Study of hyperfine structure in simple atoms and precision tests of the bound state QED

S. G. Karshenboim\textsuperscript{ab}, S. I. Eidelman\textsuperscript{c}, P. Fendel\textsuperscript{a}, V. G. Ivanov\textsuperscript{d}, N. N. Kolachevsky\textsuperscript{e}, V. A. Shelyuto\textsuperscript{b}, and T. W. H"{a}nsch\textsuperscript{a}

\textsuperscript{a}Max-Planck-Institut f"{u}r Quantenoptik, 85748 Garching, Germany
\textsuperscript{b}D. I. Mendeleev Institute for Metrology (VNIIM), St. Petersburg 190005, Russia
\textsuperscript{c}Budker Institute for Nuclear Physics and Novosibirsk State University, Novosibirsk, 630090, Russia
\textsuperscript{d}Pulkovo Observatory, St. Petersburg 196140, Russia
\textsuperscript{e}P. N. Lebedev Physics Institute, Moscow, 119991, Russia

We consider the most accurate tests of bound state QED, precision theory of simple atoms, related to the hyperfine splitting in light hydrogen-like atoms. We discuss the HFS interval of the 1\textit{s} state in muonium and positronium and of the 2\textit{s} state in hydrogen, deuterium and helium-3 ion. We summarize their QED theory and pay attention to involved effects of strong interactions. We also consider recent optical measurements of the 2\textit{s} HFS interval in hydrogen and deuterium.

1. Introduction

Light simple atoms are basically described by quantum electromagnetic theory. Quantum electrodynamics (QED) is well established and in particular it covers all interactions of leptons (electrons and muons) and photons. Such a lepton-photon theory is obviously incomplete because even pure leptonic systems are not free of hadronic effects which enter through virtual hadronic intermediate states. Effects of strong interactions cannot be calculated \textit{ab initio} and additional experimental data and/or phenomenological models are needed. Here we consider QED tests with hyperfine splitting in light hydrogen-like atoms paying attention to both: basic \textit{ab initio} QED theory and relatively small, but most uncertain, hadronic contributions.

An application of QED to the bound state problem, bound state QED, is much more complicated than ordinary QED and it deserves serious tests. Some of such tests are significant for the determination of fundamental constants and in particular of the fine structure constant $\alpha$, which may be obtained from the hyperfine structure (HFS) interval in muonium (see reviews \cite{1,2,3} for more detail).

The HFS interval in hydrogen and some other light atoms has been known for a while with an experimental accuracy at the level of a part in $10^{12}$. Meanwhile, the related theory suffers from uncertainties of the nuclear structure effects at one-nanopm level.

Here, we consider a few possibilities to perform QED tests going far beyond this level of accuracy.

2. Studying the 1\textit{s} hyperfine splitting

2.1. The 1\textit{s} hyperfine interval in muonium

Problems in accurate calculations of the proton or nuclear structure effects drew attention to studies of pure leptonic atoms such as a bound system of a positive muon and an electron, the muonium. In contrast to the hydrogen atom, the nucleus, a muon, is free of effects of strong interactions. Nevertheless, those effects enter through hadronic vacuum polarization. That sets an ultimate limit on any QED tests with muonium.
Uncertainties of the QED theory and of calculations of the hadronic effects are presented in [11]. Muonium is of metrological interest due to determination of the fine structure $\alpha$, muon-to-electron mass ratio $m_\mu/m_e$ and some other fundamental constants [3].

A calculation of the hadronic effects [4] is similar to those for the anomalous magnetic moment of the muon [5]. It is based on the low energy $e^+e^-$ data which accuracy, although fast improving, is still behind the measurement of the muon $g-2$ value [6]. The current difference between the experimental value and its theoretical prediction differs from zero by almost three standard deviations [7]. Attempts to increase the accuracy of the prediction by adding data on the decays revealed one more possible deviation from theory and the theory of the 1$s$ hyperfine splitting, is still behind the measurement of the muon $2s$ transition, is in a sense similar to the HFS theory and some other fundamental numbers, respectively, and $m_R$ is the reduced mass.

Enhancement of the recoil effects has one more consequence. In conventional atoms (such as hydrogen), theory of the spin-independent energy shifts (the Lamb shift) is completely different from that for the HFS effects. In the Lamb shift theory and the theory of the 1$s$ − 2$s$ transition, higher-order two-loop external-field effects dominate in the uncertainty budget, while the recoil and the hyperfine effects are responsible for relatively small corrections. In the theory of the HFS interval, the recoil effects are most important for the uncertainty, while the external field effects are under control.

For positronium, the theory of the 1$s$ − 2$s$ transition is in a sense similar to the HFS theory and dominant uncertainty comes from the HFS effects (see, e.g., [11]). However, the related accuracy is somewhat lower than that of the 1$s$ HFS interval.

### 3. The 2s hyperfine interval: Theory of the specific difference $D_{21}$

Another accurate QED test is possible with ordinary light hydrogen-like atoms. One can combine the HFS intervals of the 1$s$ and 2$s$ states in the same atom

$$D_{21} = 2^3 \cdot E_{\text{HFS}}(2s) - E_{\text{HFS}}(1s)$$  \hspace{1cm} (1)

to eliminate the leading nuclear contributions.

A substantial cancellation of the nuclear structure contributions takes place because the nuclear contributions in the leading approximation are of the factorized form

$$\Delta E(\text{Nucl}) = A(\text{Nucl}) \times |\Psi_{nl}(r = 0)|^2 ,$$  \hspace{1cm} (2)

i.e., the correction is a product of the nuclear-structure parameter $A(\text{Nucl})$ and the wave function at the origin

$$|\Psi_{nl}(r = 0)|^2 = \frac{1}{\pi} \left( \frac{Z \alpha m_R}{\hbar} \right)^3 \delta_{l0} ,$$  \hspace{1cm} (3)

where $n, l$ are the principal and orbital quantum numbers, respectively, and $m_R$ is the reduced mass.

Higher-order corrections due to nuclear effects are of a more complicated form and some of them survive this cancellation. Still, they are much smaller and under control [3]. The theory of $D_{21}$ in light hydrogen-like atoms is presented in Table [11] [52], [3].

The 1$s$ and 2$s$ hyperfine intervals have been measured much more accurately compared to the theoretical prediction which can be made for each of them separately. Meanwhile, for the difference $D_{21}$ the experimental and theoretical accuracy are competitive. While for $^3\text{He}^+$ the experiment [10] is still somewhat more accurate than theory [9], in the case of hydrogen and deuterium, the theory is more accurate than the measurement of the HFS interval in the 2$s$ state.

### 4. The 2s hyperfine interval: optically measured in hydrogen and deuterium

Measurements of the 2$s$ HFS interval in hydrogen [11] and deuterium [12] by microwave means...
Table 1
Theory of the specific difference \( D_{21} = 8E_{\text{HFS}}(2s) - E_{\text{HFS}}(1s) \) in light hydrogen-like atoms. The numerical results are presented for the related frequency \( D_{21}/h \). QED3 and QED4 stands for the third and fourth order QED corrections in units of the so-called Fermi energy.

| Contribution to HFS in | Hydrogen, [kHz] | Deuterium, [kHz] | \(^3\text{He}^+\) ion, [kHz] |
|------------------------|----------------|-----------------|-----------------------------|
| \( D_{21}(\text{QED3}) \) | 48.937 | 11.3056 | -1.189.253 |
| \( D_{21}(\text{QED4}) \) | 0.018(5) | 0.0044(10) | -1.13(14) |
| \( D_{21}(\text{Nucl}) \) | -0.002 | 0.0026(2) | 0.307(35) |
| \( D_{21}(\text{theo}) \) | 48.953(5) | 11.3125(10) | -1.190.08(15) |

have nearly a fifty year history. The hydrogen result was somewhat improved in 2000 \[13\] by traditional microwave means.

Recently a new generation of optical experiments was launched using a hydrogen spectrometer developed at Max-Planck-Institut für Quantenoptik for the ultraviolet \( 1s - 2s \) transition \[14\]. The spectrometer was developed in order to build a natural frequency standard.

Figure 1. The \( 1s \) and \( 2s \) levels in the hydrogen atom. Not to scale.

The fractional uncertainty of the former measurements \[13\] was at the level of a few parts in \( 10^{14} \) or 30–40 Hz and was due to various systematic effects. Expecting that dominant systematic effects are spin-independent, one can hope that a comparison of spin components of the \( 1s - 2s \) line can be performed with a higher absolute accuracy. The \( 1s - 2s \) transition lies in the ultraviolet domain (see Fig. 1) and for the triplet case the result is \( 246660110274851(34) \) Hz \[13\].

We have compared the \( 1s - 2s \) ultraviolet frequencies for different HFS components in hydrogen \[13\] and deuterium \[16\] and with the value of the \( 1s \) HFS intervals known for both atoms with a high accuracy we obtained new results for the \( 2s \) HFS interval.

Our optically measured results

\[
\begin{align*}
 f_{\text{H}}^{\text{HFS}}(2s) &= 177556860(16) \text{ Hz} , \quad [15], \\
 f_{\text{D}}^{\text{HFS}}(2s) &= 40924454(7) \text{ Hz} , \quad [16],
\end{align*}
\]

agree with early microwave data and are somewhat more precise.

5. The HFS tests of bound state QED: the summary

We summarize state-of-the-art in the precision tests of the bound state QED theory of the hyperfine structure in Table 2. The theoretical accuracy is limited by our ability to calculate higher-order radiative, recoil and radiative recoil effects (see review \[11\] for more detail). The higher-order contributions crucial for the uncertainty are related to the same diagrams and thus all tests listed in the table are really competitive. Theory and experiment are generally in good agreement. There is a minor discrepancy for positronium up
Table 2
Comparison of experiment and theory of hyperfine structure in light hydrogen-like atoms. The experimental references can be found in [1]. Here $\Delta$ is a deviation of theory from experiment and $\sigma$ is a combined uncertainty.

| Atom, quantity | Experiment, [kHz] | Theory, [kHz] | $\Delta/\sigma$ |
|----------------|-------------------|---------------|-----------------|
| $^6$Li, 1s HFS | 4 463 302.78(5)   | 4 463 302.88(55) | -0.18           |
| $^3$Ps, 1s HFS | 203 389 100(740)  | 203 391 700(500)  | -2.9            |
| $^3$Ps, 1s HFS | 203 397 500(1600) |               | -2.5            |
| H, $D_{21}$    | 49.13(13)         | 48.953(3)     | 1.4             |
| H, $D_{21}$    | 48.53(23)         |               | -1.8            |
| H, $D_{21}$    | 49.13(40)         |               | 0.4             |
| D, $D_{21}$    | 11.28(56)         | 11.312 5(5)   | -0.58           |
| D, $D_{21}$    | 11.16(16)         |               | -1.0            |
| $^3$He$^+$, $D_{21}$ | -1 189.979(71)  | -1 190.08(15) | 0.6             |
| $^3$He$^+$, $D_{21}$ | -1 190.1(16)    |               | 0.0             |

to approximately 3 standard deviations, but statistically that is acceptable if the tests as a whole are considered.

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