Improved theory of helium fine structure

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Improved theoretical predictions for the fine-structure splitting of 2^3P_J levels in helium are obtained by the calculation of contributions of order \( \alpha^5 \) Ry. New results for transition frequencies, \( \nu_{01} = 2961.943.01(17) \) kHz, and \( \nu_{12} = 2901.161.13(30) \) kHz, disagree significantly with the experimental values, indicating an outstanding problem in bound state QED.

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The fine-structure splitting of the helium 2^3P_J states is an intrinsically relativistic effect, and arises from the interaction of spins and orbital angular momentum. The value of this splitting has been measured with increasing precision over the last years [1, 2, 3, 4, 5]. Since the splitting is proportional to \( \alpha^2 \) Ry, these accurate measurements make helium a candidate for determining the fine structure constant \( \alpha \), provided that the higher order in \( \alpha \) corrections can be sufficiently well understood. The most accurate determination of \( \alpha \) at present comes from the \( q = 2 \) of the electron. This determination depends sensitively on complicated multi-loop calculations performed by Kinoshita and by Remiddi and coworkers [6], and therefore requires independent confirmation. In response to significant experimental effort [1, 2, 3, 4, 5], we present here the calculation of the \( \alpha^5 \) Ry contribution to helium fine structure, so that these experiments can be used to provide an independent determination of \( \alpha \).

Several recent advances in bound state Quantum Electrodynamics (QED) have made the calculation of higher order corrections to helium fine structure possible. Specifically, Yelkhovsky in Ref. [8] has shown how to use dimensional regularization in the calculation of helium energy levels, and together with Korobov has obtained in [9] numerical values for the \( \alpha^5 \) Ry contributions to the ground state. Next, in Ref. [10] a Foldy-Wouthuysen transformed QED Langrangian was used to derive all effective \( \alpha^4 \) Ry operators for arbitrary states of few electron atoms. More recently, together with Jentschura and Czarnecki, we have obtained in Ref. [11] general formulæ for \( \alpha^5 \) Ry correction to hydrogenic energy levels, including the fine structure. The calculational approach of these works [8, 11] and the present paper is based on dimensionally regularized QED. The parameter \( \epsilon \), related to the space dimension \( d = 3 - 2 \epsilon \), plays the role of both infrared and ultraviolet regulator, as some \( \alpha^5 \) Ry terms are divergent in \( d = 3 \) space. This artificial parameter \( \epsilon \) is used to derive various terms, and we will explicitly demonstrate its cancellation in their sum. Natural relativistic units will be used with \( \hbar = c = \epsilon_0 = m = 1 \), so that \( \epsilon^2 = 4 \pi \alpha \).

The fine structure in order \( \alpha^5 \) (\( \alpha^5 \) Ry) can be written as [13]

\[
E^{(7)} = \langle H^{(7)} \rangle + 2 \left\langle H^{(4)} \right\rangle \frac{1}{(E_0 - H_0)} H^{(5)} + E_L \tag{1}
\]

where \( E_L \) is the Bethe logarithmic correction of Eq. [15], and \( H^{(i)} \) is an effective Hamiltonian of order \( m \alpha^i \). We will concentrate in this work on a complete derivation of \( H^{(7)} \), as the other terms contributing to order \( m \alpha^7 \) (\( \alpha^5 \) Ry), \( E_L \) and the second order term called \( E_S \), have already been obtained in [13]. Important terms of order \( m \alpha^7 \) \( \ln \alpha \) first calculated in Ref. [15] are confirmed in the present calculation. \( H^{(7)} \) consists of exchange terms and radiative corrections, where a photon is emitted and absorbed by the same particle. We consider first the exchange terms. Their derivation in general is quite complicated. We note that only two-photon exchange diagrams contribute and there are no three-body terms, which is a result of an internal cancellation. A feature of the calculation that leads to considerable simplification is the fact that the order being calculated in nonanalytic in \( \alpha^2 \). For example, \( H^{(5)} \) includes only two terms

\[
H^{(5)} = -\frac{7}{6 \pi} \frac{\alpha^2}{\pi^3} + 38 \frac{Z \alpha^2}{45} \left[ \delta^3(r_1) + \delta^3(r_2) \right],
\tag{2}
\]

and they can be derived from the two-photon exchange splitting has been measured with increasing precision over the

\[
\int d^D k \frac{1}{k + q/2} \frac{1}{(k - q/2)^2} \left[ \tilde{u}(p'_1) \gamma^\mu (k + (p'_1 + p'_2))/2 - 1 \gamma^\nu u(p_1) \right]
+ \tilde{u}(p'_1) \gamma^\nu (k + (p_1 + p'_2))/2 - 1 \gamma^\mu u(p_1) \right]
\times \tilde{u}(p'_2) \gamma^\nu (k + (p_2 + p'_2))/2 - 1 \gamma^\mu u(p_2) \tag{3}
\]

where \( q = p'_1 - p_1 = p_2 - p'_2 \). If one expands this amplitude in small external momenta one obtains

\[
\delta_1 H = \alpha^2 \left\{ \sigma_1(j, q) \sigma_2(j, q) \left[ -\frac{19}{18} + \frac{1}{3 \epsilon} + \frac{1}{2} \ln(q) \right] + i \left[ \sigma_1(p'_1, p_1) + \sigma_2(p'_2, p_2) \right] \left[ \frac{5}{12} - \frac{1}{3 \epsilon} + \frac{1}{6} \ln(q) \right] + i \left[ \sigma_1(p'_2, p_2) + \sigma_2(p'_1, p_1) \right] \left[ \frac{11}{12} - \frac{2}{3 \epsilon} + \frac{4}{3} \ln(q) \right] \right\}
\]
\begin{equation}
\frac{1}{8} \sigma_1(j, p_1 + p'_1) \sigma_2(j, p_2 + p'_2) \\
- \frac{1}{8} \sigma_1(j, p_2 + p'_2) \sigma_2(j, p_1 + p'_1) \\
+ \frac{17}{72} \sigma_1(j, p_1 - p_2 + p'_1 - p'_2) \\
\times \sigma_2(j, p_1 - p_2 + p'_1 - p'_2) \right) \tag{4}
\end{equation}

where $\sigma^{ij} = -i/2 [\sigma^i, \sigma^j]$ and $\sigma(j, q) = \sigma^{ij} q^i$. The $1/\epsilon$ divergences cancel out with the low energy part where photon momenta are of the order of the binding energy. This low energy contribution gives the Bethe logarithm, described later in Eq. (15), and the correction

\begin{equation}
\delta E_L = e^2 \int_{\Lambda}^{\infty} \frac{d^3k}{(2\pi)^d 2k^2} \left( \delta^{ij} - \frac{k^i k^j}{k^2} \right) \\
\times \delta \left( \phi \left| p_1 \frac{1}{E - H - k} p_2 \right| \phi \right) + (1 \leftrightarrow 2), \tag{5}
\end{equation}

which is the transition term from dimensional regularization to the direct $\Lambda = m (Z \alpha)^2$ cut-off in the photon momenta. Here $\delta$ denotes the first order correction to $\phi$, $H$ and $E$ due to the spin dependent part of the Breit-Pauli Hamiltonian $H^{(b)}$. The resulting correction is a sum of two terms. The first one contributes to $\langle H^{(b)}/(E_0 - H_0) \rangle$ in Eq. (11), and the second term is the effective Hamiltonian

\begin{equation}
\delta_2 H = \alpha^2 \left[ \frac{5}{9} + \frac{1}{3\epsilon} + \frac{2}{3} \ln[(Z \alpha)^{-2}] \right] \left[ i \sigma_1(p'_1, p_1) \\
i \sigma_2(p'_2, p_2) + 2i \sigma_1(p'_2, p_2) + 2i \sigma_2(p'_1, p_1) \\
- \sigma_1(j, q) \sigma_2(j, q) \right], \tag{6}
\end{equation}

where we omitted a $\ln 2\Lambda$ term. Together with Eq. (4) this gives the complete contribution due to exchange terms. When calculating expectation values on $^3P_J$ states further simplifications can be performed. Namely, the expectation value of a Dirac delta function with both momenta on the right or on the left hand side vanishes. Moreover, the nonrelativistic wave function is a product of a symmetric spin and an antisymmetric spatial function. This means that the expectation value of $\sigma_1$ is equal to that of $\sigma_2$. As a result the total exchange contribution $H_E = \delta_1 H + \delta_2 H$ is

\begin{equation}
H_E = \alpha^2 \left[ 6 + 4 \ln[(Z \alpha)^{-2}] + 3 \ln q \right] i \sigma_1(p'_1, p_1) \\
+ \alpha^2 \left[ \frac{23}{9} - \frac{2}{3} \ln[(Z \alpha)^{-2}] + \frac{1}{2} \ln q \right] \\
\times \sigma_1(j, q) \sigma_2(j, q). \tag{7}
\end{equation}

The treatment of the radiative correction is different. We argue that radiative corrections can be incorporated by the use of electromagnetic formfactors and a Uehling correction to the Coulomb potential

\begin{equation}
F_1(-q^2) = 1 + \frac{\alpha}{\pi} \left( \frac{1}{8} + \frac{1}{6 \epsilon} \right) q^2 \\
F_2(-q^2) = \frac{\alpha}{\pi} \left( \frac{1}{2} - \frac{1}{12} q^2 \right) \\
F_V(-q^2) = \frac{\alpha}{\pi} \left( \frac{1}{15} q^2 \right) \tag{8}
\end{equation}

The possible additional corrections are quadratic in electromagnetic fields: see Ref. [11]. However, terms formed out of $\vec{E}, \vec{B}, \vec{p}, \vec{\sigma}$ can contribute only at higher order and thus can be neglected. Corrections due to the slope of formfactors and the vacuum polarization are obtained analogously to the Breit-Pauli Hamiltonian $H^{(b)}$, by modifying electromagnetic vertices and the photon propagator. The result is

\begin{equation}
\delta_3 H = \pi Z \alpha (F_1' + 2 F_2' + F_V') [i \sigma_1(p'_1, p_1) + \sigma_2(p'_2, p_2)] \\
\pi \alpha (2 F_1' + 2 F_2' + F_V') [i \sigma_1(p'_1, p_1) + \sigma_2(p'_2, p_2)] \\
- \pi \alpha (2 F_1' + 2 F_2' + F_V') [i \sigma_1(p'_2, p_2) + \sigma_2(p'_1, p_1)] \\
+ \pi \alpha (2 F_1' + 2 F_2' + F_V') \sigma_1(j, q) \sigma_2(j, q), \tag{9}
\end{equation}

where by $\rho''$ we denote momentum scattered off the Coulomb potential of a nucleus, and $F' = F'(\alpha)$. There is also a low-energy contribution which is calculated in a way similar to this in Eq. (5), namely

\begin{equation}
\delta E_L = e^2 \int_{\Lambda}^{\infty} \frac{d^3k}{(2\pi)^d 2k^2} \left( \delta^{ij} - \frac{k^i k^j}{k^2} \right) \\
\times \delta \left( \phi \left| p_1 \frac{1}{E - H - k} p_2 \right| \phi \right) + (1 \leftrightarrow 2) \tag{10}
\end{equation}

The resulting effective Hamiltonian is

\begin{equation}
\delta_4 H = \alpha^2 \left[ \frac{5}{9} + \frac{1}{3\epsilon} + \frac{2}{3} \ln[(Z \alpha)^{-2}] \right] \\
\times \left[ i \frac{Z}{2} \sigma_1(p''_1, p_1) + i \frac{Z}{2} \sigma_2(p''_2, p_2) \\
- i \sigma_1(p'_1, p_1) - i \sigma_2(p'_2, p_2) - 2i \sigma_2(p'_1, p_1) \\
- 2i \sigma_1(p'_2, p_2) + \sigma_1(j, q) \sigma_2(j, q) \right] \tag{11}
\end{equation}

The complete radiative correction is a sum of Eqs. (9) and (11), namely $H_R = \delta_3 H + \delta_4 H$. Using symmetry $1 \leftrightarrow 2$ it takes the form

\begin{equation}
H_R = Z \alpha^2 \left[ \frac{91}{180} + \frac{2}{3} \ln[(Z \alpha)^{-2}] \right] i \sigma_1(p'_1, p_1) \\
+ \alpha^2 \left[ \frac{73}{180} + \frac{2}{3} \ln[(Z \alpha)^{-2}] \right] \sigma_1(j, q) \sigma_2(j, q) \\
- \alpha^2 \left[ \frac{21}{10} + 4 \ln[(Z \alpha)^{-2}] \right] i \sigma_1(p'_1, p_1) \tag{12}
\end{equation}

It is convenient to consider a sum of Eqs. (7) and (12), as several logarithmic terms cancel out

\begin{equation}
H_Q = H_E + H_R = \sum_{i=1}^{5} Q_i \tag{13}
\end{equation}

The logarithmic terms agree with Refs. [15, 16], while non-logarithmic terms $Q_i$ are presented in Table I.
The remaining contribution is the anomalous magnetic moment change to the spin dependent operators. We derive it with the help of a nonrelativistic QED Hamiltonian obtained by a Foldy-Wouthuysen transformation of the Dirac Hamiltonian including the magnetic moment anomaly $\kappa$ \[11\]

$$H_{FW} = \frac{\vec{p}^2}{2} + e A^0 - \frac{e}{2} (1 + \kappa) \vec{B} \cdot \vec{B} - \frac{\vec{A}^2}{4}$$
$$- \frac{e}{8} (1 + 2 \kappa) \left[ \vec{A} \cdot \vec{E} + \vec{\sigma} \cdot (\vec{E} \times \vec{B} - \vec{E} \times \vec{B}) \right]$$
$$+ \frac{e}{8} \left\{ (\vec{\sigma} \cdot \vec{E}^2) + \kappa \left[ \vec{\sigma} \cdot (\vec{B} \times \vec{B} \cdot \vec{\sigma}) \right] \right\}$$
$$- \frac{3 + 4 \kappa}{64} \left\{ \vec{p}^2, \vec{E} \times \vec{B} \cdot \vec{p} \right\}$$

(14)

All the $m \alpha^6$ operators obtained by Douglas and Kroll (DK) in \[17\] can also be obtained from this Hamiltonian in Eq. (14), see Ref. [10]. The anomalous magnetic moment operators are derived in a very similar way. They differ (see Table II) only by multiplicative factors from the DK operators. There is a one to one correspondence with Table I of Ref. [18] with 3 exceptions. The operator $H_S$ from Table II canceled out in DK calculation. The other two exceptions are related to the different spin structure of the next to last term in Eq. (14), which leads to operators $H_{16}$ and $H_{17}$ in our Table II.

Apart from the $H_i$ and $Q_i$ operators, second order contributions and low energy Bethe-logarithmic type corrections contribute to the fine structure. These contributions have already been considered in our former work [13]. The second order contribution $E_S$, beyond the anomalous magnetic moment terms is the second term of Eq. (1). The low energy contribution $E_L$ is

$$E_L = - \frac{2 \alpha}{3 \pi} \delta \left( \phi \right) \left( \vec{p}_1 + \vec{p}_2 \right) \left( H - E \right) \ln \left[ \frac{2 (H - E)}{(\Delta \alpha)^2} \right]$$
$$\left( \vec{p}_1 + \vec{p}_2 \right) \phi + \frac{i 2 \alpha^3}{3 \pi} \phi \left( \vec{r}_1 + \vec{r}_2 \right)$$
$$\times \left( \vec{\sigma}_1 + \vec{\sigma}_2 \right) \frac{2}{2} \ln \left[ \frac{2 (H - E)}{(\Delta \alpha)^2} \right] \cdot \left( \vec{r}_1 + \vec{r}_2 \right) \phi,$$

(15)

where $\delta(...)$ denotes the correction to the matrix element $\langle ... \rangle$ due to $H^{(4)}$. Numerical results for all these contributions is presented in Table III.

| Operator | $\nu_{10}[kHz]$ | $\nu_{12}[kHz]$ |
|----------|-----------------|-----------------|
| $Q_1$    | 2.854           | 5.709           |
| $Q_2$    | 10.866          | -4.355          |
| $Q_3$    | 4.132           | -1.653          |
| $Q_4$    | 5.186           | 10.372          |
| $Q_5$    | -1.328          | -2.656          |

$E_Q = \sum_{i=1,5} Q_i$

21.731 7.418

TABLE II: Summary of contributions to helium fine structure, $E^{(4)}$ and $E^{(6)}$ including nuclear recoil corrections and the electron anomalous magnetic moment at the level of the Breit-Pauli Hamiltonian: $\alpha^{-1} = 137.0359991(46)$, $m_e/m_p = 1.37093355575(61)10^{-4}$. Ry $c = 3.289841960360(22)10^{15}$. Hz. Not indicated is the uncertainty due to $\alpha$, which is 0.0 kHz for $\nu_{10}$. The last row includes the most recent experimental values.

| Operator | $\nu_{10}[kHz]$ | $\nu_{12}[kHz]$ | Ref. |
|----------|-----------------|-----------------|------|
| $H_Q$    | 21.73           | 7.42            |      |
| $H_{11}$ | -4.21           | 4.05            |      |
| $H_{17}$ | 11.37(02)       | -12.51(27)      | [13] |
| $E_{18}$ | -29.76(16)      | -23.09(27)      |      |
| $E_{17}^{(7)}$ | -0.87(16) | -2.30(27) |      |
| $E_{17}^{(8)}$ | 82.59     | -10.09         |      |
| $E_{17}^{(10)}$ | -1557.50(06) | -654.32(12) | [12, 14, 19, 20] |
| $E_{17}^{(14)}$ | 296184187.09(01) | 2977178.84 | [14,19] |
| total    | 296184934.01(17) | 2291161.13(30) |      |
| Drake    | 296184964.2(18) | 2291154.62(31) | [14] |
| exp.     | 296185155.67(10) | 2291175.59(51) | [1, 2, 3, 4, 5, 6] |

Since all relevant contributions to helium fine structure splitting now seem to be known, we are at a position to present final theoretical predictions, which is done in Table III. Although we have included all terms up to order $m \alpha^7$, theoretical predictions are in apparent disagreement with the mea-
measurements, as can be seen from the last row of Table [11]. Let us analyze possible sources of this discrepancy. The numerical calculation involves variational nonrelativistic wave function. The parameter which controls its accuracy is the non-relativistic energy. Our wave function, consisting at maximum of 1500 explicitly correlated exponential functions reproduces energy with 18 significant digits in agreement with the result of Drake in [14]. Matrix elements with this wave function are not as accurate as nonrelativistic energy, but they are sufficiently accurate for leading fine structure operators, and results agree with more accurate and independent calculation of Drake in [14]. For example, $E^{(4)}$ agrees to 0.01 kHz and $E^{(6)}$ to 0.1 kHz. In fact almost all numerical calculations have been performed by us and by Drake independently with one exception; we have not obtained recoil correction to the second order matrix element with Breit operators in $E^{(6)}$. More important is the complexity of the derivation of $m \alpha^7$ operators, namely $H_t$ and $Q_t$. We purposely derived $H_t$ in a way very similar way to the derivation of the D-K operators to avoid accidental mistakes. We note that the $Q_t$ operators were obtained from the one-loop scattering amplitude in an almost automatic way, in contrast to the former very lengthy derivation of Zhang [21][22][23], with which we are in disagreement (see summary of Zhang results in Ref. [14]). In our previous papers with Sapirstein [13][20] we pointed out several computational mistakes and inconsistencies in Zhang’s calculations, and therefore we consider the result of Drake, see Table [11] to be incomplete. While it is possible that we have made a mistake somewhere, the other probable explanation of the discrepancy with experiments is the neglect of higher order terms, namely $m \alpha^8$. An indication of their importance is the recoil correction to the second order contribution, obtained by Drake in [14]. In spite of the small electron-alpha particle mass ratio, this correction is very significant; for example $\delta v_{101} = -10.81$ kHz. The mass ratio $m_e/m_\alpha \approx 0.00014$ is not much different from $\alpha^2 \approx 0.000053$, and for this reason one can expect that iteration of Breit-Pauli Hamiltonian in the third order might also be significant. However, most $m \alpha^8$ operators should be negligible, as $E^{(7)}$ is already at the few kHz level, so that an additional power of $\alpha$ will make these operators contribute well below the experimental accuracy.

In summary, we have obtained the complete $\alpha^5$ Ry contribution to helium fine structure splitting. Theoretical predictions, including this result, are in disagreement with measurements [12][13][14][15]. Therefore the determination of $\alpha$ from helium spectroscopy requires both checking the calculation of $E^{(7)}$ and the reliable estimation of the higher order $E^{(9)}$ contribution, which is a challenging task. Therefore, at present, helium fine structure splitting is not competitive with respect to other determinations of $\alpha$, for example, from the recent experiment on the photon recoil [24].

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