On the accuracy of the optical determination of the proton charge radius

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Determination of the proton charge radius by different methods has produced an inconsistency. The most precise value (from spectroscopy of muonic hydrogen) strongly disagrees with three less accurate values (from spectroscopy of ordinary hydrogen and deuterium, from relative measurements of the cross section of the elastic electron-proton scattering at MAMI and from evaluation of the world data on absolute measurements of $e^-p$ cross sections). Here, we question the accuracy of the determination of the proton charge radius by means of spectroscopy of ordinary hydrogen and deuterium and demonstrate that its accuracy was probably overestimated. In particular, we revisit determination from each relevant transition and find that the results of two optical experiments, which are the most statistically important, are not perfectly consistent. The inconsistency is rather a 'tension' between the results than their discrepancy, however, it implies that a more conservative estimation of the uncertainty is needed. With the more realistic estimation of the uncertainty, the results for the proton charge radius from spectroscopy of ordinary and muonic atoms are rather in fair agreement.

PACS numbers: 12.20.-m, 31.30.J-, 36.10.Gv 32.10.Fn

I. INTRODUCTION

For a few last years, since the publication in 2010 [1], the so-called proton-radius puzzle became a part of physics landscape. The present-day statement is that the determination of the proton charge radius from the Lamb shift in muonic hydrogen [2, 3] has an uncertainty much smaller than that of the other determinations, but its value is in a strong contradiction with them. The situation with the proton rms charge radius $R_p$ is graphically presented in Fig. 1 where the results are plotted following [4], based on the CODATA analysis [5].

The $H&D$ value is a result of the CODATA evaluation [5] of spectroscopic data on 24 transitions in atomic hydrogen and deuterium and it is roughly $5\sigma$ away from the muonic $PSI$ value [2]. Two more points are from the elastic electron-proton scattering. The $Sick$ result is from an evaluation of world data on the absolute measurements of the cross sections [6], while the $MAMI$ data point results from a relative measurement of the cross sections at the Mainzer Mikrotron (MAMI) [7]. The former is within $3\sigma$, while the latter is within $5\sigma$ from the result from Paul Scherrer Institut (PSI). Those three results, $H&D$, $MAMI$ and $Sick$'s, are apparently consistent. Averaging them, one finds the mean CODATA value [5] $7\sigma$ away from the muonic one, which is indeed a strong discrepancy. There is also one more point from combining the isotopic-shift measurement of the $1s-2s$ transition in hydrogen and deuterium with a result of the electron-deuteron scattering [8], however, it is not conclusive.

This controversy is challenging, and various solutions have been proposed including some unrealistic properties of the proton and unreasonable behavior of higher-order QED effects as well as new physical phenomena. No reasonable explanation within the standard physics has been suggested.

We believe that the solution lies in a different direction. The statement on the discrepancy is valid only if we rely on the accuracy of the mentioned results as they have been claimed. However, it often happens that the accuracy is overestimated and here we revisit the accuracy of the spectroscopic determination, which, as we mentioned, is within $5\sigma$ from the muonic result.

We have revisited determination of the proton charge radius from spectroscopy of ordinary hydrogen and deuterium. We basically follow the evaluation in [5]. There 24 measurements of various transitions in hydrogen and deuterium were utilized, which produced 22 partial values of the proton radius. Below we consider those values...
in detail.

II. EXTRACTION OF THE RYDBERG CONSTANT AND THE PROTON CHARGE RADIUS FROM SPECTROSCOPY OF HYDROGEN AND DEUTERIUM

The frequency of any transition in the hydrogen atom can be expressed in terms of the Rydberg constant and the proton charge radius. The expressions are very complicated, however, the dominant dependence on these two parameters is very simple (see, e.g., [9])

\[ hf(n'l' - nl) = -\frac{hcR_\infty}{n'^2 - n^2} + E_L(nl) - E_L(n'l') + \ldots \] (1)

where the Lamb shift of the \( nl \) state includes dependence on the rms proton charge radius

\[ E_L(nl) = \frac{4\alpha^4mc^2}{3}\frac{m^2c^4R^2_\infty}{\hbar^2} \frac{\delta_0}{n^3} + E'_L(nl) \] (2)

The remaining terms in \( E'_L(nl) \) and \( E'_L(nl) \) indeed also depend on \( R_\infty \) and \( R_p \). However, the required accuracy is relatively low and does not interfere with any determination of the Rydberg constant and the proton charge radius. Still, \( E'_L(nl) \) contributes to the final uncertainty of the determination of those constants (see, e.g., [5]).

Many experimentally measured frequencies, such as those of \( 1s - 2s \) or \( 2s - 8d_{5/2} \), depend both on the proton-radius term and the Rydberg-constant term. Thus, one has to combine the two hydrogen frequencies to obtain a value of the radius. On the contrary, certain experimental frequencies, e.g., \( f(2s - 2p) \), do not include the Rydberg-constant term and the proton radius can be found immediately. To obtain a value of the Rydberg constant one has to combine such a transition with one frequency, which contains the Rydberg-constant term.

Deuteron data can be described in a similar way. Combining two deuteron results one can find a value of the Rydberg constant and, applying it to a hydrogen transition, one can extract a value of the proton radius.

Below we consider the hydrogen and deuteron data and their required combinations in detail. The relevant spectroscopic data are summarized in Table I. The frequencies listed there are ‘effective’ frequencies after introduction of the appropriate hyperfine-structure correction to the originally measured transition frequencies. While describing the data, we follow [3] (see Table XI there).

There are a few important components of the evaluation of the hydrogen and deuteron spectroscopic data. At first, we have to mention the results on the \( 1s - 2s \) transition frequencies in hydrogen and deuteron measured at MPQ (Max-Planck-Institut für Quantenoptik)\[10, 11\]. These measurements are much more accurate than all other optical measurements (see Table I) and they are to be used as their ‘companions’ to find the values of the proton radius (from the H transitions) or the value of the Rydberg constant (from the D transitions).

Below we consider the hydrogen and deuterium spectroscopic data. The frequencies listed there are ‘effective’ frequencies after introduction of the appropriate hyperfine-structure correction to the originally measured transition frequencies. While describing the data, we follow [3] (see Table XI there).

| Transition(s) | Frequency [kHz] | Ref. |
|--------------|-----------------|-----|
| \( f_H(1s - 2s) \) | 2466061413187080(34) | [10] |
| \( f_D(1s - 2s) - f_H(1s - 2s) \) | 670994334606(15) | [11] |
| \( f_H(2s - 8s) \) | 77064935001208(6.6) | [13] |
| \( f_H(2s - 8d_{5/2}) \) | 770649504450.8(3.3) | [13] |
| \( f_H(2s - 8d_{3/2}) \) | 770649561584.2(6.4) | [13] |
| \( f_D(2s - 8s) \) | 77085904124576(9.3) | [13] |
| \( f_D(2s - 8d_{5/2}) \) | 770859253849.5(5.9) | [13] |
| \( f_H(2s - 12d_{5/2}) \) | 799191710472.7(9.4) | [14] |
| \( f_H(2s - 12d_{3/2}) \) | 7991917274037(7.0) | [14] |
| \( f_D(2s - 12d_{5/2}) \) | 79940916803808(6.6) | [14] |
| \( f_D(2s - 12d_{3/2}) \) | 79940918496686(8.8) | [14] |
| \( f_H(1s - 3s) \) | 2922743278678(13.15) | [13] |
| \( f_H(2s - 4s) - \frac{1}{2} f_D(1s - 2s) \) | 479733810(18) | [16] |
| \( f_H(2s - 4d_{5/2}) - \frac{1}{2} f_D(1s - 2s) \) | 469014424(18) | [18] |
| \( f_D(2s - 4s) - \frac{1}{2} f_D(1s - 2s) \) | 469069320(18) | [18] |
| \( f_D(2s - 4d_{5/2}) - \frac{1}{2} f_D(1s - 2s) \) | 469484141(18) | [18] |
| \( f_H(2s - 6s) - \frac{1}{2} f_H(1s - 2s) \) | 479760021(19) | [19] |
| \( f_H(2s - 6d_{5/2}) - \frac{1}{2} f_H(1s - 2s) \) | 469909910(19) | [19] |
| \( f_H(2s - 4p_{1/2}) - \frac{1}{2} f_H(1s - 2s) \) | 466426915(20) | [20] |
| \( f_H(2s - 4p_{3/2}) - \frac{1}{2} f_H(1s - 2s) \) | 603537310(20) | [20] |

TABLE I: The H and D transition frequencies relevant for determination of the Rydberg constant and the proton charge radius following Table XI of [3]. Those 24 transition frequencies include 2 anchor \( 1s - 2s \) transitions, 11 other absolutely measured transitions, 8 combinations of optical transitions (‘beat frequencies’) and 3 microwave frequencies.

\[1\] Following [3], we are to ignore more recent measurements of the \( 1s - 2s \) transition [12], which have a superficial accuracy for our purposes.
of any other optical transitions by more than an order of magnitude. We may neglect any correlations between the extracted values of \( R_p \) due to use of data on the \( 1s - 2s \) transitions.

Let’s consider the relevant data in more detail. We do not follow the historic chronological way and list the data according to their relevance. As well as in \[3\], we consider 24 transition frequencies. Two of them, namely, \( 1s - 2s \) in hydrogen and deuterium, serve as the ‘anchor’ transitions in our evaluation. They are used as the auxiliary companions to each of the other 22 transition frequencies to find \( R_\infty, R_p \) and \( R_d \). The most important among those 22 transition frequencies are the optical data. All relevant absolute frequency measurements, except for the anchor measurements of the \( 1s - 2s \) transition, were performed at LKB (Laboratoire Kastler Brossel). Three experiments include a measurement of six \( 2s - 8s/d \) \[13\], four \( 2s - 12d \) \[14\] and one \( 1s - 3s \) transition \[15\]. Except for the latter, the other measurements were performed on both hydrogen and deuterium and they are the most statistically important because of their accuracy (see below).

To take advantage of a possibility to extract \( R_\infty \) by combining the \( 1s - 2s \) frequency with the other one, e.g., \( 2s - nl \), one has to be able either to calculate \( E_L \) for various levels or to find a relation between them. An appropriate relation is based on a possibility to obtain the difference \[\delta E_L(n) = E_L(1s) - n^3E_L(ns) = E_L'(1s) - n^3E_L'(ns) \] (3)

for various \( ns \) states, the most important of which is the \( 2s \) state. Meantime, for \( l \neq 0 \) a calculation of the \( E_L'(nl) \) is not a problem. That allows us to express all the transitions in terms of \( R_\infty \) and \( E_L(2s) \), while all the other contributions are under control and do not require accurate knowledge either of \( R_\infty \) or of \( R_p \). To extract \( R_p \) from \( E_L(2s) \) one has to deal with a complete theory of the Lamb shift in hydrogen. In the CODATA evaluation \[5\] the expression for \( \Delta L(n) \) has not been used explicitly, but their suggestions on the character of the \( n \)-dependence of various contributions are roughly equivalent to this approach. Eventually, we follow the summary \[2\] of a relevant theoretical contributions to the energy levels in H and D atoms (see also \[24\]).

Note that the deuterium values of \( R_p \) involve absolutely the same theory as hydrogenic ones. One can have in mind a picture, in which we first find \( R_d \) and next, applying the result on the isotopic shift of the \( 1s - 2s \) transition as a constraint, obtain \( R_p \). In this way we need a theory of the deuterium Lamb shift and of the isotopic shift and such theories are in general more complicated and less reliable than the one for the hydrogen atom. The issue is the deuterium polarizability, which may involve additional uncertainty. However, the contribution of the deuterium polarizability eventually cancels out for \( R_p \). That is easy to understand if we choose a different prescription to utilize the same data. We use the isotopic shift to find the \( 1s - 2s \) frequency in D, next we combine it with a deuterium transition of interest to find a value of the Rydberg constant. All that does not require any theory for the deuteron polarizability (since it has a trivial state dependence being proportional to \( \delta_{21}/n_3 \) and does not contribute to \( \Delta L(n) \) for deuterium).

With the value of the Rydberg constant extracted from deuterium, we obtain a value of the proton radius from the \( 1s - 2s \) transition in hydrogen. All that requires a theory of the Lamb shift in hydrogen, but not in deuterium.

## III. The Data and the Results

The relevant transitions are summarized in Table \[1\] and Fig. \[2\]. We present in Fig. \[2\] the partial results of a determination of the proton charge radius and the Rydberg constant. The partial results on determination of the deuteron radius look similar, because \( R_d, R_p, R_\infty \) are strongly correlated to each other. As we mentioned, the most accurate results on the proton charge radius come from a comparison of 11 optical transitions \[13\] \[15\] with the anchor data on the \( 1s - 2s \) transitions. The other experiments \[13\] \[20\] and \[21\] \[23\] produce frequencies which do not include the Rydberg term and allow us to determine \( R_p \) directly. However, they are statistically substantially less important as clearly seen in Fig. \[2\] where we summarize all the 22 determinations. To determine the Rydberg constant from the experiments, which produce a value of the proton radius without involving of the anchor data, one has to combine the derived proton radius with the \( 1s - 2s \) transition frequency.

Various experimental correlations are presented and the extracted values of the Rydberg constant are as [in]dependent from each other as the data are. The additional correlations due to the evaluation procedure are marginal for the Rydberg constant. Besides, for the proton radius there is an additional (to the determination of the Rydberg constant) theoretical correlation due to the application of the same value of \( E_L'(2s) \) to all the evaluations. This may shift all the values of the proton radius, extracted from H & D spectroscopy, the same way but does not affect their scatter.

The extracted partial values in Fig. \[2\] are strongly correlated not only because some use similar methods and perform measurements at a similar set up, but also because those 22 transition frequencies were measured in 9 experiments only and, in particular, ten most statistically significant results originate from two experiments \[13\] \[14\] performed at essentially the same set up.

While \( \chi^2 \) of the distribution around the average value \[3\] seems reasonable, we note that the distribution of the results in Fig. \[2\] around the mean value is not random. A comparison of the two most accurate experiments \[13\] and \[14\] shows that there is a certain systematic effect which has been missed in the evaluation of data and which is responsible for the difference between these two groups of the results. While most of \( 2s - 8s/d \) transi-
FIG. 2: Determination of the proton charge radius and the Rydberg constant from various H and D transitions. Each of 22 partial values of the proton radius and the Rydberg constant is obtained by using a certain unique measurement of a transition frequency or their combination (the transition is used as the label) and the frequency of one or two anchor $1s - 2s$ transitions as explained in the text. The transitions are grouped by experiments; the related references could be found in Table I. The closed circles are for 11 absolute optical frequency measurements, 8 open ones are for the differential optical frequency measurements, and 3 squares are for the microwave transitions. The long blue broad belt is for the CODATA-2010 all-spectroscopic value (see adjustment 6 in Table XXXVIII of [3]). The long narrow red belt (which looks as a bold line) is for the value from the muonic hydrogen Lamb shift [2,3]. The other filled areas are for the average value of two crucial experiments [13] and [14], performed at LKB. The ‘dark’ part of each area is for the mean value without taking any correlations into account while the ‘light’ one is with taking them into account following [14].

We have to comment on the theory applied to produce values of $R_p$ in Fig. 2 from the $2s - 8s/8d/12d$ transitions. As we have explained, we use for the extraction basically the same theory, a theory of the Lamb shift in hydrogen. There is a small difference in theoretical expressions because we studied different $2s - nl$ transitions. Since $n$ is rather high ($n = 8, 12$), we find that details of the theory of the higher excited states $8s, 8d, 12d$ are rather of marginal importance for the accuracy of the extraction. In other words, a small inconsistency, which shows up in the extraction, already exists in the experimental data of two experiments [13] and [14], since all the transitions are evaluated in approximately the same way. In particular, one can find an effective value of the frequency for the $2s - 8d_{5/2}$ transition in hydrogen from each of ten H or D transitions under question. The results are plotted in Fig. 3. The QED computational uncertainty is substantially below 1 kHz as well as the standard uncertainty (from H & D spectroscopy) due to applied values of the Rydberg constant and the proton radius (cf. [24, 25]). (If one uses a value of the Rydberg constant consistent from H & D spectroscopy) due to applied values of the Rydberg constant and the proton radius (cf. [24, 25]). (If one uses a value of the Rydberg constant consistent with the $\mu$H Lamb shift to find an effective value of the $2s - 8d_{5/2}$ frequency from a $2s - 12d$ transition, such an effective value is to be higher by roughly 1 kHz, which does not remove the systematic pattern).

We expect the value of the proton radius to lie between 0.85 and 0.89 fm. Until the nature of the systematic effect is clarified, we see no conclusive reasons to expect that the spectroscopic value of the proton radius is more than a small inconsistency with the CODATA-2010 all-spectroscopic value.

Contrary to the 1998 edition, we study different $2s - 12d$ transitions. Since $n$ is rather high ($n = 8, 12$), we find that details of the theory of the higher excited states $8s, 8d, 12d$ are rather of marginal importance for the accuracy of the extraction. In other words, a small inconsistency, which shows up in the extraction, already exists in the experimental data of two experiments [13] and [14], since all the transitions are evaluated in approximately the same way. In particular, one can find an effective value of the frequency for the $2s - 8d_{5/2}$ transition in hydrogen from each of ten H or D transitions under question. The results are plotted in Fig. 3. The QED computational uncertainty is substantially below 1 kHz as well as the standard uncertainty (from H & D spectroscopy) due to applied values of the Rydberg constant and the proton radius (cf. [24, 25]). (If one uses a value of the Rydberg constant consistent with the $\mu$H Lamb shift to find an effective value of the $2s - 8d_{5/2}$ frequency from a $2s - 12d$ transition, such an effective value is to be higher by roughly 1 kHz, which does not remove the systematic pattern).

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accurate. Indeed, the suggested constraint still does not agree literally with the muonic-hydrogen value, however, the discrepancy is not statistically significant. It is also important that two LKB experiments are correlated. It is possible that both series are affected by the same systematic effect and the true value of the proton radius from the H & D spectroscopy might be considered as disputable. One may in principle object our estimation of the required expansion, but not the presence of a systematic effect by itself. The latter must require a certain extension of the uncertainty. In spite of the apparent presence of a systematic effect, it would be helpful if the LKB experiments will be re-done in one or other way, in order to check whether their results are reproducible. (Indeed, a competitive independent measurements of any transition in hydrogen and deuterium would be also greatly appreciated to resolve the problem.)

The systematic pattern in the distribution of the individual results in Figs. 2 and 3 has not drawn attention previously in part because the overall procedure has a good $\chi^2$ value, thanks to the less accurate determinations and thanks to the fact that the ten questionable transitions produce a non-random distribution with all the data being roughly one sigma above [13] or below [14] the average value. We also note, that the attention was for various reasons concentrated on internal consistency of the pure hydrogenic data (cf., e.g., [14]) As for the hydrogen values by themselves, the difference between the results of [13] and [14] is not that statistically significant.

Concluding, the distribution of the data for the LKB experiments [13] and [14] shows perfect internal agreement between different measurements within each group and a small, but clear difference between the two groups of the data, apparently caused by a certain systematic effect. The effect should be understood before making any statement about a contradiction between the results on the proton radius from spectroscopy of muonic and ordinary atoms.

The question of an expansion of the uncertainty for the derived value of the proton radius from the H & D spectroscopy might be considered as disputable. One may in principle object our estimation of the required expansion, but not the presence of a systematic effect by itself. The latter must require a certain extension of the uncertainty. In spite of the apparent presence of a systematic effect, it would be helpful if the LKB experiments will be re-done in one or other way, in order to check whether their results are reproducible. (Indeed, a competitive independent measurements of any transition in hydrogen and deuterium would be also greatly appreciated to resolve the problem.)

The result of the systematic effect is not a ‘contradiction’ between different parts of the optical data. We should rather speak about a ‘tension’ between the data. However, it crucially affects the accuracy of any overall statistical evaluation of the data. Actually, it rather prevents it at a desirable level of accuracy. The level of accuracy below one percent for the radius cannot be claimed until the effect is understood. The present situation on this issue is summarized in Fig. 4.

With such an extended understanding of the uncertainty of the spectroscopic value, the contradiction is now between the muonic result and the elastic-scattering results [6, 7] only. Those scattering results have been obtained by somewhat different techniques, and, in particular, the MAMI cross sections were measured in arbitrary units in [7], while the world data, evaluated in [6], were obtained from absolute measurements. Nevertheless, the fitting procedure has various features in common. We cannot claim any longer that the muonic value disagrees with results, obtained by a few independent methods. The discrepancy in the determination of the proton radius might in principle be attributed to underestimation of the systematic uncertainty due to the fitting procedure.

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