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Hydrogen and deuterium energy levels theory

Hydrogen/deuterium energy levels based on bound-state Quantum Electrodynamics:

...related to the electron mass and the fine-structure constant

 m_e electron-to-nucleus mass ratio m_N

Hydrogen and deuterium energy levels theory

Hydrogen/deuterium energy levels based on bound-state Quantum Electrodynamics:

$$E_{nlj} = hc R_{\infty} \left(-\frac{1}{n^2} + f_{nlj}(\alpha, \frac{m_e}{m_N}) + \frac{\delta_{l0}}{n^3} \left(C_{\rm NS} r_N^2 + C_{\rm pol} + \text{h.o.n.e.} \right) \right)$$
QED effects with point-like nucleus
$$\frac{1 + \log \text{ pop ED: vac-pol.}}{\alpha \alpha^2 \times \alpha^3 \ln(\alpha^2)} \xrightarrow{1 + \log \text{ pop ED: vac-pol.}} \alpha \alpha^2 \times \alpha^3 \alpha^3 \left(\frac{1 + \log \text{ pop ED: vac-pol.}}{\alpha \alpha^2 \times \alpha^3 \ln(\alpha^2)} \right)$$

$$\frac{1 + \log \text{ pop ED: vac-pol.}}{\alpha \alpha^2 \times \alpha^4} = 0$$

$$\frac{1 + \text{ other terms}}{\alpha \alpha^2 \times \alpha^4} + 0$$

$$\frac{1 + \text{ higher order nuclear effects (h.o.n.e.)}}{\alpha \alpha^2 \times \alpha^2 + \alpha^2 \ln(\alpha^2)}$$

H 2S-6P vs D 2S-6P: contributions to transition frequency



		Hydrogen $2S_{1/2}$ - $6P_{1/2}$ (Hz)	Deuterium $2S_{1/2}$ - $6P_{1/2}$ (Hz)
e'	Dirac (with $m_e \to m_{red}$) Rel. nuclear recoil Radiative recoil	$730691021696054\\1129173\\1540$	730 889 842 123 184 566 917 771
$e' \longrightarrow e'e' \\ f'e' e' $	1-loop QED self-energy vacuum-polarization $\mu^+\mu^-$ vacuum-pol. hadronic vacuum-pol. 2-loop QED 3-loop QED	$\begin{array}{r} -1071679859\\ 26853088\\ 634\\ 425\\ -90477\\ -236\end{array}$	$\begin{array}{r} -1072517882\\ 26875014\\ 634\\ 425\\ -90551\\ -236\end{array}$
	Finite nuclear size $\propto \alpha^4$ $\propto \alpha^5$ $\propto \alpha^6$	-138394 5 -74	-885943 19 -433
excitation	Nuclear polarizability $\propto \alpha^5$ $\propto \alpha^6$	8 49	2722 68
	Total	730 689 977 771 255	730 888 796 074 559
-	Theory uncertainty Uncert. from constants Total uncertainty	130 089 977 771 255 199 1532 1545	181 1529 1539

Hydrogen 2S-6P: higher-order nuclear size effects and polarizability < 0.1 kHz Deuterium 2S-6P: higher-order nuclear size 0.4 kHz, polarizability 2.7 kHz

N =

 $N \Longrightarrow$



Considering hydrogen and deuterium separately: 1S-2S transition measurement in hydrogen or deuterium combined with other transition measurement:



but so far no recent data from deuterium spectroscopy







Hydrogen: I = 1/2







Deuterium: I = 1





Additionally allowed transitions

Deuterium: I = 1

compared to hydrogen require to consider:

1) simultaneous excitation of different hyperfine levels





Additionally allowed transitions

Deuterium: *I* = 1

compared to hydrogen require to consider:

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Residual circular polarization S changes the dipole ratio of excited hyperfine state manifolds

Introduced polarization monitor in our improved active fiber-based retroreflector [1]

Shift from non-zero circular polarization cancels for equal population of initial states

[1] V. Wirthl et al., Opt. Express 29(5), 7024 (2021)



Additionally allowed transitions

Deuterium: I = 1

compared to hydrogen require to consider:

1) simultaneous excitation of different hyperfine levels

2) quantum interference between unresolved hyperfine transitions [1]



[1] Th. Udem et al., Ann. Phys. 531(5), 1900044 (2019)





- for π decays q. i. effect cancels [2] for each initial state

- for σ^{\pm} decays q. i. effect cancels [2] for equal population of initial states or equal detection of σ^+ and σ^- decays e

possible sensitivity ξ_\circ of e⁻ yield upon **circular polarization**

[1] Th. Udem et al., Ann. Phys. 531(5), 1900044 (2019) [2] V. Wirthl, PhD Thesis, LMU Munich (2023)

V. Wirthl, MPQ

 $\sigma^- \mathbf{e^-}$

Al detector





Both effects from additional transitions in deuterium doubly suppressed

[1] Th. Udem et al., Ann. Phys. 531(5), 1900044 (2019)

V. Wirthl, MPQ

Initial state population asymmetry: estimation from Boltzmann



Both effects from additional transitions in deuterium depends on the **initial state population asymmetry**:

$$v = \frac{N_{i2} - N_{i1}}{N_{i2} + N_{i1}}$$

Spin-polarizing effects in the nozzle?





Deuterium: l = 1

Symmetric nozzle: **symmetry breaking induced by magnetic field**, which leads to the energy difference $\Delta E_{\iota} = \frac{2}{3}\mu_{\rm B}B$ between the two initial states. Estimate assuming thermalization (Boltzmann distribution):

$$\frac{N_{i1}}{N_{i2}} = \exp\left(-\frac{\Delta E_{\iota}}{k_{\rm B}T_{\rm N}}\right) \quad \Rightarrow \quad \iota \simeq \frac{\mu_{\rm B}B}{3k_{\rm B}T_{\rm N}} \sim 3 \times 10^{-7}$$

Initial state population asymmetry: Stern-Gerlach effect





Initial state population asymmetry: Stern-Gerlach effect





Initial state population asymmetry: Stern-Gerlach effect





Initial state asymmetry originates only from asymmetries in the apparatus

Estimate of initial state asymmetry from Stern-Gerlach effect in the atomic beam:

$$\iota \simeq 10^{-6} \dots 5 \times 10^{-5}$$

Depends on velocity of atoms: velocity-resolved detection sensitive to this effect Estimates of line shifts due to initial state population asymmetry



Estimates of initial state asymmetry:



Calculation of systematic shifts coupled to population asymmetry yields [1]:

Shift due to simultaneous excitation with
residual circular polarization fraction S: $2S-6P_{1/2}$:
 $\Delta \nu_{\iota s} \simeq \iota s \times 75 \, \mathrm{kHz}$ $2S-6P_{3/2}$:
 $\iota s \times 37 \, \mathrm{kHz}$ Shift due to unresolved Q.I. with circular
polarization sensitivity of the detector ξ_{\circ} : $\Delta \nu_{\iota \xi_{\circ}} \simeq \iota \xi_{\circ} \times 100 \, \mathrm{kHz}$ $\iota \xi_{\circ} \times 5 \, \mathrm{kHz}$

With the estimated initial state population asymmetry of $< 10^{-4}$, both effects lead to shifts < 1 Hz even for the worst case of other imperfections

+ sensitive to velocity-resolved detection + different for $2S-6P_{1/2}$ and $2S-6P_{3/2}$ [1] V. Wirthl, *PhD Thesis, LMU Munich* (2023)

Possible measurement of initial state population asymmetry







Observed deuterium 2S-6P transition signal with a high count rate, low background:



Test measurement: ~ 300 deuterium 2S-6P precision line scans



Preliminary deuterium 2S-6P measurement campaign result:



 \rightarrow feasible with a similar precision as in hydrogen

Setup upgrade for O₂ flushing of UV mirrors: differential pumping

Main problem for continuos operation of the experiment: **UV mirror degradation** for the 243nm enhancement cavity

→ Solution: in the future planned to rebuild setup for differential pumping to flush mirrors with ~1mbar of oxygen



Setup upgrade for O₂ flushing of UV mirrors: differential pumping





Upgrade to differential pumping required to disassemble the whole apparatus







Thank you for your attention!

Hydrogen team







Weis

Vincent

Omer

Amit



Vitaly Wirthl



Lothar Maisenbacher (UC Berkeley)

Looking for new PhD students!



Randolf Pohl



Thomas Udem



Theodor W. Hänsch