theory and experiment. However, further corrections of order $\alpha^4 Z^4$ a.u. from crossed-box and vertex diagrams could well be as large as the discrepancies. For example, relativistic corrections of $O(\alpha^4 Z^5)$ to the lowest-order Lamb shift contribute -51.99 MHz, calculated in a one-electron approximation modified by the correct electron density at the nucleus for helium (see Drake and Yan [1], and Drake [2,3] for further details). The renormalization of the electron density at the nucleus is expected to account for the majority of the two-electron effects [18], but residual corrections of $O(\alpha^4 Z^4)$ undoubtedly remain. Further progress in the comparison of theory and experiment will require a full calculation of two-electron QED corrections of this order. However, the logarithmic part evaluated here is likely to be numerically the most significant. The shifts for some of the higher-lying S-states may also be large enough to be observable, but they are much less than current uncertainties in the two-electron Bethe logarithm. For $L \geq 3$, the shifts are unobservably small.

TABLE III. Contributions to the energy of the $1s2s\ ^1S$ state of helium, relative to $He^+(1s)$, in units of MHz. The various terms are as defined by Drake and Yan [1].

Term	Contribution
$\Delta E_{\rm nr}$	$-960\,331\,428.82$
$\Delta E_M^{(1)}$	8 570.43
$\Delta E_M^{(2)}$	-16.72
$\Delta E_{\rm rel}$	$-11\,969.81$
$(\Delta E_{\rm RR})_M$	-14.83
$(\Delta E_{\rm RR})_X$	9.84
$\Delta E_{\rm nuc}$	2.00
$\Delta E_{L,1}$	3 136.34(18)[a]
$\Delta E_{L,2}$	-330.35
$\Delta E'_{L,2}$	2.49
Higher-order QED	± 1[b]
Total	$-960\,332\,039.43(18) \pm 1$

[a] Electron-nucleus Lamb shift, including a shift of 93.54(18) MHz due to the Bethe logarithm calculation of Baker *et al.* [16] relative to the $1/Z$ expansion result of Goldman and Drake [17].
[b] Estimate.

ACKNOWLEDGMENTS

This work was supported by the Natural Sciences and Engineering Research Council of Canada and by the Russian Fund for Fundamental Research.

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