

Deuteron charge radius and Rydberg constant from spectroscopy data in atomic deuterium

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We give a pedagogical description of the method to extract the charge radii and Rydberg constant from laser spectroscopy in regular hydrogen (H) and deuterium (D) atoms, that is part of the CODATA least-squares adjustment (LSA) of the fundamental physical constants. We give a deuteron charge radius r_d from D spectroscopy alone of 2.1415(45) fm. This value is independent of the measurements that lead to the proton charge radius, and five times more accurate than the value found in the CODATA Adjustment 10. The improvement is due to the use of a value for the $1S \rightarrow 2S$ transition in atomic deuterium which can be inferred from published data or found in a PhD thesis.

I. INTRODUCTION

For quite a while now, a 7σ discrepancy has existed between the proton rms charge radius (r_p) determined using electrons and muons. On the one hand, the value from laser spectroscopy of the exotic muonic hydrogen atom (μp),

$$r_p(\mu p) = 0.8409(4) \text{ fm} \quad (1)$$

has been reported by the CREMA collaboration [1, 2]. On the other hand, the most recent CODATA-2010 ‘‘world average’’ value

$$r_p(\text{CODATA-2010}) = 0.8775(51) \text{ fm} \quad (2)$$

has been determined by a self-consistent least-squares adjustment (LSA) of the fundamental physical constants [3]. The discrepancy of $\sim 7\sigma$ between these two values has been coined the ‘‘Proton Radius Puzzle’’ [4, 5].

The CREMA collaboration has just published a value of the deuteron charge radius r_d from laser spectroscopy of muonic deuterium (μd) [6]

$$r_d(\mu d) = 2.1256(8) \text{ fm}, \quad (3)$$

again more than 7σ smaller than the CODATA-2010 value of r_d

$$r_d(\text{CODATA-2010}) = 2.1424(21) \text{ fm}. \quad (4)$$

However, comparison of the new $r_d(\mu d)$ value with the CODATA-2010 value may be considered inadequate or redundant, because the CODATA values of r_d and r_p are highly correlated, with a correlation coefficient $c(r_p, r_d) = 0.9989$ (see

Ref. [3], Eq. (92)). This large correlation is the result of the very precisely measured isotope shift of the $1S \rightarrow 2S$ transition in atomic hydrogen (H) and deuterium (D) [7, 8], which yields a very accurate value for the *difference* of the (squared) deuteron and proton charge radii [9]

$$r_d^2 - r_p^2 = 3.82007(65) \text{ fm}^2. \quad (5)$$

One could thus argue that the CODATA deuteron charge radius is larger than the muonic deuterium value only because the correlated, and very accurately determined, proton charge radius is larger than the muonic hydrogen value.

Here we use the available data on spectroscopy of atomic deuterium to deduce a precise value of r_d which does *not* depend on r_p through Eq. (5). In our analysis we use a value of the $1S \rightarrow 2S$ transition in atomic deuterium (see Tab. VI) that has not been used by CODATA. Its value can either be inferred from published data or found in a PhD thesis [10]. This $1S \rightarrow 2S$ value helps improve the accuracy of the deuteron charge radius by a factor of five, compared to the CODATA Partial Adjustment 10 [3].

A. CODATA Partial Adjustments

The final CODATA-2010 recommended values of the fundamental constants are deduced in the so-called ‘‘Adjustment 3’’. As detailed in Sec. XIII.B.2 on page 1577 ff. of the CODATA-2010 report [3], there are additional adjustments that use only a subset of the available input data. ‘‘Adjustments 6-12’’ are the ones relevant for r_p , r_d and the Rydberg constant R_∞ , and the results are summarized in Tab. XXXVIII of Ref. [3].

These auxiliary Partial Adjustments serve two purposes: On the one hand, they verify the internal consistency of the CODATA LSA, as results from different subsets of the data are in good agreement with each other. On the other hand,

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these adjustments provide uncorrelated values of r_p and r_d . These can then be compared with their muonic counterparts to obtain a clearer picture of the issues surrounding the “proton radius puzzle”.

For the proton, the value of r_p that is deduced from data obtained by precision spectroscopy in atomic hydrogen alone (omitting both elastic electron-proton (e-p) scattering results and measurements in deuterium) is determined in Adjustment 8, see Tab. XXXVIII of Ref. [3]:

$$r_p(\text{H spectr.}, \text{CODATA}) = 0.8764(89) \text{ fm.} \quad (6)$$

This value is in excellent agreement with Eq. (2), and only slightly less accurate, see Fig. 1. The “atomic physics” part of the proton radius puzzle is the 4.0σ discrepancy between Eq. (1) and Eq. (6). It is unaffected by the problems that may exist in the analysis of e-p scattering data [11–15].

The situation is somewhat less favorable for the deuteron charge radius r_d . The CODATA-2010 value from the full Adjustment 3 given in Eq. (4) is very precise: $r_d(\text{CODATA}) = 2.1424(21) \text{ fm}$. The value from laser spectroscopy of atomic deuterium from Adjustment 10, on the other hand, is less so [69]:

$$r_d(\text{D spectr.}, \text{CODATA}) = 2.1214(253) \text{ fm.} \quad (7)$$

This value is not accurate enough for a useful comparison with the new result from muonic deuterium, see Fig. 2.

B. The “missing” $1S \rightarrow 2S$ measurement in D

The reason for this significantly worse accuracy of r_d in Eq. (7) is the apparent lack of a precise measurement of the $1S \rightarrow 2S$ transition in atomic deuterium. Only the isotope shift, *i.e.* the *difference* of the $1S \rightarrow 2S$ transitions in H and D, is used in the CODATA LSA, see Ref. [3], Tab. XI.

This is perfectly valid for the “full” CODATA Adjustment 3 using all available input data. However, for Adjustment 10 of spectroscopy data in D, the lack of a precise value for the $1S \rightarrow 2S$ transition in D results in a much larger uncertainty.

In this note we argue that the $1S \rightarrow 2S$ transition frequency in atomic deuterium has been measured very accurately by some of the authors at MPQ. The published isotope shifts [7, 8] are in fact the calculated differences of the measured $1S \rightarrow 2S$ transitions in atomic deuterium and hydrogen.

We can thus proceed to deduce a precise value of the deuteron radius from deuterium spectroscopy alone, combining the $1S \rightarrow 2S$ transition in D, measured by some of the authors at MPQ, with the $1S \rightarrow 8S$, $8D$, and $12D$ transitions in D, measured by some of the authors at LKB. The new value is five times more precise as the one in Eq. (7), and can be usefully compared to the muonic deuterium value of r_d [6].

Next we proceed with a pedagogical introduction to the theory of the energy levels in atomic H and D. We determine the *proton* charge radius from atomic hydrogen data alone. Our value is in excellent agreement with the one from CODATA Adjustment 8. Afterwards we apply the same formalism to the deuterium data.

II. ENERGY LEVELS IN HYDROGEN AND DEUTERIUM

The energy levels in H and D, E/h in frequency units [kHz] due to the Planck constant h , can be parameterized [16] as a function of principal quantum number n , orbital quantum number ℓ , and total angular momentum j , as

$$E(n, \ell, j)/h = -\frac{cR_\infty}{n^2} \frac{m_{\text{red}}}{m_e} + \frac{E_{NS}}{n^3} \delta_{\ell 0} + \Delta(n, \ell, j). \quad (8)$$

The first term on the right hand side is the famous Bohr result for the energy levels of an electron orbiting an infinitely heavy nucleus $-R_\infty/n^2$, corrected for the leading order nuclear motion by the reduced mass ratio m_{red}/m_e . Here, R_∞ denotes the Rydberg constant, c is the speed of light in vacuum, and the reduced mass of the atom with an electron of mass m_e and a nucleus of mass m_N is given by

$$m_{\text{red}} = \frac{m_e m_N}{m_e + m_N} = \frac{m_e}{1 + \frac{m_e}{m_N}}. \quad (9)$$

The mass ratios m_e/m_N are tabulated in Ref. [3].

The second term in Eq. (8) is the finite nuclear size correction, whose leading order is given in kHz by [3, 16]

$$E_{NS}^{(0)} = \frac{2}{3h} \left(\frac{m_{\text{red}}}{m_e} \right)^3 (Z\alpha)^4 m_e c^2 \left(\frac{r_N}{\lambda_C} \right)^2. \quad (10)$$

Here, $\alpha \approx 1/137.036$ is the fine structure constant, $Z = 1$ is the nuclear charge for H and D, $\lambda_C \approx 386.16 \text{ fm}$ is the reduced Compton wavelength of the electron, and r_N is the rms charge radius of the nucleus, *i.e.* r_p for H and r_d for D.

The charge radius contribution E_{NS} is significant only for S-states ($\ell = 0$), as indicated by the Kronecker symbol $\delta_{\ell 0}$ in Eq. (8).

The $1/n^3$ dependence of E_{NS} in Eq. (8) originates from the overlap of the electron’s wave function with the extended nuclear charge distribution. For our purposes it is convenient to sum $E_{NS}^{(0)}$ and all other finite nuclear size effects that are proportional to $1/n^3$. These higher-order nuclear size corrections are 2×10^{-4} of E_{NS} and thus very small, see Ref. [3] Eqs. (75), (77) and (78). We obtain

$$E_{NS}(\text{H}) = 1564.60 \times r_p^2 \text{ kHz/fm}^2, \quad (11)$$

$$E_{NS}(\text{D}) = 1565.72 \times r_d^2 \text{ kHz/fm}^2, \quad (12)$$

both with negligible uncertainty on the level of a few Hz/fm². For reference, E_{NS} amounts to approx. 1100 kHz and 7100 kHz for the $1S$ ground state in H and D, respectively.

The third ingredient of Eq. (8), $\Delta(n, \ell, j)$, summarizes all the remaining corrections. The largest part of $\Delta(n, \ell, j)$ is due to the use of the Dirac equation instead of the simple Bohr formula. Other contributions are the fine- and hyperfine-splittings, the relativistic, QED, radiative, recoil and Darwin-Foldy corrections, finite size corrections for P -states, nuclear polarizability, and many higher-order contributions. These are listed in Sec. IV.A.1 of Ref. [3].

The $\Delta(n, \ell, j)$ can be calculated very accurately using the detailed formulas found e.g. in Refs. [3, 17, 18]. We list in

TABLE I: Values of $\Delta(n, \ell, j)$ in kHz for relevant energy levels in atomic hydrogen. $\Delta(n, \ell, j)$ includes all relevant corrections to the energy levels from fine structure splittings and QED effects. The uncertainties are taken from Ref. [3], Tab.XVIII. They arise mostly from the estimated uncertainty of uncalculated two-loop corrections [16]. An uncertainty of “(0)” denotes “negligibly small”.

n	$S_{1/2}$	$P_{1/2}$	$P_{3/2}$	$D_{3/2}$	$D_{5/2}$
1	-35 626 637.5(2.5)				
2	-12 636 167.73(31)	-13 693 861.67(3)	-2 724 820.10(3)		
3	-4 552 757.02(9)			-1 622 832.29(0)	-539 495.09(0)
4	-2 091 350.05(4)	-2 224 408.70(0)	-853 278.87(0)	-855 566.25(0)	-398 533.10(0)
8	-293 431.56(1)			-138 996.24(0)	-81 867.09(0)
12				-44 349.61(0)	-27 422.46(0)

TABLE II: Values of $\Delta(n, \ell, j)$ in kHz for relevant energy levels in atomic deuterium. The caption of Tab. I applies.

n	$S_{1/2}$	$P_{1/2}$	$P_{3/2}$	$D_{3/2}$	$D_{5/2}$
1	-35 621 512.1(2.3)				
2	-12 638 504.55(29)	-13 696 839.80(3)	-2 724 804.25(3)		
3	-4 553 743.34(9)			-1 623 126.89(0)	-539 493.99(0)
4	-2 091 828.14(4)	-2 224 966.95(0)	-853 462.87(0)	-855 752.49(0)	-398 594.64(0)
8	-293 502.94(1)			-139 031.16(0)	-81 886.41(0)
12				-44 361.10(0)	-27 429.34(0)

Tab. I and Tab. II the values of $\Delta(n, \ell, j)$ for relevant states in H and D, respectively. For reference, the sum of all so-called QED corrections, included in $\Delta(1, 0, 1/2)$ of the $1S$ ground state in H and D amount to $8\,171\,663.8 \pm 2.5$ kHz and $8\,176\,795.7 \pm 2.3$ kHz, respectively. The dominant uncertainties arise from the two-loop corrections [16], and they are responsible for almost all of the uncertainties of the $\Delta(n, \ell, j)$. The hyperfine splittings of the $1S$ and $2S$ states have been measured very accurately [19–21].

All constants except R_∞ and the radii r_N in Eqs. (8)-(12) are known with sufficient accuracy [3] from measurements other than H or D spectroscopy. This leaves R_∞ and r_N to be determined from H or D spectroscopy. Note that we will later only be concerned with *transition frequencies* between different energy levels, so the Planck constant h on the left hand side of Eq. (8) drops out.

The Rydberg constant R_∞ appears in Eq. (8) explicitly only for the 1st (Bohr) term. This is to emphasize that the full accuracy of $\sim 10^{-12}$ is required only for the Bohr term, because only the measurements of optical transitions between levels with different principal quantum number n are accurate on the 10^{-12} level or better, see Tab. III. These measurements achieve accuracies in the kHz range or better, for transition frequencies of a several hundred THz.

Technically, also the 2nd (finite size) and 3rd ($\Delta(n, \ell, j)$) terms contain the Rydberg constant, acting as a “unit converter” between atomic units, used in the calculation of E_{NS} and $\Delta(n, \ell, j)$, and the SI unit of frequency, in which the measurements are done. The accuracy required in the latter terms is much lower, on the order of a few times 10^{-8} . This becomes obvious from kHz-accuracy required for the E_{NS} (1100 kHz and 7100 kHz for H and D, respectively), or for the $\Delta(1S)$ (-35.6×10^6 kHz). Thus, these terms do not require the full 10^{-12} accuracy in R_∞ . Instead, one can *calculate* R_∞ with

an accuracy of a few parts in 10^8 from the definition

$$R_\infty = \frac{\alpha^2 m_e c}{2h}, \quad (13)$$

and the values of α , m_e and h from measurements other than spectroscopy of H or D [22–26].

The CODATA-2010 report lists 24 transition frequencies in H and D that enter the LSA, see Ref. [3], Tab. XI. We reproduce the most relevant numbers, and a few more, in Tabs. III, V and VI. In particular, we list several measurements of the $1S \rightarrow 2S$ transition frequency in D.

Next we introduce the *modified* transition frequencies

$$\tilde{\nu}[(n, \ell, j) \rightarrow (n', \ell', j')] = \nu_{\text{meas}} + \Delta(n, \ell, j) - \Delta(n', \ell', j') \quad (14)$$

where all fine-, hyperfine-, and QED contributions (except for the finite size effect of S states) have been removed. These *modified* transition frequencies can then be used to extract r_N and R_∞ using

$$\tilde{\nu}[(n, \ell, j) \rightarrow (n', \ell', j')] = cR_\infty \frac{m_{\text{red}}}{m_e} \left(\frac{1}{n^2} - \frac{1}{n'^2} \right) - E_{NS} \left(\frac{\delta_{\ell 0}}{n^3} - \frac{\delta_{\ell' 0}}{n'^3} \right), \quad (15)$$

which of course follows from Eq. (8).

III. PROTON RADIUS FROM HYDROGEN SPECTROSCOPY

Table III lists 14 transition frequencies in atomic hydrogen. These can be separated in three blocks.

TABLE III: Some recent measurements in atomic hydrogen. An asterisk following the reference denotes items considered in the most recent CODATA-2010 report. Following our nomenclature, the $2S \rightarrow 2P_{1/2}$ transition must be assigned a negative frequency, because the final state $(n', \ell', j') = 2P_{1/2}$ is lower than the initial $(n, \ell, j) = 2S_{1/2}$ state.

#	$(n, \ell, j) - (n', \ell', j')$	ν_{meas} (kHz)	rel. unc.	Source	Ref.
H1	$2S_{1/2} \rightarrow 2P_{1/2}$	-1 057 862(20)	1.9×10^{-5}	Sussex 1979	[27] *
H2		-1 057 845.0(9.0)	8.5×10^{-6}	Harvard 1986	[28] *
H3	$2S_{1/2} \rightarrow 2P_{3/2}$	9 911 200(12)	1.2×10^{-6}	Harvard 1994	[29] *
H4	$2S_{1/2} \rightarrow 8S_{1/2}$	770 649 350 012.0(8.6)	1.1×10^{-11}	LKB 1997	[30] *
H5	$2S_{1/2} \rightarrow 8D_{3/2}$	770 649 504 450.0(8.3)	1.1×10^{-11}	LKB 1997	[30] *
H6	$2S_{1/2} \rightarrow 8D_{5/2}$	770 649 561 584.2(6.4)	8.3×10^{-12}	LKB 1997	[30] *
H7	$2S_{1/2} \rightarrow 12D_{3/2}$	799 191 710 472.7(9.4)	1.1×10^{-11}	LKB 1999	[31] *
H8	$2S_{1/2} \rightarrow 12D_{5/2}$	799 191 727 403.7(7.0)	8.7×10^{-12}	LKB 1999	[31] *
H9	$1S_{1/2} \rightarrow 2S_{1/2}$	2 466 061 413 187.103(46)	1.9×10^{-14}	MPQ 2000	[32]
H10		2 466 061 413 187.080(34)	1.4×10^{-14}	MPQ 2004	[33] *
H11		2 466 061 413 187.035(10)	4.2×10^{-15}	MPQ 2011	[34]
H12		2 466 061 413 187.018(11)	4.5×10^{-15}	MPQ 2013	[35]
H13	$1S_{1/2} \rightarrow 3S_{1/2}$	2 922 743 278 678(13)	4.4×10^{-12}	LKB 2010	[36] *
H14		2 922 743 278 659(17)	5.8×10^{-12}	MPQ 2016	[37]

1. Radio-frequency measurements within $n = 2$

The first block in Tab. III, items H1-H3, are radio-frequency measurements of $2S \rightarrow 2P$ transition frequencies in H. Modifying the measured frequencies by $\Delta(2S_{1/2}) - \Delta(2P_{j'})$ from Tab. I, each of these three measurements can be used individually to determine a value of the proton charge radius r_p from Eq. (11)

$$\tilde{\nu}(2S_{1/2} \rightarrow 2P_{1/2}) = \frac{1}{8} E_{NS}. \quad (16)$$

Each of these three measurements H1-H3 thus yields, a value of r_p , listed in Tab. IV.

As explained above, these three r_p values are in fact independent of the *exact* value of the Rydberg constant: The relative uncertainties of the radio-frequency measurements are on the order of 10^{-6} , so only the 6 most significant digits of R_∞ enter the calculation. The ‘‘proton radius puzzle’’ could ultimately require a change of R_∞ by 7σ , or 10^{-11} , as explained below. But such a change would not affect the r_p values obtained from items H1-H3.

2. Optical measurements between levels with different n

The 2nd block in Tab. III, items H4-H8, lists the five most accurate measurements of transition frequencies between the metastable $2S$ state and higher- n ‘‘Rydberg’’ states with $n=8$ or 12. Because these transitions are between levels with different principal quantum number n , one has to combine each of these measurements with a 2nd measurement to obtain a pair of values for r_p and R_∞ , using Eq. (8). Ideally, one combines each of the items H4-H8 with a measurement of the $1S \rightarrow 2S$ transition from block 3 in Tab. III, solving pairs of equations

like

$$\tilde{\nu}(1S \rightarrow 2S) = \frac{3}{4} cR_\infty - \frac{7}{8} E_{NS} \quad (17)$$

$$\tilde{\nu}(2S \rightarrow 8S) = \frac{15}{64} cR_\infty - \frac{63}{512} E_{NS}. \quad (18)$$

Considering the uncertainties of the experimental values in Tab. III and of the $\Delta(n, \ell, j)$ in Tab. I one sees immediately, that the dominant uncertainty is always given by the $2S \rightarrow n\ell$ measurements with their experimental uncertainty of the order of ~ 7 kHz. Several measurements of the $1S \rightarrow 2S$ transition exist with uncertainties of much less than 1 kHz. Hence one can choose any of the items H9-H12 to reach the same conclusion.

We choose the 2004 measurement [33] H10 with an uncer-

TABLE IV: Proton charge radii from hydrogen. The row labeled ‘‘CODATA Adjustment 8’’ is the value using all hydrogen data, listed in Ref. [3], Tab. XXXVIII. Also given are the radii from combining the $2S \rightarrow n\ell$ transitions in H with either $1S \rightarrow 2S$ or $1S \rightarrow 3S$. All values agree very well. ‘‘avg’’ denotes the average of all values in the rows above, also considering correlations.

#	Transition(s)	r_p [fm]
H1	$2S \rightarrow 2P_{1/2}$	0.9270 ± 0.0553
H2	$2S \rightarrow 2P_{1/2}$	0.8788 ± 0.0262
H3	$2S \rightarrow 2P_{3/2}$	0.8688 ± 0.0354
H10 + H4	$1S \rightarrow 2S + 2S \rightarrow 8S_{1/2}$	0.8666 ± 0.0211
H10 + H5	$1S \rightarrow 2S + 2S \rightarrow 8D_{3/2}$	0.8789 ± 0.0204
H10 + H6	$1S \rightarrow 2S + 2S \rightarrow 8D_{5/2}$	0.8911 ± 0.0155
H10 + H7	$1S \rightarrow 2S + 2S \rightarrow 12D_{3/2}$	0.8551 ± 0.0222
H10 + H8	$1S \rightarrow 2S + 2S \rightarrow 12D_{5/2}$	0.8641 ± 0.0164
$1S \rightarrow 2S$ (H10) + all H($2S \rightarrow n\ell$)		0.8747 ± 0.0091 avg.
$1S \rightarrow 3S$ (H13+H14) + all H($2S \rightarrow n\ell$)		0.8780 ± 0.0108
CODATA Adj. 8		0.8764 ± 0.0089 Eq. (19)

tainty of 0.034 kHz, which was also used in CODATA-2010. The results are summarized in Tab. IV.

A trivial weighted average of all individual r_p values in Tab. IV yields r_p from H spectroscopy alone, of $r_p(\text{H}) = 0.8746 \pm 0.0076$ fm, 4.4σ larger than the μp value. This number is in good agreement with a recent evaluation [18], which finds a 0.035(7) fm, or 4.9σ , difference between H and μp .

However, relevant correlations exist between the various measurements of block 2, see Ref. [3], Tab. XIX. These correlations increase the uncertainty of the derived $r_p(\text{H}) = 0.8747(91)$ fm.

Alternatively, one can, instead of the $1S \rightarrow 2S$ transition (H10) combine the $1S \rightarrow 3S$ transitions (H13 and H14) with all $2S \rightarrow n\ell$ transitions. This yields (including correlations) $r_p(\text{H}') = 0.8780(108)$ fm, in very good agreement with the value above, and only slightly less accurate.

A reliable value for the proton rms charge radius deduced from H data alone, which takes into account all data in H listed in Tab. XI of Ref. [3], as well as the correlations between all input parameters, is given in Adjustment 8 of the CODATA-2010 LSA, see Ref. [3], Tab. XXXVIII.

$$r_p(\text{H spectroscopy}) = 0.8764(89) \text{ fm.} \quad (19)$$

This value is 4.0σ larger than the value from muonic hydrogen, see Fig. 1.

Considering elastic electron-proton (e-p) scattering data together with H spectroscopy, as done in Adjustment 9 of the CODATA-2010 LSA, yields $r_p(\text{H and e-p}) = 0.8796(56)$ fm, which is 6.9σ larger than the μp value. This is the “proton radius puzzle” between measurements with electrons and muonic hydrogen.

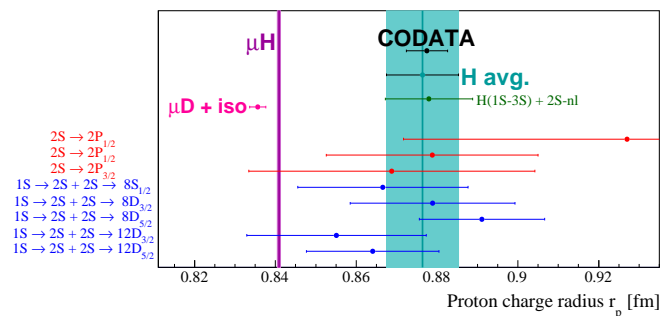


FIG. 1: Proton rms charge radii from muonic hydrogen (μH , the stripe includes the uncertainty) and muonic deuterium [6] (“ $\mu\text{D} + \text{iso}$ ”, obtained using Eq.(5)), in comparison with the CODATA-2010 value (Eq.(2)), the value from hydrogen spectroscopy alone (Eq.(19)), and the alternative value from using the $1S \rightarrow 3S$ measurement in hydrogen instead of the $1S \rightarrow 2S$ transition, see text. Also shown are the individual values from $2S \rightarrow 2P$ and from combining $1S \rightarrow 2S$ and $2S \rightarrow n\ell$, see Tab. IV.

IV. DEUTERON RADIUS FROM DEUTERIUM SPECTROSCOPY ALONE

The principle of determining the deuteron radius from deuterium spectroscopy is exactly analogous to the one described for hydrogen above. However, not all measurements were done for deuterium. Table VI lists the relevant deuterium data.

First, we note that there are no radio-frequency measurements of $2S \rightarrow 2P$ transitions (i.e. no “block 1”). Thus there are no “Rydberg-free” r_d values such as the r_p values H1-H3.

Moreover, no measurement of the $1S \rightarrow 2S$ transition in “deuterium only” is listed in the CODATA list of measurements, see Ref. [3], Tab. XI. Only the $1S \rightarrow 2S$ isotope shift, i.e. the difference of the $1S \rightarrow 2S$ transition in D and H, is listed there. We give the two most recent values of the H/D isotope in Tab. V.

This apparent lack of a precise measurement of the $1S \rightarrow 2S$ transition in D seems to make it impossible to apply the procedure outlined above for hydrogen, in which pairs of (R_∞, r_d) are obtained by combining $1S \rightarrow 2S$ and $2S \rightarrow n\ell$ measurements. CODATA instead performs their Adjustment 10 of all “deuterium only” measurements using only $2S \rightarrow n\ell$ measurements (plus some much less accurate differences of $2S \rightarrow 4S/D$ and $1/4$ of the $1S \rightarrow 2S$ transition [38], which we omit here for brevity). This has the serious drawback that the “long lever-arm” provided by the extremely accurate $1S \rightarrow 2S$ transition is lost, which is reflected by the large uncertainty of r_d obtained in Adjustment 10 of CODATA-2010 of $r_d = 2.1207(253)$ fm, see Eq. (7).

Several very precise values for the $1S \rightarrow 2S$ transition in atomic deuterium exist, however, see Tab. VI. The most precise value is obtained by simply adding the $1S \rightarrow 2S$ transition frequency in H and the $1S \rightarrow 2S$ H/D isotope shift. Indeed, the published values of the H/D isotope shift are obtained by subtracting two frequency measurements of $1S \rightarrow 2S$ transitions in H and D [7, 8]. For the full CODATA adjustment 3, this choice makes no difference. However, without the $1S \rightarrow 2S$ transition in D one does not obtain the best possible deuteron radius from D spectroscopy in Adjustment 10.

Any frequency measurement is nothing more than a frequency *comparison*. The so-called “absolute frequency measurements” are characterized by a comparison to a Cs clock [39]. Technically, all these comparisons between H and Cs involve intermediate comparisons with “transfer oscillators”.

For example, items I1, D9 and D10 used a CH_4 -stabilized HeNe laser, which was then transported to the German Standards Institute PTB for comparison with a Cs clock. In between, a plethora of local oscillators were used in two “frequency chains” [10]. More recently, items H9-H12 used a hydrogen maser as a transfer oscillator. This maser was then compared to a Cs fountain clock [39].

The isotope shift measurement I2 is a frequency comparison between D($1S \rightarrow 2S$) and the same hydrogen maser, using GPS calibration. The maser was then compared to the hydrogen $1S \rightarrow 2S$ transition. The practical reason to use hydrogen as an intermediate transfer oscillator to the Cs SI

TABLE V: Some recent measurements of the H-D isotope shift. An asterisk following the reference denotes items considered in the most recent CODATA-2010 report.

#	Transitions	Frequency (kHz)	rel. unc.	Source	Ref.
I1	$D(1S_{1/2} \rightarrow 2S_{1/2}) - H(1S_{1/2} \rightarrow 2S_{1/2})$	670 994 334.64(15)	2.2×10^{-10}	MPQ 1998 [7]	
I2		670 994 334.606(15)	2.2×10^{-11}	MPQ 2010 [8] *	

TABLE VI: Some recent measurements in atomic deuterium. An asterisk following the reference denotes items considered in the most recent CODATA-2010 report. Items D9 and D10 are direct measurements using a CH_4 stabilized He:Ne laser as a transfer oscillator, while D11 and D12 have been measured using the $1S \rightarrow 2S$ transition in hydrogen and a hydrogen maser as transfer oscillators.

#	$(n, \ell, j) - (n', \ell', j')$	ν_{meas} (kHz)	rel. unc.	Source	Ref.
D4	$2S_{1/2} \rightarrow 8S_{1/2}$	770 859 041 245.7(6.9)	8.9×10^{-12}	LKB 1997	[30] *
D5	$2S_{1/2} \rightarrow 8D_{3/2}$	770 859 195 701.8(6.3)	8.2×10^{-12}	LKB 1997	[30] *
D6	$2S_{1/2} \rightarrow 8D_{5/2}$	770 859 252 849.5(5.9)	7.7×10^{-12}	LKB 1997	[30] *
D7	$2S_{1/2} \rightarrow 12D_{3/2}$	799 409 168 038.0(8.6)	1.1×10^{-11}	LKB 1999	[31] *
D8	$2S_{1/2} \rightarrow 12D_{5/2}$	799 409 184 966.8(6.8)	8.5×10^{-12}	LKB 1999	[31] *
D9	$1S_{1/2} \rightarrow 2S_{1/2}$	2 466 732 407 521.8(1.5)	6.1×10^{-13}	MPQ 1997	[10]
D10		2 466 732 407 522.88(91)	3.7×10^{-13}	MPQ 1997	[10]
D11		2 466 732 407 521.74(20)	7.9×10^{-14}	MPQ 1998/2000 H9 +I1	
D12		2 466 732 407 521.641(25)	1.0×10^{-14}	MPQ 2010/2011 H11+I2	

clock was that it did not require the availability of a primary Cs frequency standard at MPQ.

Thus, we combine items H9 and I1, and H11 and I2, to obtain two values for the $D(1S \rightarrow 2S)$ transition frequency, D11 and D12. This avoids double-counting, because item H10 has been used above to determine the proton radius. For simplicity, we add the uncertainties linearly, although a more rigorous evaluation of the combined uncertainty, including all correlations, would certainly yield a smaller uncertainty of the $D(1S \rightarrow 2S)$ transition frequency.

If one wishes, one could also use the values D9 or D10 which can be found in the PhD thesis of Th. Udem [10]. These values are “absolute” frequency measurements without the use of hydrogen as a transfer oscillator.

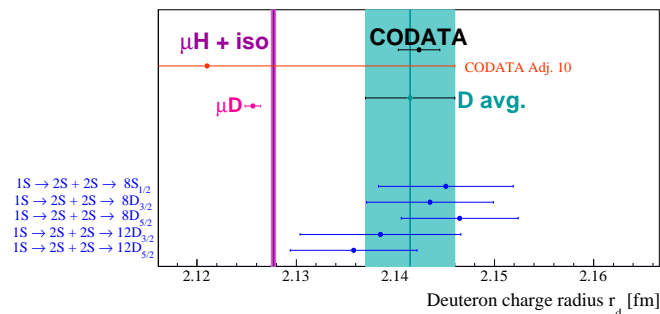


FIG. 2: Deuteron rms charge radii from spectroscopy of deuterium alone, see Tab. VII, and muonic atoms. Also shown are the CODATA value Eq. (4), and the value from CODATA Adjustment 10 (Eq. (7)) that does not use the value for the $1S \rightarrow 2S$ transition in D (see text). The value “ $\mu\text{H} + \text{iso}$ ” [2] is obtained from Eq. (5) using the proton charge radius from muonic hydrogen Eq. (1). The discrepancy is the same “proton radius puzzle” as the one in Fig. 1. The new deuteron radius from muonic deuterium [6] (μD) is 3.5σ smaller than the average value from deuterium spectroscopy (Eq. (20)).

TABLE VII: Deuteron charge radii from deuterium. The value labeled “Eq. (20)” is our result. It is the average of the individual values above it, taking into account the known correlations between the $2S \rightarrow n\ell$ measurements. The next two values use items D9 and D10, which have not been measured using atomic hydrogen as a transfer oscillator (see text).

#	Transitions	r_d [fm]	
D12 + D4	$1S \rightarrow 2S + 2S \rightarrow 8S_{1/2}$	2.1451 ± 0.0068	
D12 + D5	$1S \rightarrow 2S + 2S \rightarrow 8D_{3/2}$	2.1435 ± 0.0064	
D12 + D6	$1S \rightarrow 2S + 2S \rightarrow 8D_{5/2}$	2.1465 ± 0.0059	
D12 + D7	$1S \rightarrow 2S + 2S \rightarrow 12D_{3/2}$	2.1385 ± 0.0081	
D12 + D8	$1S \rightarrow 2S + 2S \rightarrow 12D_{5/2}$	2.1358 ± 0.0064	
	D12 + all $D(2S \rightarrow n\ell)$	2.1415 ± 0.0045	Eq. (20)
	D9 + all $D(2S \rightarrow n\ell)$	2.1414 ± 0.0045	
	D10 + all $D(2S \rightarrow n\ell)$	2.1411 ± 0.0045	

All of the four values D9...D12 are sufficiently accurate to proceed with the determination of r_d values from combining $1S \rightarrow 2S$ and $2S \rightarrow n\ell$ for $n=8,12$, see Tab. VII.

The trivial weighted average of the values in Tab. VII is $r_d = 2.1422(30)$ fm, *i.e.* 5.3σ larger than the μd value. Again, however, correlations [70] between the $2S \rightarrow n\ell$ measurements increase the uncertainty. Taking into account these correlations we obtain

$$r_d(\text{D spectroscopy}) = 2.1415(45) \text{ fm.} \quad (20)$$

This value is 3.5σ larger than the new value from muonic deuterium.

For comparison, using, instead of D12, the $1S \rightarrow 2S$ measurements D9 or D10, yields $r_d = 2.1414(45)$ fm and $r_d = 2.1411(45)$ fm, respectively, including the correlations.

The agreement of these three values shows that it is not important which of the available $D(1S \rightarrow 2S)$ measurements is chosen (see Tab. VII).

Moreover, this ‘‘D spectroscopy’’ value is in excellent agreement with the global CODATA value from Adjustment 3, $r_d = 2.1424 \pm 0.0021$ fm. This is a strong indication for the internal consistency of CODATA LSA. This agreement is also evident in the agreement of the Rydberg constants from H spectroscopy on the one hand, and D spectroscopy on the other. This is further discussed in section VI.

We emphasize again that this 3.5σ discrepancy between muonic and electronic deuterium spectroscopy measurements is as independent as possible of any measurement used in the proton charge radius determination. Correlations may exist because of unidentified systematic shifts in any of the electronic or muonic measurements, or missing or wrong theory contributions in electronic or muonic atoms. In the absence of any indication for such an unknown correlation, the new μd measurement [6] constitutes an independent discrepancy.

V. THE DEUTERON STRUCTURE RADIUS

In the preceding sections we were concerned with hidden or implicit correlations between the (CODATA) values of r_p and r_d , which originate from the nature of performing a least-squares adjustment using all available input data in H and D. Here, we could provide values of r_p and r_d which are ‘‘as uncorrelated as possible’’ by separating the analysis of H and D data.

Physics, on the other hand, is also the source of an explicit correlation between r_p and r_d , simply because the deuteron contains a proton. The deuteron charge radius is related to the proton charge radius by [9, 40]

$$r_d^2 = r_{\text{struct.}}^2 + r_p^2 + r_n^2 + \frac{3\hbar^2}{4m_p^2 c^2}, \quad (21)$$

where $r_{\text{struct.}} = 1.97507(78)$ fm [9] is the deuteron structure radius, *i.e.* the proton-neutron separation, r_n is the neutron mean square charge radius $\langle r_n^2 \rangle = -0.114(3)$ fm [41, 42], and the rightmost term is the Darwin-Foldy correction of 0.0331 fm² due to the zitterbewegung of the proton, see [9] and also the Appendix of Ref. [43].

The 0.8% smaller deuteron charge radius from muonic deuterium in Eq. (3) is very consistent with the 4% smaller proton radius from muonic deuterium Eq. (1), inserted in Eq. (21). This is the reason why the new $r_d(\mu d)$ is understood to confirm the smaller proton radius from muonic hydrogen [6].

VI. THE RYDBERG CONSTANT

The correlation coefficient between the proton radius r_p and the Rydberg constant R_∞ is as large as 0.989 in the CODATA LSA. Therefore, a change of r_p by $x\sigma$ will normally result in a change of R_∞ by almost the same $x\sigma$.

This can be understood by considering Eq. (8), and the accuracy of the measurements in H listed in Tab. III:

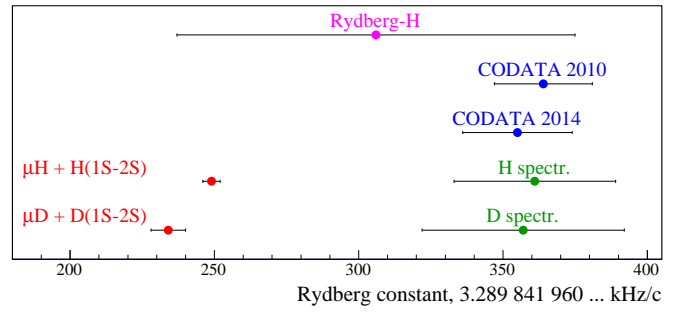


FIG. 3: Rydberg constant from CODATA-2010 [3], Eq. (25) and CODATA-2014 [44], from spectroscopy of regular H and D, Eqs. (26) and (27), respectively, and from combining the muonic charge radius of the proton and the deuteron and the measurement of the $1S \rightarrow 2S$ transition in H and D, Eqs. (22) and (23), respectively. Also shown is the result from spectroscopy of high-lying ($n = 27 \dots 30$) circular Rydberg states of atomic hydrogen [45], Eq. (28).

The accuracy of each of the $2S \rightarrow n\ell$ transitions ($n = 8, 12$), which determine the accuracy of R_∞ , is about 1 part in 10^{11} . As a consequence, the uncertainty of the Rydberg constant in CODATA-2010 is about 6 parts in 10^{12} . The $1S \rightarrow 2S$ transition, on the other hand, has been measured with an uncertainty of 4 parts in 10^{15} , *i.e.* a factor of 1000 more accurately.

A look at Eq. (17) reveals the correlation: The left side is measured with an accuracy of 0.010 kHz. The 1st term on the right side is known only to ~ 10 kHz (3/4 of the 17 kHz uncertainty of the CODATA value of cR_∞) [3].

Adopting the muonic values of r_p and r_d in E_{NS} will thus shift the central value of E_{NS} , which must immediately be compensated by a corresponding change in R_∞ because of the 1000-fold more precisely determined left side of Eq. (17). At the same time, the smaller uncertainty of the muonic charge radii will yield more accurate values of R_∞ , when combined with the electronic $1S \rightarrow 2S$ transitions:

$$R_\infty [H(1S \rightarrow 2S); r_p(\mu p)] = 3.289\,841\,960\,249(3) \times 10^{12} \text{ kHz/c} \quad (22)$$

from electronic and muonic hydrogen [2], and

$$R_\infty [D(1S \rightarrow 2S); r_d(\mu d)] = 3.289\,841\,960\,234(6) \times 10^{12} \text{ kHz/c} \quad (23)$$

from electronic and muonic deuterium [6].

The value in Eq. (22) is in good agreement with the one from CODATA Adjustment 11,

$$R_\infty (\text{Adjustment 11}) = 3.289\,841\,960\,255(4) \times 10^{12} \text{ kHz/c} \quad (24)$$

see Tab. XXXVIII of Ref. [3], which includes r_p from muonic hydrogen in the global LSA. Because of its tiny uncertainty, the muonic r_p value dominates Adjustment 11, yielding r_p (Adjustment 11) = 0.84225(65) fm, and this change of r_p is accompanied by a change of R_∞ , as described above.

For reference, the CODATA recommended value of the Rydberg constant is

$$R_{\infty} (\text{CODATA} - 2010) = 3.289\,841\,960\,364(17) \times 10^{12} \text{ kHz}/c \quad (25)$$

which is 7σ larger.

For completeness, the values of the Rydberg constant from hydrogen data alone, taken from CODATA Adjustment 8, is

$$R_{\infty} (\text{H spectroscopy}) = 3.289\,841\,960\,361(28) \times 10^{12} \text{ kHz}/c. \quad (26)$$

The one we deduce from deuterium data alone, including the $1S \rightarrow 2S$ transition is

$$R_{\infty} (\text{D spectroscopy}) = 3.289\,841\,960\,357(35) \times 10^{12} \text{ kHz}/c. \quad (27)$$

A measurement of transition frequencies between high-lying circular Rydberg states of atomic H, with $n = 27\dots30$, which are insensitive to the proton charge radius, yielded [45]

$$R_{\infty} (\text{Rydberg} - \text{H}) = 3.289\,841\,960\,306(69) \times 10^{12} \text{ kHz}/c. \quad (28)$$

This result is unfortunately not accurate enough to discriminate the muonic and the “purely electronic” values, see Fig. 3.

New insight into the “proton radius puzzle” is expected from several new atomic physics measurements: The $2S \rightarrow 4P$ transitions in H [46, 47] will yield an independent value of the Rydberg constant. A new measurement of the classical Lamb shift in H [48] will yield a proton charge radius that is independent of the exact value R_{∞} , see Sec. III 1. Improved measurements of the $1S \rightarrow 3S$ transition in H are underway at MPQ and LKB [49, 50]. Measurements of the $1S$ - $2S$ transition in H-like He^+ ions [51–53] will, when combined with a new value of the alpha particle charge radius from muonic helium spectroscopy [54], yield a Rydberg constant or test higher-order QED contributions. The Rydberg constant can also be determined from high-precision spectroscopy of molecules and molecular ions of hydrogen isotopes [55–59], combined with improved calculations [60]. One-electron ions in circular Rydberg states [61, 62] will also yield a Rydberg constant free from nuclear radius effects.

As a final remark, we may attribute the small 2.2σ difference between the two Rydberg values using the muonic radii (Eq. (22) and Eq. (23)) to the deuteron polarizability contribution [63–67], summarized in Ref. [6].

VII. CONCLUSIONS

The most accurate value of the deuteron rms charge radius from laser spectroscopy of regular (electronic) deuterium only is $r_d = 2.1415(45)$ fm. It is obtained using a value for the $1S \rightarrow 2S$ transition in atomic deuterium which can be inferred from published data [8, 34], or found in a PhD thesis [10]. Our value is in excellent agreement with the CODATA value [3], and only twice less accurate.

In contrast to the CODATA value, the deuteron radius above is as uncorrelated as possible to measurements that determine the proton rms charge radius r_p . The CODATA Adjustment 10, which is also independent of r_p , is five times less accurate than the value above, because of a more conservative treatment of the deuterium $1S \rightarrow 2S$ measurements.

Note added: After the submission of this manuscript, the updated CODATA-2014 paper was published [44]. The numbering of the partial Adjustments remained the same. What was Tab. XXXVIII in CODATA-10 is now Tab. XXIX on page 54 of CODATA-14.

The partial Adjustments 8 (H spectroscopy) and 10 (D spectroscopy) yield identical values compared to CODATA-10, our Eqs. (6) and (7), respectively. The only new input data is our item H12, the 2013 measurement of the $1S \rightarrow 2S$ transition from MPQ.

The change of the recommended values of r_p , r_d , and R_{∞} (from the full Adjustment 3) is exclusively from a reassessment of the uncertainty of the electron scattering data [68]. None of the conclusions of the present manuscript are changed.

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- [70] See Ref. [3], Tab. XIX