Higher Order Recoil Corrections to Helium Fine Structure

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Abstract

A class of recoil corrections of order $\alpha^4 \frac{m_e}{m_\alpha} \mathrm{Ry}_\infty c$ to the fine structure of helium is calculated. The present status of the fine structure constant determined from comparison of theory with recent accurate experiments of the large interval ν_{01} is described, and possible explanations for significant discrepancies between theory and experiment for ν_{01} as well as the small interval ν_{12} discussed.

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I. INTRODUCTION

The study of nuclear recoil corrections to light atomic spectra is a challenging problem. In the nonrelativistic limit these corrections are accounted for by introducing the mass polarization term and replacing the electron mass with its reduced mass equivalent μ. Relativistic recoil corrections are much more difficult to treat. It is incorrect, for example, to simply use the reduced mass in the Dirac equation. A generally accepted method of accounting for recoil corrections in the relativistic case is provided by the Bethe-Salpeter equation; however its implementation in atomic physics is very complicated. Recoil corrections have been worked out in greatest detail in hydrogenic systems [1]. For light few electron atoms, one can take advantage of the smallness of the nuclear charge and perform a nonrelativistic expansion within QED (quantum electrodynamic theory). This is the effective Hamiltonian approach, which has been applied to a number of corrections to helium fine structure [2]. The leading relativistic recoil corrections in helium are well understood, and were first derived by Stone [3]. The problem we will be concerned with here is the evaluation of corrections of order $\alpha^4 \frac{m_e}{m_\alpha}\,\mathrm{Ry}_\infty c$. Although they are small, they are still significant for the determination of α from the measurement of helium fine structure.

In a recent paper [4] we presented a convenient formula which can be used to extract the fine structure constant from measurements of the splitting $\nu_{01} \equiv E(2^3P_0) - E(2^3P_1)$ in helium,

$$\nu_{01} - \delta\nu_{01} = \alpha^2 \cdot 556\ 200\ 289.5(1)\,\mathrm{MHz}. \tag{1}$$

Here $\delta\nu_{01}$ represents QED corrections starting in order $\alpha^4\ \mathrm{Ry}_\infty c$, and the factor multiplying α^2 is determined from the leading contribution of order $\alpha^2\ \mathrm{Ry}_\infty c$, with the electron anomalous magnetic moment and recoil corrections treated to all orders. The two most accurate experiments are those of Inguscio's group [5], which has an accuracy of 68 ppb,

$$\nu_{01} = 29\ 616.949\ 7(20)\,\mathrm{MHz}, \tag{2}$$

and those of Hessels' group [6], which have an accuracy of 30 ppb,

$$\nu_{01} = 29\ 616.950\ 9(9)\,\mathrm{MHz}. \tag{3}$$

The form of the higher order corrections is given by

$$\delta\nu_{01} \equiv \nu_{01}^{(4)} + \nu_{01}^{(4r)} + \nu_{01}^{(5)} + \nu_{01}^{(6)}, \tag{4}$$

where each term is small enough so that it suffices to use the CODATA [7] value of α to determine it. The first term, $\nu_{01}^{(4)}$, consists of contributions from second-order perturbation theory in the Breit Hamiltonian, which contribute in order α^4 Ry$_\infty c$, along with a set of operators first calculated by Douglas and Kroll [8] which contribute in the same order. These terms were evaluated several decades ago [9], [10], but were first calculated at the ppm level by Yan and Drake [11]. We have found good agreement with these calculations [4], and this term can be regarded as completely understood. Its value is -1.547 06(10) MHz. We note that this value includes the electron anomalous magnetic moment in the second order perturbation theory terms. The second term, $\nu_{01}^{(4r)}$, is the subject of this paper, and involves recoil corrections of order $\alpha^4 \frac{m_e}{m_\alpha}$ Ry$_\infty c$. These were left incompletely evaluated in Ref. [4], and as individual terms in a part of the calculation that was carried out could be as large as 5 kHz, it is clearly important to complete them. The third term, $\nu_{01}^{(5)}$, of order α^5 Ry$_\infty c$, has also been only partially calculated. While we will not complete the calculation here, we will discuss its feasibility in the conclusion. The value of the terms so far calculated, which include terms proportional to lnα [12] and constant terms [13], is 0.070 29 MHz. Finally, the fourth term, $\nu_{01}^{(6)}$, which involves α^6 Ry$_\infty c$ contributions, was evaluated [4] to leading order in ln α, and found to be quite small, 0.000 08 MHz. If the associated constant is small, the completion of the calculation of $\nu_{01}^{(5)}$ should allow a determination of α of accuracy approaching that of the precision available from the electron $g-2$ [14] and cesium recoil [15]. We now discuss the calculation of $\nu_{01}^{(4r)}$.

This recoil correction can be divided into three parts, discussed now in turn. The first part deals with the 15 operators first listed by Douglas and Kroll [8] that contribute to $\nu_{01}^{(4)}$. Recoil corrections affect these in two ways: firstly, use of the reduced mass in place of the electron mass leads to scaling factors of order $(\mu/m)^4$ and $(\mu/m)^5$ that are trivially implemented. Secondly, the effect of mass polarization can be included by reevaluating the 15 expressions in between wave functions determined with mass polarization included. This calculation was carried out in Ref. [4], and is in perfect agreement with results compiled by Drake in [16]. The second set of recoil corrections arises from second-order perturbation theory. This also requires use of wave functions including mass polarization and reduced mass scaling factors. Results for these have been presented by Drake [16], and we will include them below. The only terms that require a new theoretical treatment are the recoil analogs of the DK operators. While our calculation is somewhat complex, the final answer is relatively compact,

$$
\begin{aligned}
V_{\rm rec}^{\rm DK} \;=\; & 2\,\alpha^4\,\frac{m_e}{m_\alpha}{\rm Ry}_\infty c \\
& \Big\{\frac{Z}{4}p_1^2\Big[\frac{i}{r_1}\vec{\sigma}_1\cdot\vec{p}_1\times\vec{p}_2 - i\,\frac{\vec{r}_1}{r_1^3}(\vec{\sigma}_1\cdot\vec{r}_1\times\vec{p}_1)\cdot(\vec{p}_1+\vec{p}_2) - \frac{3}{r_1^3}\,\vec{\sigma}_1\cdot\vec{r}_1\times(\vec{p}_1+\vec{p}_2)\Big] \\
& +Z^2\Big[\vec{\sigma}_1\cdot\frac{\vec{r}_1}{r_1^3}\times\frac{\vec{r}_2}{r_2^3}\,(\vec{r}_1\cdot\vec{p}_1) - \frac{1}{2}\vec{\sigma}_1\cdot\frac{\vec{r}_1}{r_1^4}\times(\vec{p}_1+\vec{p}_2) - \frac{1}{4}\vec{\sigma}_1\cdot\frac{\vec{r}_2}{r_2^3}\,\vec{\sigma}_2\cdot\frac{\vec{r}_1}{r_1^2}\Big] \\
& +Z\Big[\vec{\sigma}_1\cdot\frac{\vec{r}_{12}}{r_1 r_{12}^3}\times(\vec{p}_1+\vec{p}_2) - \vec{\sigma}_1\cdot\left(\frac{\vec{r}_1}{r_1^3}\times\frac{\vec{r}_{12}}{r_{12}^3}\right)\,\vec{r}_1\cdot(\vec{p}_1+\vec{p}_2)\Big]\Big\}\,. \qquad (5)
\end{aligned}
$$

The derivation of this expression will be given below. Corrections of this order have previously been considered by Zhang [17], [18], and we will compare with his results, with which we have differences, in the conclusion.

The general approach we use is the effective Hamiltonian technique [2], in which diagrams involving relativistic electron propagators and retarded photon propagators are compared with diagrams obtained from a nonrelativistic field theory, with the difference identified with operators that are subsequently treated as perturbations in bound state perturbation theory. If these perturbations enter in higher order, spurious ultraviolet infinities are encountered that must be carefully cancelled, but for $\nu^{(4r)}$ such subtleties do not arise. The relevant diagrams are shown in Figs. 1 a-h. In the following, all operators will be expressed in atomic units, and a common prefactor of $2\,\alpha^4\frac{m_e}{m_\alpha}{\rm Ry}_\infty c = 2.558$ kHz is understood.

Figure 1a, which also accounts for the leading recoil correction [3] of order $\alpha^2\frac{m_e}{m_\alpha}\,{\rm Ry}_\infty\,c$, leads to three additional operators contributing in the order of interest

$$
\begin{aligned}
V_1 \;=\; & \frac{i\,Z}{4}\,p_1^2\,\frac{1}{r_1}\vec{\sigma}_1\cdot\vec{p}_1\times\vec{p}_2 - \frac{i\,Z}{4}\,p_1^2\,\frac{\vec{r}_1}{r_1^3}\,(\vec{\sigma}_1\cdot\vec{r}_1\times\vec{p}_1)\cdot(\vec{p}_1+\vec{p}_2) \\
& -\frac{3\,Z}{4}\,p_1^2\,\vec{\sigma}_1\cdot\frac{\vec{r}_1}{r_1^3}\times(\vec{p}_1+\vec{p}_2). \qquad (6)
\end{aligned}
$$

In these expressions p_1^2 is understood to operate to the left, and while only one electron spin is present, the effect of the second has been included as an overall multiplicative factor. This convention will be used in the remaining expressions. Figure 1b involves the third term in the expansion of the propagator, which we call retardation

$$
\frac{1}{E-H_0-k} = -\frac{1}{k} + \frac{(E-H_0)}{k^2} - \frac{(E-H_0)^2}{k^3} + ... \qquad (7)
$$

The first term has already been treated in Figure 1a and the second is associated with the Salpeter correction, which does not contribute to fine structure, and which is why no

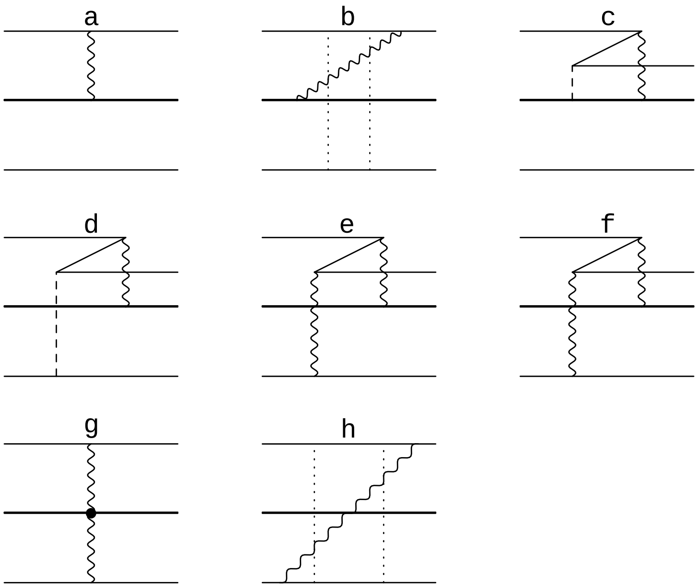

FIG. 1: Time ordered diagrams contributing to helium fine structure at order $m^2/M\,\alpha^6$. Dashed line is a Coulomb photon, the wavy line is a transverse photon, the dotted lines denotes retardation, the thicker middle horizontal line denotes the nucleus, and the thiner outer horizontal lines denote electrons.

diagram with a single dotted line is treated here. The remaining term leads to

$$V_2 = \frac{Z^2}{2}\vec{\sigma}_1 \cdot \frac{\vec{r}_1}{r_1^4} \times \vec{p}_1 + \frac{Z^2}{2}\vec{\sigma}_1 \cdot \frac{\vec{r}_2}{r_1 r_2^3} \times \vec{p}_1 + \frac{Z^2}{2}\vec{\sigma}_1 \cdot \frac{\vec{r}_1}{r_1^3} \times \frac{\vec{r}_2}{r_2^3}\,(\vec{r}_1 \cdot \vec{p}_1). \tag{8}$$

Figures 1c and 1d, sometimes referred to as Z diagrams, account for the fact the electron propagator has negative energy components. Specifically, one can divide a free electron propagator using

$$\frac{1}{E\gamma_0 - \vec{\gamma}\cdot\vec{p} - m} = \frac{\sum_s u_s(\vec{p})\bar{u}_s(\vec{p})}{E - \sqrt{\vec{p}^2 + m^2}} + \frac{\sum_s v_s(\vec{p})\bar{v}_s(\vec{p})}{E + \sqrt{\vec{p}^2 + m^2}} \tag{9}$$

where u_s and v_s are positive and negative energy solutions of the Dirac equation. The second part is represented by the Z shape in the upper electron propagators in Figures 1c and 1d. The contribution from Figure 1c is

$$V_3 = -\frac{Z^2}{2}\vec{\sigma}_1 \cdot \frac{\vec{r}_1}{r_1^4} \times (\vec{p}_1 + \vec{p}_2) \tag{10}$$

and from Figure 1d

$$V_4 = \frac{Z}{2}\vec{\sigma}_1 \cdot \frac{\vec{r}_{12}}{r_1 r_{12}^3} \times (\vec{p}_1 + \vec{p}_2) + \frac{Z}{2}\vec{\sigma}_1 \cdot \left(\frac{\vec{r}_{12}}{r_{12}^3} \times \frac{\vec{r}_1}{r_1^3}\right) \vec{r}_1 \cdot (\vec{p}_1 + \vec{p}_2). \tag{11}$$

When the negative energy component of an electron propagator is sandwiched between two transverse photon vertices, the net effect is to create the pointlike interaction described by the A^2 term in the well-known nonrelativistic expression

$$\frac{(\vec{p} - e\vec{A})^2}{2m}, \tag{12}$$

and this is used in Figures 1e-g. They give the contributions

$$V_5 = \frac{Z}{2}\vec{\sigma}_1 \cdot \frac{\vec{r}_{12}}{r_1 r_{12}^3} \times (\vec{p}_1 + \vec{p}_2) - \frac{Z}{2}\vec{\sigma}_1 \cdot \frac{\vec{r}_1}{r_1^3} \times \frac{\vec{r}_{12}}{r_{12}^3}\, \vec{r}_1 \cdot (\vec{p}_1 + \vec{p}_2)) \tag{13}$$

$$V_6 = -\frac{Z^2}{2}\vec{\sigma}_1 \cdot \frac{\vec{r}_1}{r_1^4} \times \vec{p}_1 \tag{14}$$

$$V_7 = -\frac{Z^2}{4}\vec{\sigma}_1 \cdot \frac{\vec{r}_2}{r_2^3}\sigma_2 \cdot \frac{\vec{r}_1}{r_1^3} - \frac{Z^2}{2}\vec{\sigma}_1 \cdot \frac{\vec{r}_1}{r_2 r_1^3} \times \vec{p}_2 - \frac{Z^2}{2}\vec{\sigma}_1 \cdot \frac{\vec{r}_1}{r_1^3} \times \frac{\vec{r}_2}{r_2^3}\, (\vec{r}_2 \cdot \vec{p}_2). \tag{15}$$

Finally, while Figure 1h is in fact vanishing to the order of interest, it has at intermediate stages of its evaluation, terms that are of order $\alpha^4 \frac{m_e}{m_\alpha}\, \mathrm{Ry}_\infty\, c$. Only rather detailed cancellations lead to the null result.

The above contributions sum to our main result, Eqn. (5). However, to do this the last term of V_7 is transformed by first exchanging indices 1 and 2, and then replacing σ_2 with σ_1, which is allowed for triplet states. This ends up combining with the third term of V_2, with both terms equal. A similar manipulation on the second term of V_7 leads to a term which cancels the second term of V_2.

The individual contributions in kHz to the large and small fine structure intervals are presented in Table 1. The method used for the treatment of angular reduction and numerical evaluation is the same as that described in Ref. [4]. While highly precise wave functions are not needed for the present calculation, we note at this point the remarkable improvement in numerical accuracy for the ground state energy recently achieved by Schwartz [19], who determined that energy to 36 decimal digits.

II. COMPARISON WITH PREVIOUS WORK AND CONSEQUENCES FOR THE FINE STRUCTURE CONSTANT

As mentioned above, operators for recoil corrections at the present order of interest were previously treated by Zhang [17], [18]. He used a Salpeter formalism that should give results equivalent to those coming from our effective Hamiltonian approach. Here, we have identified

TABLE I: Results in kHz for the recoil correction operators, listed with prefactor $2\,\alpha^4 \frac{m_e}{m_\alpha} \mathrm{Ry}_\infty c$ understood, for the large and small helium fine structure intervals

Contribution	ν_{01}	ν_{12}
$\frac{iZ}{4} p_1^2 \frac{1}{r_1} \vec{\sigma}_1 \cdot (\vec{p}_1 \times \vec{p}_2)$	0.480	0.959
$-\frac{iZ}{4}\, p_1^2\, \frac{\vec{r}_1}{r_1^3}\, (\vec{\sigma}_1 \cdot \vec{r}_1 \times \vec{p}_1) \cdot (\vec{p}_1 + \vec{p}_2)$	0.165	0.330
$-\frac{3Z}{4}\, p_1^2\, \vec{\sigma}_1 \cdot \frac{\vec{r}_1}{r_1^3} \times (\vec{p}_1 + \vec{p}_2)$	-1.103	-2.206
$Z\, \vec{\sigma}_1 \cdot \frac{\vec{r}_{12}}{r_1\, r_{12}^3} \times (\vec{p}_1 + \vec{p}_2)$	0.129	0.258
$Z\, \vec{\sigma}_1 \cdot \frac{\vec{r}_{12}}{r_{12}^3} \times \frac{\vec{r}_1}{r_1^3}\, (\vec{r}_1 \cdot (\vec{p}_1 + \vec{p}_2))$	0.042	0.085
$Z^2\, \vec{\sigma}_1 \cdot \frac{\vec{r}_1}{r_1^3} \times \frac{\vec{r}_2}{r_2^3}\, (\vec{r}_1 \cdot \vec{p}_1)$	-0.236	-0.472
$-\frac{Z^2}{2}\, \vec{\sigma}_1 \cdot \frac{\vec{r}_1}{r_1^4} \times (\vec{p}_1 + \vec{p}_2)$	-0.471	-0.941
$-\frac{Z^2}{4} \vec{\sigma}_1 \cdot \frac{\vec{r}_2}{r_2^3}\, \vec{\sigma}_2 \cdot \frac{\vec{r}_1}{r_1^3}$	-0.354	0.141
sum	-1.348	-1.847

four terms in which we differ by sign. These are the first two terms of Eqn. (351) in Ref. [17] and the first two terms of Eq. (18) in Ref. [18]. These correspond to the last two terms in V_2 and V_7 respectively. Unfortunately, we have not been able to trace the origin of this difference, due to the complexity of Zhang's derivation.

We now turn to a discussion of the consequences of accounting for the contributions to $\delta\nu_{01}^{(4r)}$ not included in our previous work [4]. In that paper, we obtained $\delta\nu_{01}^{(4r)} = 0.001\,78$ MHz. The calculation presented here decreases this by -0.001 35 MHz, and Drake's calculation [16] of the second order perturbation contributions decreases it by even more, -0.010 81 MHz. The present status of our theory for $\delta\nu_{01}$ is then summarized below:

$$\begin{aligned}
\nu_{01}^{(4)} &= -1.547\,06(10)\,\mathrm{MHz} \\
\nu_{01}^{(4r)} &= -0.010\,38\,\mathrm{MHz} \\
\nu_{01}^{(5)} &= 0.070\,29(500)\,\mathrm{MHz} \\
\nu_{01}^{(6)} &\approx 0.000\,08(30)\,\mathrm{MHz}
\end{aligned} \tag{16}$$

and current value for $\delta\nu_{01}$ using Eq. (4) is then

$$\delta\nu_{01} = -1.487\,07(500)\,\mathrm{MHz}. \tag{17}$$

This corresponds, using Eqs. (1) and (3), to a value of

$$\alpha_{\rm fs}^{-1} = 137.035\,955(12). \tag{18}$$

which does not agree well with the CODATA value of $\alpha^{-1} = 137.035\,999\,76(50)$. If we used this value of α, we have the prediction for the large interval $\nu_{01} = 29\,616.931(5)$ MHz. The poor agreement between theory and experiment mirrors that already observed in Ref. [4] for the small interval. Taking our former result $\delta\nu_{12} = -6.564\,20(500)$ MHz, together the result of Table 1 for the DK recoil corrections of -0.001 85 MHz with Drake's calculation of recoil corrections to second order perturbation theory [16] 0.010 19 MHz leads to $\delta\nu_{12} = -6.555\,86(500)$ MHz and to a prediction for the small interval of

$$\nu_{12} = 2\ 291.162(5)\,\text{MHz}, \tag{19}$$

in poor agreement with the two most accurate experiments,

$$\nu_{12} = \begin{cases} 2\,291.1759(10)\,\text{MHz} & [20] \\ 2\,291.1740(14)\,\text{MHz} & [21] \end{cases}$$

The most obvious possibility to explain this situation is that our estimate of uncalculated terms in $\delta\nu^{(5)}$, which is 5 kHz, is not conservative enough. The only way to settle this issue is of course the completion of this difficult calculation. This entails a derivation of a set of operators along with their numerical evaluation. A set of operators contributing to $\delta\nu^{(5)}$ have been derived by Zhang [17], but considering the discrepancies with his formulas noted in this paper along with problems with his one-electron contributions to $\nu^{(5)}$ discussed in Ref. [13], we think it is important that an agreed on set of operators, ideally derived by different groups using different methods, be established for helium fine structure.

Less likely is the possibility that the matrix elements of the second-order perturbation theory component of $\delta\nu^{(4r)}$ or the logarithmic terms of $\delta\nu^{(5)}$ are in error. At present, though, they have been evaluated only by Drake in [16], and an independent check of the calculation is desirable. We conclude by noting that, while considerable work clearly needs to be done in precision calculations of helium fine structure, once the corrections have been finally settled, the precision of both theory and experiment will be sufficient to make the study of helium fine structure a valuable way of determining the fine structure constant, whose comparison with values determined from electron $g-2$ [14] and cesium recoil [15] will either strongly test the internal consistency of QED or else point the way to possible new physics.

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