University of Windsor Scholarship at UWindsor

Physics Publications

Department of Physics

1993

Energy corrections of order mc2 α 6ln α in helium

Gordon W. F. Drake University of Windsor

I. B. Khriplovich

A. I. Milstein

A. S. Yelkhovsky

Follow this and additional works at: https://scholar.uwindsor.ca/physicspub

Part of the Physics Commons

Recommended Citation

Drake, Gordon W. F.; Khriplovich, I. B.; Milstein, A. I.; and Yelkhovsky, A. S.. (1993). Energy corrections of order mc2α6lnα in helium. *Physical Review A*, 48 (1), R15-R17. https://scholar.uwindsor.ca/physicspub/71

This Article is brought to you for free and open access by the Department of Physics at Scholarship at UWindsor. It has been accepted for inclusion in Physics Publications by an authorized administrator of Scholarship at UWindsor. For more information, please contact scholarship@uwindsor.ca.

VOLUME 48, NUMBER 1

JULY 1993

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

G. W. F. Drake

Department of Physics, University of Windsor, Windsor, Ontario, Canada N9B 3P4

I. B. Khriplovich, A. I. Milstein, and A. S. Yelkhovsky Budker Institute of Nuclear Physics, 630090 Novosibirsk, Russia (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 ${}^{1}S_{0}$ state to higher-lying 1snp ${}^{1}P_{1}$ [7] and 1snd ${}^{1}D_{2}$ [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 $^{1}S_{0}$ 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 $\hbar = c = 1$)

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

where σ_1 and σ_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

$$\delta E(n,l) = \frac{4}{3} \frac{\mu^5}{M^2 m^2} \alpha^6 \ln \alpha^{-1} \sigma_1 \cdot \sigma_2 \frac{\delta_{l,0}}{n^3} , \qquad (2)$$

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

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

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

The above is an order of α smaller than the leading Araki-Sucher terms $\Delta E_{L,2}$ [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

R16

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

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

Deviations from LS coupling come from the spindependent 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

$$\langle V_{e-e}^{\mathbf{s}} \rangle_{n,L} = \langle 1snl \ ^{1}L | V_{e-e}^{\mathbf{s}} | 1snl \ ^{1}L \rangle \tag{6}$$

is the expectation value of V_{e-e}^{s} for the singlet state in pure LS coupling, then the energy shifts for the mixed states are

$$\Delta E_{L,2}'(\text{singlet}) = \langle V_{e-e}^{s} \rangle_{n,L} \cos^2 \theta_{n,L}, \qquad (7)$$

$$\Delta E_{L,2}'(\text{triplet}) = \langle V_{e-e}^{s} \rangle_{n,L} \sin^2 \theta_{n,L}.$$
(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 $\langle V_{e-e}^s \rangle_{n,L}$ 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 = 10and 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-

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.

\boldsymbol{n}	$\pi \langle \delta({f r}_{12}) angle$
1	0.334 093 840(4)
2	0.027169868(4)
3	0.007644317(5)
4	0.003136293(5)
5	0.0015778616(17)
6	0.00090216798(7)
7	0.00056314772(12)
8	0.0003747406(11)
9	0.0002618049(12)
10	0.0001900427(15)

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 $1s^{2}$ $^{1}S_{0}$ 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 ${}^{1}S_{0}$ state. The theoretical contributions to its (negative) ionization energy are summarized in Table III. The electron-nucleus QED term $\Delta E_{L,1}$ 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 $\Delta E_{\mathrm{L},2}$ 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 II. Energy shifts $\Delta E'_{L,2}$ of $O(mc^2\alpha^6 \ln \alpha)$ for various states of helium, including singlet-triplet mixing (in units of kHz).

State	$\Delta E'_{\mathrm{L},2}(\mathrm{singlet})$	$\Delta E'_{\mathrm{L,2}}(\mathrm{triplet})$	$\sin heta_{n,L}$
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		
9 <i>S</i>	24.031		
10 <i>S</i>	17.444		
2P	211.997	0.000 0164	0.000278
3P	72.672	0.0000048	0.000256
4P	32.143	0.000 0020	0.000250
5P	16.817	0.000 0010	0.000247
6P	9.847	0.000 0006	0.000246
7P	6.246	0.0000004	0.000245
8P	4.204	0.000 0003	0.000245
9 P	2.963	0.0000002	0.000244
10 P	2.165	0.000 0001	0.000 244
3 D	0.659	0.000 1607	0.015610
4D	0.388	0.0000504	0.011 396
5D	0.226	0.0000231	0.010114
6D	0.139	0.0000127	0.009529
7 D	0.091	0.0000077	0.009207
8D	0.062	0.0000051	0.009 009
9 D	0.045	0.0000035	0.008878
10 D	0.033	0.0000025	0.008 786
4F	0.00076	0.00044	0.604 102
5 F	0.00071	0.00031	0.549929
6F	0.00054	0.00020	0.518074
7 F	0.00039	0.00013	0.498418
8F	0.00029	0.000 09	0.485577
9 F	0.00021	0.000 06	0.476762
10 F	0.00016	0.00005	0.470459

1s2s ${}^{1}S_{0}$ state to the 1snp ${}^{1}P_{1}$ states [7] and 1snd ${}^{1}D_{2}$ states [8] can be used to extract an experimental value for the 1s2s ${}^{1}S_{0}$ 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

-960332041.52(21)	MHz	from	\mathbf{the}	Ρ	states,
-960332040.87(15)	MHz	from	\mathbf{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 twoelectron effects [18], but residual corrections of $O(\alpha^4 Z^4)$ TABLE III. Contributions to the energy of the 1s2s ^{1}S state of helium, relative to He⁺(1s), in units of MHz. The various terms are as defined by Drake and Yan [1].

Term	Contribution	
$\Delta E_{ m nr}$	-960331428.82	
$\Delta E_M^{(1)}$	8 570.43	
$\Delta E_M^{(2)}$	-16.72	
$\Delta E_{ m rel}$	-11969.81	
$(\Delta E_{ m RR})_M$	-14.83	
$(\Delta E_{ m RR})_{ m X}$	9.84	
$\Delta E_{ ext{nuc}}$	2.00	
$\Delta E_{\mathrm{L,1}}$	3 136.34(18) ^a	
$\Delta E_{{f L},{f 2}}$	-330.35	
$\Delta E'_{{f L},{f 2}}$	2.49	
Higher-order QED) ±1 ^b	
${f Total}$	$-960332039.43(18){\pm}1$	

^aElectron-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].

^bEstimate.

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.

ACKNOWLEDGMENTS

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

- G. W. F. Drake and Z.-C. Yan, Phys. Rev. A 46, 2378 (1992).
- [2] G. W. F. Drake in Long-Range Casimir Forces: Theory and Recent Experiments in Atomic Systems, edited by F. S. Levin and D. A. Micha (Plenum, New York, 1993).
- [3] G. W. F. Drake, Adv. At. Mol. Opt. Phys. (to be published).
- [4] G. W. F. Drake, Adv. At. Mol. Opt. Phys. (to be published).
- [5] J. D. Morgan III, in Relativistic, Quantum Electrodynamic, and Weak Interaction Effects in Atoms, Proceedings of the program held at the Institute of Theoretical Physics, Santa Barbara, CA, 1988 edited by W. Johnson, P. Mohr, and J. Sucher, AIP Conf. Proc. No. 189 (AIP, New York, 1988), p. 123.
- [6] G. W. F. Drake, Nucl. Instrum. Methods Phys. Res. Sect. B 31, 7 (1988).
- [7] C. J. Sansonetti and J. D. Gillaspy, Phys. Rev. A 45, R1 (1992).

- [8] W. Lichten, D. Shiner, and Z.-X. Zhou, Phys. Rev. A 43, 1663 (1991).
- [9] R. N. Fell, Phys. Rev. Lett. 68, 25 (1992)
- [10] W. E. Caswell and G. P. Lepage, Phys. Rev. A 20, 36 (1979).
- [11] I. B. Khriplovich, A. I. Milstein, and A. S. Yelkhovsky, Phys. Scr. (to be published).
- [12] I. B. Khriplovich, A. I. Milstein, and A. S. Yelkhovsky, Phys. Lett. B 282, 237 (1992).
- [13] H. Araki, Prog. Theor. Phys. 17, 619 (1957).
- [14] J. Sucher, Phys. Rev. 109, 1010 (1958).
- [15] W. C. Martin, Phys. Rev. A 29, 1883 (1984).
- [16] J. Baker, R. C. Forrey, R. N. Hill, M. Jerziorska, J. D. Morgan III, and J. Schertzer (unpublished).
- [17] S. P. Goldman and G. W. F. Drake, J. Phys. B 17, L197 (1984).
- [18] G. Feldman, T. Fulton, and J. Ingham, Ann. Phys. (N.Y.) 219, 1 (1992).