

2s Hyperfine Structure in Hydrogen Atom and Helium-3 Ion

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Abstract. The usefulness of study of hyperfine splitting in the hydrogen atom is limited on a level of 10 ppm by our knowledge of the proton structure. One way to go beyond 10 ppm is to study a specific difference of the hyperfine structure intervals $8\Delta\nu_2 - \Delta\nu_1$. Nuclear effects for are not important this difference and it is of use to study higher-order QED corrections.

1 Introduction

The hyperfine splitting of the ground state of the hydrogen atom has been for a while one of the most precisely known physical quantities, however, its use for tests of QED theory is limited by a lack of our knowledge of the proton structure. The theoretical uncertainty due to that is on a level of 10 ppm. To go farther with theory we need to eliminate the influence of the nucleus. A few ways have been used (see e. g. [1]):

- to remove the proton from the hydrogen atom and to study a two-body system, which is similar hydrogen, but without any nuclear structure, namely: muonium [2] or positronium [3];
- to compare the hyperfine structure intervals of the 1s and 2s states (this work);
- to measure the hyperfine splitting in muonic hydrogen and to compare it with the one in a normal hydrogen atom (a status report on the $n = 2$ muonic hydrogen project is presented in Ref. [4]; comparison of the 1s and 2s *hfs* and possibility to measure 1s *hfs* is considered in Ref. [5].

Recently there has been considerable progress in measurement and calculation of the hyperfine splitting of the ground state and the $2s_{1/2}$ state in the hydrogen atom. The $2s_{1/2}$ hyperfine splitting in hydrogen was determined to be [6]

$$\Delta\nu_2(\text{H}) = 177\,556.785(29) \text{ kHz} , \quad (1)$$

While less accurate than the classic determination of the ground state hyperfine splitting, the combination of 1s and 2s *hfs* intervals

$$D_{21}(\text{H}) = 8\Delta\nu_2 - \Delta\nu_1 . \quad (2)$$

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which is determined in the hydrogen atom [6] as

$$D_{21}(H) = 48.528(232) \text{ kHz} ,$$

has more implications for tests of bound state QED because there is significantly less dependence on the poorly understood proton structure contributions. Specifically, the theoretical uncertainty for the ground state from the proton structure is about 10 kHz, while the uncertainty for the combination is estimated to be few Hz.

On the theoretical front, there has been considerable progress in the calculation of the ground state hyperfine splitting. Taken together with earlier calculations of D_{21} [14,15], which were possible because of cancellations of a number of large terms, one can now give quite accurate values for $\Delta\nu_1$ and $\Delta\nu_2$,

We collect in Tables 1 and 2 along with the hydrogen results, the known experimental and theoretical results for the deuterium atom and the $^3\text{He}^+$ ion. The helium results [7]

$$\Delta\nu_1(^3\text{He}^+) = 8665\,649.867(10) \text{ kHz} \quad (3)$$

and [8]

$$\Delta\nu_2(^3\text{He}^+) = 1083\,354.969(30) \text{ kHz} \quad (4)$$

lead to the most accurate value for the difference

$$D_{21}(^3\text{He}^+) = 1\,189.979(71) \text{ kHz} . \quad (5)$$

Table 1. Comparison of the QED part of the theory to the experiment for hydrogen and deuterium atoms and for the $^3\text{He}^+$ ion. The results are presented in kHz

Atom	Experiment		QED theory for D_{21}	
	$D_{21}(\text{exp})$	Refs.: 2s/1s	Old	New
H	48.528(232)	[6]/[9]	48.943	48.969(2)
H	49.13(40)	[10]/[9]		
D	11.16(16)	[11]/[12]	11.307	11.3132(4)
$^3\text{He}^+$	1 189.979(71)	[8]/[7]	1 189.795	1 191.126(40)
$^3\text{He}^+$	1 190.1(16)	[13]/[7]		

2 Theory

We consider a hydrogen-like system with a nucleus of charge Z , mass M , spin I , and magnetic moment μ . The basic scale of the hyperfine splitting is then given

by the Fermi formula,

$$E_F = \frac{8}{3} Z^3 \alpha^2 Ryd \frac{|\mu|}{\mu_B} \frac{2I+1}{2I} \left(\frac{M}{m+M} \right)^3. \quad (6)$$

Here we take the fine structure constant α derived from $g-2$ value of electron $\alpha^{-1} = 137.035\,999\,58(52)$. In addition we use a value the Rydberg constant of $Ryd = c Ry = 3.289\,841\,931 \cdot 10^{12}$ kHz.

We present the hyperfine structure as a sum

$$\Delta\nu_n = \Delta\nu_n(QED) + \Delta\nu_n(\text{nuclear structure}). \quad (7)$$

2.1 Non-recoil limit

First we consider the external-field approximation. For a point-like nucleus, they can be compactly parameterized by the equation

$$\Delta\nu_n(\text{N-R}) = \frac{E_F}{n^3} \left[B_n + \frac{\alpha}{\pi} D_n^{(2)}(Z\alpha) + \left(\frac{\alpha}{\pi} \right)^2 D_n^{(4)}(Z\alpha) + \dots \right].$$

Here, with $\gamma = \sqrt{1 - (Z\alpha)^2}$, [22] the Breit relativistic contribution is

$$B_1 = \frac{1}{\gamma(2\gamma-1)} \simeq 1 + \frac{3}{2} (Z\alpha)^2 + \frac{17}{8} (Z\alpha)^4 + \dots \quad (8)$$

and

$$B_2 = \frac{2(2(1+\gamma) + \sqrt{2(1+\gamma)})}{(1+\gamma)^2 \gamma (4\gamma^2 - 1)} \simeq 1 + \frac{17}{8} (Z\alpha)^2 + \frac{449}{128} (Z\alpha)^4 + \dots \quad (9)$$

and the functions $D_n^{2r}(Z\alpha)$ represent r loop radiative corrections. In the limit $Z\alpha = 0$ they reduce to the power series expansion of the electron $g-2$ factor, and the difference is referred to a binding correction. For the ground state,

$$\begin{aligned} D_1^{(2)} = & \frac{1}{2} + \pi(Z\alpha) \left(\ln(2) - \frac{5}{2} \right) + (Z\alpha)^2 \left[-\frac{8}{3} \ln^2(Z\alpha) \right. \\ & \left. + \left(\frac{16}{3} \ln(2) - \frac{281}{180} \right) \ln(Z\alpha) + G_1^{\text{SE}}(Z\alpha) + G_1^{\text{VP}}(Z\alpha) \right] \end{aligned} \quad (10)$$

and for the excited state

$$\begin{aligned} D_2^{(2)} = & \frac{1}{2} + \pi(Z\alpha) \left(\ln(2) - \frac{5}{2} \right) + (Z\alpha)^2 \left[-\frac{8}{3} \ln^2(Z\alpha) \right. \\ & \left. + \left(\frac{32}{3} \ln(2) - \frac{1541}{180} \right) \ln(Z\alpha) + G_2^{\text{SE}}(Z\alpha) + G_2^{\text{VP}}(Z\alpha) \right]. \end{aligned} \quad (11)$$

At present the functions G^{SE} have been determined numerically at $Z = 1$ and $Z = 2$ [16],

$$G_1^{SE}(Z = 1) = 16.079(15) \quad (12)$$

and

$$G_1^{SE}(Z = 2) = 15.29(9) \quad (13)$$

while G_1^{VP} is known analytically [17]:

$$G_1^{VP} = -\frac{8}{15} \ln(2) + \frac{34}{225} + \pi(Z\alpha) \left[-\frac{13}{24} \ln \frac{Z\alpha}{2} + \frac{539}{288} \right] + \dots \quad (14)$$

To present results for the $2s$ state, we can use the results of Ref. [14] for D_{21} , which however include terms only up to order $\alpha(Z\alpha)^2 E_F$. After we recalculated some integrals from paper [14] the result is

$$G_2^{SE} = G_1^{SE} + \left(-7 + \frac{16}{3} \ln(2) \right) \ln(Z\alpha) - 5.221233(3) + \mathcal{O}(\pi(Z\alpha)) \quad (15)$$

and

$$G_2^{VP} = G_1^{VP} - \frac{7}{10} + \frac{8}{15} \ln(2) + \mathcal{O}(\pi(Z\alpha)) . \quad (16)$$

Continuing to the two-loop corrections, all terms known to date are state-independent, so we give only the ground state result [18,19,20],

$$D_1^{(4)} = a_e^{(4)} + 0.7718(4) \pi(Z\alpha) - \frac{4}{3} (Z\alpha)^2 \ln^2(Z\alpha) .$$

Non-leading terms, including single powers of $\ln(Z\alpha)$ and constants, are both state-dependent, but unknown.

When the nucleus is not point-like, the leading correction is known as the Zemach correction,

$$\Delta\nu_n(\text{Zemach}) = \frac{8E_F}{\pi n^3} (Z\alpha m) \int \frac{dp}{p^2} \left(G_E(p) \tilde{G}_M(p) - 1 \right) . \quad (17)$$

Inaccuracy arisen from uncertainties in the form factors G_E and \tilde{G}_M , which are both normalized to unity at zero momentum, and from the lack of knowledge of polarization effects, is as large as about 10 ppm or 4 ppm respectively, but those leading terms are state-independent and do not contribute into the difference D_{12} .

For atoms with nuclear structure the following result was found [15]

$$\begin{aligned} \Delta D_{21}(\text{Rec}) = (Z\alpha)^2 \frac{m}{M} \left\{ -\frac{9}{8} + \left[-\frac{7}{32} + \frac{\ln(2)}{2} \right] \left(1 - \frac{1}{x} \right) \right. \\ \left. - \left[\frac{145}{128} - \frac{7}{8} \ln(2) \right] x \right\} , \end{aligned} \quad (18)$$

where $gM/Zm_p = x = (\mu/\mu_B)(M/m)(1/ZI)$. It does not depend on the nuclear structure effects such a distribution of the nuclear charge and magnetic moment. Contrary, the leading recoil term for the $\Delta\nu_n$ (which has order $(Z\alpha)(m/M) \ln(M/m)$ [21] is essentially nuclear-structure dependent.

3 Present status of D_{21} theory

3.1 Old theory and recent progress

The Breit, Zwanziger and Sternheim corrections [22,14,15] lead to a result

$$\begin{aligned}
 D_{21} = E_F (Z\alpha)^2 \times & \left\{ \left[\frac{5}{8} + \frac{177}{128} (Z\alpha)^2 \right] \right. \\
 & + \frac{\alpha}{\pi} \left[\left(-7 + \frac{16}{3} \ln(2) \right) \ln(Z\alpha) - 5.37(6) \right] \\
 & + \frac{\alpha}{\pi} \left[-\frac{7}{10} + \frac{8}{15} \ln(2) \right] \\
 & + \frac{m}{M} \left[-\frac{9}{8} + \left(-\frac{7}{32} + \frac{\ln(2)}{2} \right) \left(1 - \frac{1}{x} \right) \right. \\
 & \left. \left. - \left(\frac{145}{128} - \frac{7}{8} \ln(2) \right) x \right] \right\}. \quad (19)
 \end{aligned}$$

Some progress was achieved before we started our work. In particular, we need to mention two results:

- Integrals, used in Ref. [14], were evaluated later by P. Mohr¹ with higher accuracy and the constant was found to be -5.2212 instead of -5.37(6). The theoretical prediction based on Eq. (19) but with a corrected value of the constant is Table 1 as “old theory”.
- Some nuclear-structure- and state-dependent corrections were found [23] for arbitrary ns .

3.2 Our results

The similar difference has been under investigation also for the Lamb shift and a number of useful auxiliary expressions have been found for calculating the state dependent corrections to the Lamb shift [24].

Let us mention that an improvement in the accuracy and new result on higher n *hfs* can be expected with progress in optical measurements and we present here a progress also for higher n , defining $D_{n1} = n^3 \Delta\nu_n - \Delta\nu_1$.

- We have reproduced the logarithmic part of the self energy contribution and found for arbitrary ns

$$\begin{aligned}
 \Delta D_{n1} = & \frac{\alpha}{\pi} (Z\alpha)^2 E_F \ln(Z\alpha) \left(-\frac{8}{3} \right) \\
 & \times \left[2 \left(-\ln(n) + \frac{n-1}{n} + \psi(n) - \psi(1) \right) - \frac{n^2-1}{2n^2} \right]. \quad (20)
 \end{aligned}$$

¹ Unpublished. The result is quoted accordingly to Ref. [8].

The calculation is based on a result in Ref. [24] for the single logarithmic correction due to the one-loop self energy and one-loop vacuum polarization.

- We have reproduced the vacuum polarization contribution and found that for arbitrary ns

$$\Delta D_{n1} = \frac{\alpha}{\pi} (Z\alpha)^2 E_F \left(-\frac{4}{15} \right) \times \left[2 \left(-\ln(n) + \frac{n-1}{n} + \psi(n) - \psi(1) \right) - \frac{n^2-1}{2n^2} \right]. \quad (21)$$

- Integrals used by Zwanziger [14] have been recalculated and the constant was found to be -5.221233(3).
- We also found two higher-order logarithmic corrections

$$\Delta D_{n1} = \frac{\alpha^2}{\pi^2} (Z\alpha)^2 E_F \ln(Z\alpha) \left(-\frac{4}{3} \right) \times \left[2 \left(-\ln(n) + \frac{n-1}{n} + \psi(n) - \psi(1) \right) - \frac{n^2-1}{2n^2} \right] \quad (22)$$

and

$$\Delta D_{n1} = \frac{\alpha}{\pi} \frac{m}{M} (Z\alpha)^2 E_F \ln(Z\alpha) \left(\frac{16}{3} \right) \times \left[2 \left(-\ln(n) + \frac{n-1}{n} - \psi(n) + \psi(1) \right) - \frac{n^2-1}{2n^2} \right]. \quad (23)$$

- We found two higher-order non-logarithmic corrections

$$\Delta D_{n1}^{SE} = \alpha (Z\alpha)^3 E_F \left\{ \left[\frac{139}{16} - 4 \ln(2) \right] \times \left[-\ln(n) + \frac{n-1}{n} + \psi(n) - \psi(1) \right] + \left[\ln(2) - \frac{13}{4} \right] \times \left[\psi(n+1) - \psi(2) - \ln(n) - \frac{(n-1)(n+9)}{4n^2} \right] \right\} \quad (24)$$

and

$$\Delta D_{n1}^{VP} = \alpha (Z\alpha)^3 E_F \times \left\{ \left[\frac{5}{24} \right] \left[-\ln(n) + \frac{n-1}{n} + \psi(n) - \psi(1) \right] \right\}$$

$$+ \left[\frac{3}{4} \right] \times \left[\psi(n+1) - \psi(2) - \ln(n) - \frac{(n-1)(n+9)}{4n^2} \right] \Bigg\}. \quad (25)$$

- We have also found a term proportional to the magnetic radius. To the best of our knowledge that is the first contribution, which is proportional to the magnetic radius and on the level of the experimental accuracy. The complete nuclear-structure correction is

$$\begin{aligned} \Delta D_{n1}^{\text{Nucl}} = & -(Z\alpha)^2 \left[\psi(n+1) - \psi(2) - \ln(n) - \frac{(n-1)(n+9)}{4n^2} \right] \\ & \times \Delta\nu_1(\text{Zemach} + \text{polarizability}) + \frac{4}{3}(Z\alpha)^2 \left[\psi(n) - \psi(1) - \ln(n) \right. \\ & \left. + \frac{n-1}{n} - \left(\frac{R_M}{R_E} \right)^2 \frac{n^2-1}{4n^2} \right] (mR_E)^2 E_F. \end{aligned} \quad (26)$$

4 Present status

To calculate the corrections presented in the previous sections, we have used an effective non-relativistic theory. In particular we have studied two kinds of terms. One is a result of the second order perturbation theory with two $\delta(\mathbf{r})$ -like potentials, evaluated in the leading non-relativistic approximation, while the other is due to a more accurate calculation of a single delta-like potential. Both kinds contribute into the state-independent leading logarithmic corrections ($\alpha^2(Z\alpha)^2 \ln^2(Z\alpha)$, $\alpha(Z\alpha)^2(m/M) \ln^2(Z\alpha)$, and $\alpha(Z\alpha)^3 \ln(Z\alpha)$) and to next-to-leading state-dependent terms ($\alpha^2(Z\alpha)^2 \ln(Z\alpha)$, $\alpha(Z\alpha)^2(m/M) \ln(Z\alpha)$, and $\alpha(Z\alpha)^3$). The crucial question is if we found all corrections in these orders. Rederiving a leading term in order $\alpha(Z\alpha)^2 \ln(Z\alpha)$ within our technics, we can easily incorporate the anomalous magnetic moment of the electron in the calculation and restore the nuclear mass dependence. Since we reproduce the well-known result for the $\alpha(Z\alpha)^2 \ln(Z\alpha)$ term, we consider that as a confirmation of two other logarithmic corrections found by us. In the case of $\alpha(Z\alpha)^3$ it might be a contribution of an effective operator, proportional to $(\Delta/m)\delta(\mathbf{r})$. That can give no logarithmic corrections, but leads to a state-dependent constant. We are now studying this possibility.

Summarizing all corrections, the final QED result is found to be:

$$\begin{aligned} D_{21}^{\text{QED}} = & E_F (Z\alpha)^2 \times \left\{ \left[\frac{5}{8} + \frac{177}{128} (Z\alpha)^2 \right] \right. \\ & \left. + \frac{\alpha}{\pi} \left[\left(-7 + \frac{16}{3} \ln(2) \right) \ln(Z\alpha) - 5.221233(3) \right] \right\} \end{aligned}$$

$$\begin{aligned}
& + \frac{\alpha}{\pi} \left[-\frac{7}{10} + \frac{8}{15} \ln(2) \right] \\
& + \frac{m}{M} \left[-\frac{9}{8} + \left[-\frac{7}{32} + \frac{\ln(2)}{2} \right] \left(1 - \frac{1}{x} \right) - \left[\frac{145}{128} - \frac{7}{8} \ln(2) \right] x \right] \Bigg\} \\
& + \frac{\alpha^2}{2\pi^2} \left(-7 + \frac{16}{3} \ln(2) \right) \ln(Z\alpha) \\
& - \frac{\alpha}{\pi} \frac{2m}{M} \left(-7 + \frac{16}{3} \ln(2) \right) \ln(Z\alpha) \\
& + \alpha(Z\alpha) \left\{ \left[\frac{139}{16} - 4 \ln(2) + \frac{5}{24} \right] \left[\frac{3}{2} - \ln(2) \right] \right. \\
& \left. + \left[\frac{13}{4} - \ln(2) - \frac{3}{4} \right] \left[\ln(2) + \frac{3}{16} \right] \right\}. \tag{27}
\end{aligned}$$

Numerical results (in kHz) for hydrogen and deuterium atoms and the helium-3 ion are collected in Table 2. One can see that the new corrections essentially shift the theoretical predictions. A comparison of the QED predictions (in kHz) against the experiments is summarized in Table 1. We take the values of the fundamental constants (like e. g. the fine structure constant α) from the recent adjustment (see Ref. [25]).

Table 2. QED contributions to the D_{21} in hydrogen, deuterium and helium-3 ion. The results are presented in kHz

Contribution	H	D	${}^3\text{He}^+$
$(Z\alpha)^2 E_F$	47.2275	10.8835	1 152.9723
$+ \alpha(Z\alpha)^2 E_F$ (SE)	1.9360	0.4461	37.4412
$+ \alpha(Z\alpha)^2 E_F$ (VP)	-0.0580	-0.0134	-1.4148
$+ (Z\alpha)^2 \frac{m}{M} E_F$	-0.1629	-0.0094	0.7966
$+ \alpha^2 (Z\alpha)^2 E_F$	0.0033(16)	0.0008(4)	0.070(35)
$+ \alpha(Z\alpha)^2 \frac{m}{M} E_F$	-0.0031(15)	-0.0004(2)	-0.022(11)
$+ \alpha(Z\alpha)^3 E_F$ (SE)	0.0282	0.0065	1.3794
$+ \alpha(Z\alpha)^3 E_F$ (VP)	-0.0019	-0.0005	-0.0967

An important point is that the difference is sensitive to 4th order corrections and so is competitive with the muonium hfs as a test of the QED. The difference between the QED part of the theory and the experiment is an indication of higher-order corrections due to the QED and the nuclear structure, which have to be studied in detail. In particular, we have to mention that while we expect that we have a complete result on logarithmic corrections and on the vacuum-

polarization part of the $\alpha(Z\alpha)^3$ term we anticipate more contributions in the order $\alpha(Z\alpha)^3$ due to the self-energy. A complete study of this term offers a possibility to determine the magnetic radius of the proton, deuteron and helion-3.

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