The 2S\(1/2\)–2P\(1/2\) Lamb Shift in He\(^+\)

U. D. Jentschura\(^1\) and G. W. F. Drake\(^2\)

\(^1\)Universität Freiburg, Physikalisches Institut (Theoretische Quantendynamik), Hermann–Herder–Straße 3, 79104 Freiburg im Breisgau, Germany
\(^2\)Department of Physics, University of Windsor, Windsor, Ontario N9B 3P4

February 3, 2022

Abstract

The current theoretical status of the Lamb shift in He\(^+\) is discussed. Recent calculations of two-loop binding corrections to the Lamb shift significantly shift the theoretical value of the “classic” Lamb shift in He\(^+\), i.e. of the 2S\(1/2\)–2P\(1/2\)-interval. In this brief research note, we present a new (theoretical) value for this interval which reads 14041.474(42) MHz. The theoretical uncertainty is reduced as well as the discrepancy between theory and experiment. Planned measurements should be of help in further elucidating the situation.

1 Introduction

One of the intriguing questions which remain to be answered in bound-state quantum electrodynamics is related to the discrepancy between the theoretical and experimental values for the Lamb shift in ionized helium, or He\(^+\), which is a hydrogenlike atomic system with a nuclear charge number \(Z = 2\). The latest measurement of the “classical” Lamb shift in He\(^+\), using the anisotropy method, has led to the result \(^1\)

\[ \nu_{\text{exp}}(2S_{1/2} - 2P_{1/2}) = 14041.13(17) \text{ MHz}. \quad (1) \]

The theoretical value given in \(^2\) is different:

\[ \nu_{\text{th,old}}(2S_{1/2} - 2P_{1/2}) = 14041.57(8) \text{ MHz}, \quad (2) \]

where the uncertainty has been assigned according to an estimate of the magnitude of higher-order contributions which had been unknown. If these higher unknown terms had turned out to increase rather than decrease the value of the Lamb shift, then a 3.0\(\sigma\) discrepancy between theory and experiment could have arisen. In the current paper, we review a shift in the theoretical value due to recently calculated higher-order two-loop self-energy corrections, and a further shift due to radiative-recoil corrections where a certain discrepancy between conflicting results has recently been eliminated.

Bound-state quantum electrodynamics (QED) energy shifts may be expressed as combined perturbation series in the parameter \(\alpha\), which is the fine-structure constant, and in \(Z\alpha\), which is a measure of the electron-nucleus interaction. Although Lamb-shift measurements in atomic hydrogen \((Z = 1)\) have a long history, it is necessary to perform at least one measurement for a different value of \(Z\) in order to test the \(Z\)-dependence of the corrections, which are generated by bound-state effects and are fundamentally different from the QED of free electrons. In He\(^+\), we have \(Z = 2\), and the series in \(Z\alpha\) converge much slower than for \(Z = 1\) (atomic hydrogen).

A more accurate measurement of the Lamb shift in He\(^+\) is currently being pursued by Hinds and Boshier \(^3\). It is perhaps worthwhile to note that He\(^+\), as it constitutes an ionic system, should also

1
be an attractive candidate for high-precision laser-spectroscopic measurements in traps, where the small Doppler shifts associated with the slow movement of the trapped ion could provide a basis for a further significant reduction in the experimental uncertainty.

2 Evaluation of Higher-Order Corrections

A detailed summary of radiative corrections which contribute to the Lamb shift of \( n = 2 \) states in \( \text{He}^+ \) has been given in Table I of [1]. Recently, the understanding of two-loop binding corrections to the Lamb shift of \( S \) states has been significantly enhanced [2]. Terms of order \( \left( \frac{\alpha}{\pi} \right)^2 \frac{(Z\alpha)^6 m_e c^2}{n^3} \ln^2[(Z\alpha)^{-2}] B_{62}(nS) \) and \( \left( \frac{\alpha}{\pi} \right)^2 \frac{(Z\alpha)^6 m_e c^2}{n^3} \ln[(Z\alpha)^{-2}] B_{61}(nS) \) (3)

have been evaluated. [Here, \( m_e \) is the electron mass, \( c \) is the speed of light, and the energy shift can be converted to frequencies via division by the natural unit of action, which is Planck’s constant \( \hbar \). In the following, we use a system of units in which \( \hbar = \epsilon_0 = c = 1 \). We will also use the notations \( m \) and \( m_e \) for the electron mass interchangeably [1], and by \( M \), we denote the mass of the \( \alpha \) particle.] These coefficients involve contributions originating from two-loop self-energy, combined self-energy vacuum-polarization, and two-loop vacuum-polarization diagrams. The final results [2] read as follows,

\[
B_{62}(1S) = \frac{104}{135} - \frac{16}{9} \ln 2 = -0.461891 ,
\]

\[
B_{62}(nS) = B_{62}(1S) + \frac{16}{9} \left( \frac{3}{4} + \frac{1}{4n^2} - \frac{1}{n} - \ln(n) + \Psi(n) + \gamma \right),
\]

where \( \gamma = 0.57721 \ldots \) is Euler’s constant, and \( \psi(z) = \Gamma'(z)/\Gamma(z) \). For \( n \to \infty \), the coefficient approaches a limiting value of

\[
\lim_{n \to \infty} B_{62}(nS) = \frac{4}{135} \left[ 71 + 60(\gamma - \ln 2) \right] = 1.897603 .
\]

The numerical value of the \( B_{62} \)-coefficient depends rather significantly on \( n \). For \( n = 2 \), we have

\[
B_{62}(2S) = \frac{419}{135} - \frac{32}{9} \ln 2 = 0.639180 .
\]

A graph of \( B_{62}(nS) \) in the range \( n = 1, \ldots, 8 \) is given in Fig. [1] [1]

Surprisingly large results have been obtained [2] for the coefficient \( B_{61} \).

\[
B_{61}(1S) = \frac{39751}{10800} + \frac{110}{9} \zeta(2) + \frac{9}{2} \zeta(2) \ln 2 - \frac{9}{8} \zeta(3) - \frac{616}{135} \ln 2 + \frac{40}{9} \ln^2 2 + \frac{4}{3} N(1S) = 50.344005 ,
\]

\[
B_{61}(nS) = B_{61}(1S) + \frac{4}{3} [N(nS) - N(1S)] + \frac{304}{135} - \frac{32}{9} \ln 2 \left( \frac{3}{4} + \frac{1}{4n^2} - \frac{1}{n} - \ln(n) + \Psi(n) + \gamma \right) ,
\]

The quantity \( N(nS) \) results from a correction to the Bethe logarithm induced by a local potential, and has been given for excited states in [4]. In particular, we have \( N(2S) = 12.032209(1) \) and \( B_{61}(2S) = 42.447669(1) \). This is a 15% deviation from the corresponding result for \( 1S \) [equation (7a)] which is indicated here in equation (7b). The \( B_{61} \)-correction, for \( 2S \), therefore does not quite enhance the \( 2S_{1/2}-2P_{1/2} \) interval as much as might be expected from the corresponding result for the \( 1S \) state [equation (7a)].
Figure 1: Dependence of the $B_{62}$-coefficient on the principal quantum number $n$ for S states. On the abscissa, we have the principal quantum number $n$, and the ordinate axis represents the numerical values of $B_{62}(nS)$ as given in equation (4). The smooth curve results from a three-parameter fit with a model of the form $a + b/n + c/n^2$ (the quantities $a$, $b$, and $c$ are fit parameters). A model of this form has been shown to lead to a satisfactory representation of the $n$-dependence of quantum electrodynamic radiative corrections in many cases (see [4] and references therein). The coefficient $B_{62}$ changes sign between $n = 1$ and $n = 2$.

Additionally, we note that the recently available [5] nonlogarithmic two-loop terms of order $(\alpha \pi)^2 (\alpha^2 Z)^6 (\alpha Z)^2 (Z\alpha)^{-6} m_e c^2 n^3 B_{60}(nS)$ result in a negative energy shift for S states and that the $B_{60}$-coefficients are surprisingly large,

$$B_{60}(1S) = -61.6(3) \pm 15\%,$$
$$B_{60}(2S) = -53.2(3) \pm 15\%.$$  

Here, the uncertainty is mainly due to an unknown high-energy contribution to this coefficient.

Recent progress has also been reported with regard to recoil corrections of first order in the mass ratio $m_e/M$, where $M$ is the mass of the atomic nucleus. For hydrogenic systems, a nonperturbative evaluation to all orders in $Z\alpha$ has been performed in [6], and the results are in agreement with the known terms of the $Z\alpha$-expansion of this effect. These are as follows: in the order $(Z\alpha)^5 (m_e/M) m_e c^2$, we have the Salpeter correction. In relative order $(Z\alpha)$, we have a correction obtained by Pachucki and Groch [7]. Finally, in relative order $(Z\alpha)^2 \ln^2[(Z\alpha)^{-2}]$, we have a further correction recently obtained by Pachucki and Karshenboim, and Melnikov and Yelkhovsky [8, 9]. The sum of these corrections, evaluated for $Z = 2$, leads to a satisfactory agreement with the numerical data published in [6] for the entire range $1 < Z \leq 100$. The nonperturbative (in $Z\alpha$) remainder can conservatively be estimated as 3 kHz, which is three times the magnitude of the term of order $(Z\alpha)^2 \ln^2[(Z\alpha)^{-2}]$ (see [8, 9]). This term is not the main source of the theoretical uncertainty.

A discrepancy in the analysis of radiative-recoil corrections of order $\alpha (Z\alpha)^5 (m_e/M) m_e c^2$ has recently been resolved. According to the fully analytic calculation [10], the coefficient multiplying this term has the value $-1.324028/n^3$ for S states (here, $n$ is the principal quantum number). In [11], a slightly different coefficient of $-1.374/n^3$ had been obtained, whereas in [11, 12, 13], a coefficient of $-1.988(4)$ has been given. Assuming the correctness of the most recent evaluation [10], the result for radiative-recoil corrections of order $\alpha (Z\alpha)^5 (m_e/M) m_e c^2$ should be taken as $-0.014$ MHz rather

3
than $-0.035 \text{ MHz}$. This concerns the entry termed \( \alpha (Z\alpha)^5 m/M \) in Table I of [1] which, in units of \( m_e c^2 \), is of relative order \( (Z\alpha)^5 m_e/M \).

Finally, we note that the uncertainty due to the nonperturbative (in \( Z\alpha \)) one-loop self-energy remainder \( G_{SE}(Z\alpha) \) has recently been eliminated [14]: the numerical result reads \( G_{SE}(2S_{1/2}, 2\alpha) = -0.64466(5) \). For the 2S state of \( \text{He}^+ \), the following energy shifts result from the results reported in equations (4)–(9):

\[
\begin{align*}
B_{62}(2S) & \rightarrow +0.037 \text{ MHz} \quad (10a) \\
(\text{entry termed } \alpha (Z\alpha)^6 \ln(Z\alpha)^{-2} \text{ in Table I of [1]}), \\
B_{61}(2S) & \rightarrow +0.289 \text{ MHz} \quad (10b) \\
(\text{entry termed } \alpha (Z\alpha)^6 \ln(Z\alpha)^{-2} \text{ in Table I of [1]}), \\
B_{60}(2S) & \rightarrow (-0.043 \pm 0.006) \text{ MHz} \quad (10c) \\
(\text{entry termed } \alpha (Z\alpha)^6 \text{ in Table I of [1]}), \\
\text{radiative recoil} & \rightarrow -0.014 \text{ MHz} \quad (10d) \\
(\text{entry termed } \alpha (Z\alpha)^5 m/M \text{ in Table I of [1]}), \\
G_{SE}(2S_{1/2}, 2\alpha) & \rightarrow -10.624 \text{ MHz} \quad (10e) \\
(\text{entry termed } (Z\alpha)^6 G_{SE}(Z\alpha) \text{ in Table I of [1]}),
\end{align*}
\]

For completeness, we should also note slight inconsistencies in the notation of the corrections in [1]. First, in Table I of [1], all corrections are given in units of \( m_e c^2 \). The Salpeter correction has inadvertently been termed \( \alpha (Z\alpha)^5 m/M \) whereas in units of \( m_e c^2 \), it should be termed \( Z \alpha (Z\alpha)^4 m/M \).

Correspondingly, the correction denoted \( \alpha (Z\alpha)^6 m_e c^2 \) should actually be termed \( Z \alpha (Z\alpha)^5 m/M \), and the correction denoted as \( \alpha (Z\alpha)^7 \ln(Z\alpha) m/M \) is of course a correction of (relative) order \( Z \alpha (Z\alpha)^6 \ln(Z\alpha) m/M \).

We now discuss the main source of the theoretical uncertainty. There exists an essentially unknown three-loop binding correction of order

\[
(\frac{\alpha}{\pi})^3 \frac{(Z\alpha)^5 m_e c^2}{n^3} C_{50}(nS), \quad (11)
\]

where we note that the \( C_{50} \)-coefficient, in analogy to the two-loop binding correction \( B_{50} \approx -21.5562(31) \), might be numerically large. With the estimate \(|C_{50}| \approx 30\) for the unknown term, the corresponding additional uncertainty for the 2S state is 0.008 MHz. The nuclear-size contribution to the uncertainty is 0.010 MHz [15, 11] (this is assuming a nuclear radius of 1.673(1) fm). There is an additional 0.015 MHz uncertainty due to unknown higher-order two-loop corrections for 2P states.

We obtain the following theoretical error budget for the theoretical value of the Lamb shift in \( \text{He}^+ \):

- unknown high-energy part of \( B_{60} \): 6 kHz.
- unknown higher-order two-loop effects for P states: 15 kHz.
- unknown three-loop binding correction \( C_{50} \): 8 kHz.
- nonperturbative remainder of nuclear recoil: 3 kHz.
- uncertainty in the nuclear charge radius: 10 kHz.

The \( \alpha \) particle charge radius has been determined to high accuracy in [15], using spectroscopic experimental data from the system \( \mu^-\text{He}^2+ \). However, the accuracy of the resulting charge radius of 1.673(1) fm has been questioned (see e.g. [16, 17]). The result obtained in combining scattering experiments is 1.674(12) fm [18] and has a considerably larger error. The above entry in the error
budget should therefore rather be interpreted as a lower limit of this problematic contribution. Because theoretical errors cannot be expected to follow a normal distribution like experimental errors, there exists no universally adopted procedure for the determination of a total theoretical error in a situation where several unknown terms contribute to an error budget. In the current work, we choose to (conservatively) add the above errors in order to obtain a total theoretical uncertainty of 42 kHz. To complete the discussion, we mention that (i) under the assumption of normally distributed theoretical errors, the total theoretical uncertainty would be reduced to 20 kHz, and (ii) under the assumption of a 0.012 fm uncertainty in the nuclear radius \[18\], the theoretical error due to the $\alpha$ particle charge radius alone would be 126 kHz.

3 Conclusions

We have re-evaluated theoretical predictions for the 2S–2P$_{1/2}$ Lamb shift in He$^+$. Taking into account recently evaluated corrections to the entries in Table I of \[11\] (see equation \(10\)), we obtain the new theoretical value of

\[
\nu_{th}(2S_{1/2} - 2P_{1/2}) = 14041.474(42)(126) \text{ MHz},
\]

where the first error is due to the error budget as discussed above, and the second error results due to the nuclear size alone, if we assign a larger nuclear charge radius uncertainty of 0.012 fm \[18\] instead of 0.001 fm \[15\]. For the 2P$_{3/2}$–2S$_{1/2}$-interval, the new theoretical prediction is

\[
\nu_{th}(2P_{3/2} - 2S_{1/2}) = 16154.029(42)(126) \text{ MHz},
\]

with the same error budgets as for 2S$_{1/2} - 2P_{1/2}$.

There remains a small discrepancy between the “new” theoretical value of 14041.474(42) MHz (equation \(12a\)) and the experimental result of 14041.13(17) MHz given in equation \(11\). However, this discrepancy is less severe than the difference of the experimental value \(11\) and the “old” theoretical value of 14041.57(8) MHz (see equation \(12\)).

The sum of the experimental (= 0.17 MHz) and the theoretical uncertainty (= 0.04 MHz) is $\sigma = 0.21$ MHz. This should be compared to the difference $\delta = 0.34$ MHz between the theoretical and experimental “expectation values” \(12a\) and \(11\). The difference $\delta$ corresponds to $1.6 \sigma$. If we assign the larger error of 0.012 fm to the nuclear radius, then the discrepancy shrinks to $1.2 \sigma$.

Even though a difference of $1.2 \sigma$ to $1.6 \sigma$ between theory and experiment remains somewhat unsettling, it is not large enough to be regarded as statistically significant. Even at this level, it still represents a better test of the unexpectedly large $B_{\text{SD}}$ two-loop binding correction to the Lamb shift ($-1.339$ MHz) than that provided by the corresponding measurement in hydrogen. In addition, the anisotropy method provides a completely independent method of measuring the Lamb shift that is not limited by the large level width of the 2P state(s), and it is the only method that is capable of comparing two different atomic or ionic species (H and He$^+$, c.f. Ref. \[19\]) within the same apparatus.

It may also be beneficial, in the near future, to re-analyze the results of the most recent measurement \[11\] in terms of QED corrections to the 2S–2P transition matrix elements which are currently under study \[20\]. In the current paper, we restrict the discussion to the theoretical predictions for the absolute frequency of the 2S–2P transitions. Further clarification of this and related questions will certainly benefit from a reduction of the experimental uncertainty of the Lamb-shift measurement to $\pm 100$ kHz or better, as is currently being pursued by Hinds and Boshier \[3\]. Finally, we stress that all theoretical predictions for transitions in He$^+$ rely on the single available accurate determination of the charge radius of the $\alpha$-particle as described in \[16\]. There is still a lack of accurate independent verifications of this determination of the charge radius. In the end, the answer to a number of questions related to Lamb-shift measurements in atomic hydrogen and He$^+$ might be as easy as a slight deviation of the proton and $\alpha$ particle charge radii from their currently accepted values. However, other, more subtle explanations cannot be ruled out at present, either.
Acknowledgements

The authors acknowledge helpful conversation with P. J. Mohr and J. Sapirstein. We are grateful for SHARCNET support extended to the University of Windsor during the organization of a workshop related to topical questions in quantum electrodynamics, on the occasion of which this research note has been completed. Research support by the Natural Sciences and Engineering Research Council of Canada is gratefully acknowledged.

References

[1] A. van Wijngaarden, F. Holuj, and G. W. F. Drake. Phys. Rev. A 63, 012505 (2001).
[2] K. Pachucki. Phys. Rev. A 63, 042503 (2001).
[3] S.A. Burrows, E.A. Hinds, F. Lison, and M.G. Boshier. in Laser Spectroscopy 14, edited by R. Blatt, J. Eschner, D. Leibfried, and F. Schmidt-Kaler (World Scientific, Singapore, 1999); E.A. Hinds and M.G. Boshier. private communication (2003).
[4] U. D. Jentschura. J. Phys. A 36, L229 (2003).
[5] K. Pachucki and U. D. Jentschura. Phys. Rev. Lett. 91, 113005 (2003).
[6] A. N. Artemyev, V. M. Shabaev, and V. A. Yerokhin. Phys. Rev. A 52, 1884 (1995).
[7] K. Pachucki and H. Grotch. Phys. Rev. A 51, 1854 (1995).
[8] K. Pachucki and S. G. Karshenboim. Phys. Rev. A 60, 2792 (1999).
[9] K. Melnikov and A. S. Yelkhovsky. Phys. Rev. A 60, 2792 (1999).
[10] M. I. Eides, H. Grotch, and V. A. Shelyuto. Phys. Rev. A 63, 052509 (2001).
[11] G. Bhatt and H. Grotch. Phys. Rev. A 31, 2794 (1985).
[12] G. Bhatt and H. Grotch. Ann. Phys. (N. Y.) 178, 1 (1987).
[13] G. Bhatt and H. Grotch. Phys. Rev. Lett. 58, 471 (1987).
[14] U. D. Jentschura, P. J. Mohr, and G. Soff. Phys. Rev. A 64, 042512 (2001).
[15] E. Borie and G. A. Rinker. Phys. Rev. A 18, 324 (1978).
[16] J. S. Cohen. Phys. Rev. A 25, 1791 (1982).
[17] L. Bracci and E. Zavattini. Phys. Rev. A 41, 2352 (1990).
[18] I. Sick, J. S. McCarthy, and R. R. Whitney. Phys. Lett. B 64, 33 (1976).
[19] A. van Wijngaarden, F. Holuj and G.W.G. Drake. Can. J. Phys. 76, 95 (1998).
[20] J. Sapirstein, private communication (2003).