Theory of the hydrogen–deuterium isotope shift

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We present an overview of the contributions to the isotope shift of the $1S$-$2S$ transition between hydrogen and deuterium. We have calculated an additional contribution to the energy, due to the exchange of a virtual transverse photon between the electron and the deuteron. We also correct the previously evaluated finite-size and recoil contributions [F. Schmidt-Kaler *et al.*, Phys. Rev. Lett. **70**, 2261 (1993)]. Our result is 670 994 445(33) kHz, which is in disagreement with the experimental value of 670 994 337(22) kHz. This discrepancy is probably caused by an incorrect value for the deuteron radius.

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I. INTRODUCTION

Recent advances in Doppler-free two-photon spectroscopy of the $1S$-$2S$ transitions in hydrogen and deuterium [1] make possible a precise measurement of the isotope shift. The most recently measured value is

$$\nu_{\rm expt} = \nu_D - \nu_H = 670\,994\,337(22)\ \text{kHz}. \tag{1}$$

Taking into account the difference in the reduced mass, the difference in the nuclear charge radii, and the deuteron polarizability, we find a theoretical value for the isotope shift

$$\nu_{\rm theo} = 670\,994\,445(33)\ \text{kHz}. \tag{2}$$

The above 33 kHz error comes from the 14 kHz uncertainty in electron–proton mass ratio and the 19 kHz uncertainty in the difference of the square charge radius of deuteron and proton. The apparent discrepancy in the above results makes a new and more precise measurement of the deuteron and proton radii neccesary. A considerable improvement of the experimental precision of the H–D isotope shift to about 1 kHz should be possible in the near future.

We present in this paper all contributions to the isotope shift at the level of 1 kHz for S states. We follow the comprehensive review of Sapirstein and Yennie in [2] and add some recently evaluated corrections: nonradiative nuclear recoil [5], and nuclear polarizability due to Coulomb interaction [6]. The calculation of an additional polarizability contribution due to the exchange of a transverse photon between the electron and deuteron is also presented. The whole polarizability correction gives a contribution of 19 kHz to the $1S$-$2S$ isotope shift and is included in the theoretical value stated above.

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We use physical constants from the 1986 adjustment [3], except for the more recent determination of the Rydberg constant [4].

$$R_\infty = 10\,973\,731.568\,41(42)\ \text{m}^{-1}, \tag{3}$$
$$c = 299\,792\,458\ \text{m}\,\text{s}^{-1}, \tag{4}$$
$$\alpha^{-1} = 137.035\,989\,5(61), \tag{5}$$
$$\frac{M_p}{m_e} = 1836.152\,701(37), \tag{6}$$
$$\frac{M_d}{M_p} = 1.999\,007\,496(6), \tag{7}$$

II. CONTRIBUTIONS TO ISOTOPE SHIFT

The dominating contribution to the isotope shift is due to the mass difference between the proton and deuteron. The main part of this is a reduced-mass correction and is calculated by taking the difference in the following term [2] between hydrogen and deuterium,

$$E_{\rm RM} = \mu\,[f(n)-1] - \frac{\mu^2}{2(m+M)}\,[f(n)-1]^2\,, \tag{8}$$

where m, M, μ are electron, nucleus, and reduced mass, respectively. $f(n)$ is a dimensionless Dirac energy and for S states with a principal number n is given by

$$f(n) = \left(1 + \frac{(Z\alpha)^2}{\left(n-1+\sqrt{1-(Z\alpha)^2}\right)^2}\right)^{-\frac{1}{2}}. \tag{9}$$

The first term in (8) is a Dirac energy with the reduced mass, and the second term is an additional correction coming from the one–photon kernel in the effective two-body equation. This formula does not, however, incorporate all corrections of this type: the remainder which comes from higher-order kernels in the two-body equation, gives contributions of order $\frac{m}{M}(Z\alpha)^5$ and $\frac{m}{M}(Z\alpha)^6$.

These are named the nonradiative nuclear recoil correction and will be given later in this paper. After evaluation of the energy difference $E_{\rm D}(2S\text{-}1S) - E_{\rm H}(2S\text{-}1S)$ we obtain

$$\Delta E_{\rm RM} = 671\,004\,059(14)\ \text{kHz}\,. \tag{10}$$

The mass difference also causes a shift in the electron self–energy and the vacuum polarization. The main part of this can be obtained by replacing the electron mass by the reduced mass in the formula for one– and two–loop (nonrecoil) contributions to Lamb shift [the terms of higher order in $(Z\alpha)$ such as A_{60}, A_{61}, A_{62} are neglected]:

$$E_{\rm QED} = \frac{m\,\alpha\,(Z\,\alpha)^4}{\pi\,n^3}\left(\frac{\mu}{m}\right)^3 \times\left(A_{40} + A_{41}\ln\left[\frac{m}{\mu}(Z\,\alpha)^{-2}\right] +(Z\,\alpha)A_{50} + \frac{\alpha}{\pi}\,B_{40}\right), \tag{11}$$

$$A_{40} = \frac{10}{9} - \frac{4}{15} - \frac{4}{3}\ln\left[k(n)\right]\,, \tag{12}$$

$$A_{41} = \frac{4}{3}\,, \tag{13}$$

$$A_{50} = 4\,\pi\left(\frac{139}{128} + \frac{5}{192} - \frac{\ln(2)}{2}\right)\,, \tag{14}$$

$$B_{40} = -\frac{4358}{1296} - \frac{10}{27}\pi^2 + \frac{3}{2}\pi^2\,\log(2) - \frac{9}{4}\zeta(3)\,, \tag{15}$$

where $\ln[k(n)]$ is the Bethe logarithm, which for $1S$ and $2S$ states amounts to

$$\ln\left[k(1)\right] = 2.984\,128\,555\,9\,, \tag{16}$$

$$\ln\left[k(2)\right] = 2.811\,769\,893\,2\,. \tag{17}$$

This correction gives for the isotope shift of $1S$-$2S$

$$\Delta E_{\rm QED} = -5562\ \text{kHz}\,. \tag{18}$$

The nonradiative (only exchange photons) nuclear recoil contribution in $(Z\alpha)^5$ order for arbitrary nucleus mass has the form [7]

$$E_{\rm RS} = \frac{\mu^3}{m\,M}\frac{(Z\,\alpha)^5}{\pi\,n^3}\left\{\frac{2}{3}\ln\left(\frac{1}{Z\,\alpha}\right) - \frac{8}{3}\ln\left[k(n)\right] - \frac{1}{9} - \frac{7}{3}\,a_n - \frac{2}{M^2-m^2}\left[M^2\ln\left(\frac{m}{\mu}\right) - m^2\ln\left(\frac{M}{\mu}\right)\right]\right\}, \tag{19}$$

$$a_n = -2\left[\ln\left(\frac{2}{n}\right) + \left(1 + \frac{1}{2} + \cdots + \frac{1}{n}\right) + 1 - \frac{1}{2\,n}\right]\,. \tag{20}$$

This contribution adds to the isotope shift of $1S$-$2S$ the amount

$$\Delta E_{\rm RS} = 1033\ \text{kHz}\,. \tag{21}$$

The radiative recoil contribution, which is not covered by the simple mass replacement in (11), in $\frac{m}{M}\alpha(Z\,\alpha)^5$ order is [8]

$$E_{\rm RR} = \frac{\alpha\,(Z\,\alpha)^5}{n^3}\,\frac{m^2}{M}\left(\frac{35}{4}\ln(2) - \frac{7333}{960} - 0.415\right)\,, \tag{22}$$

and gives for the isotope shift of $1S$-$2S$

$$\Delta E_{\rm RR} = -9\ \text{kHz}\,. \tag{23}$$

The most difficult part of the evaluation is the nonradiative recoil contribution of order $\frac{m}{M}\,(Z\,\alpha)^6$. This has been calculated recently, in the context of the $(2S$-$2P)$ Lamb shift, by Doncheski, Grotch, and Ericson [5]:

$$E_{\rm RE} = \frac{m^2}{M}\frac{(Z\,\alpha)^6}{n^3}\left[\frac{5}{2} - \ln\left(\frac{2}{\alpha}\right) + 2\ln\left(\frac{1}{\alpha}\right) - 4.25\right]\,. \tag{24}$$

Although it was not stated in their paper, which we have checked by solving the single-photon-kernel two-body equation, this contribution complements the formula (8) in $\frac{m}{M}\,(Z\,\alpha)^6$ order for the S-state energy shift. This contribution amounts for the $1S$-$2S$ isotope shift to

$$\Delta E_{\rm RE} = 11\ \text{kHz}\,. \tag{25}$$

The nucleus-finite-size energy shift is given by

$$E_{\rm FS} = \frac{2}{3\,n^3}\,(Z\alpha)^4\,\mu^3\,\langle r^2\rangle\,. \tag{26}$$

For evaluation of the difference of charge square radii r^2 we take results from [9], where a careful evaluation of the deuteron mean–square matter radius based on the existing electron-deuteron scattering data has been performed.

$$r_{Ed} = 1.953(3)\ \text{fm}\,. \tag{27}$$

After combining this result with the mean–square neutron radius

$$r_n^2 = -0.1192(18)\ \text{fm}^2\,, \tag{28}$$

into formula (1.1) from that paper, we obtain

$$\langle r^2\rangle = r_{\rm ch}^2 - r_p^2 = r_{Ed}^2 + r_n^2 + \frac{3}{4}\frac{1}{M_p^2} = 3.728(14)\ \text{fm}^2\,. \tag{29}$$

Although the dependence on the proton charge radius cancels to the first order in m/M, it contributes to the small nuclear mass dependent part (about 3 kHz). Inserting the square charge radius difference, together with proton radius $r_p = 0.862(12)$ fm, we obtain for the $1S$-$2S$ isotope shift

$$\Delta E_{\rm FS} = -5107(19)\ \text{kHz}. \tag{30}$$

The last contribution listed in this paper is due to the deuteron polarizability (the proton polarizability gives a neglible shift of the order of 30 Hz [6]). Its main contribution due to exchange of a Coulomb photon, has been evaluated in [6] and has the form

$$\Delta E = -4\, m\, \alpha\, \phi(0)^2\, \alpha_d \left[1 + \ln\left(2\frac{\overline{E}}{m}\right)\right], \tag{31}$$

where α_d is a deuteron polarizability and $\overline{E}$ is an average deuteron excitation energy

$$\alpha_d = 0.635\ \text{fm}^3, \tag{32}$$

$$\overline{E} = 4.915\ \text{MeV} \approx 2\, E_{\rm binding}. \tag{33}$$

The additional polarizability correction, the evaluation of which we now present, is due to the exchange of a transversal photon. The diagrams are given in Fig. 1, where the wavy lines denote a spatial part of the photon propagator in the Coulomb gauge, and the two straight lines denote electron and proton (with the reduced mass) propagators. In a simplified picture we can imagine the deuterium as a system of two atoms: the first is a proton-neutron atom and the second is an electron in the average Coulomb field from the proton. If we have two atoms, far away, they interact by fluctuation of dipole moments (van der Waals forces) or by photon exchange. In our case the distance is zero but the nature of forces is the same.

The expression related to these diagrams is

$$\begin{aligned}\Delta E = i \int_{C_F} \frac{d\omega}{2\pi} \int d^3x_1\, d^3x_2 d^3x_1' d^3x_2' \\ \times \Big\{ \bar\psi(\mathbf{x}_1)\, (-i\, e\, \gamma^i)\, i\, S(\mathbf{x}_1, \mathbf{x}_2, E_\psi - \omega)\, (-i\, e\, \gamma^j)\, \psi(\mathbf{x}_2) \\ \times \phi(\mathbf{x}_1') \left(-i\, e\, \frac{p^{i'}}{M}\right) i\, S_d(\mathbf{x}_1', \mathbf{x}_2', E_\phi - \omega) \left(-i\, e\, \frac{p^{j'}}{M}\right) \phi(\mathbf{x}_2')(-i) G_{ij'}(\mathbf{x}_1 - \mathbf{x}_2', \omega)\, (-i)\, G_{i'i}(\mathbf{x}_1' - \mathbf{x}_2, \omega) \\ + \bar\psi(\mathbf{x}_1)\, (-i\, e\, \gamma^i)\, i\, S(\mathbf{x}_1, \mathbf{x}_2, E_\psi + \omega)\, (-i\, e\, \gamma^j)\, \psi(\mathbf{x}_2) \\ \times \phi(\mathbf{x}_1') \left(-i\, e\, \frac{p^{i'}}{M}\right) i\, S_d(\mathbf{x}_1', \mathbf{x}_2', E_\phi - \omega) \left(-i\, e\, \frac{p^{j'}}{M}\right) \phi(\mathbf{x}_2')(-i) G_{ii'}(\mathbf{x}_1 - \mathbf{x}_1', \omega)\, (-i)\, G_{jj'}(\mathbf{x}_2 - \mathbf{x}_2', \omega) \Big\},\end{aligned} \tag{34}$$

where

$$S(\mathbf{x}_1, \mathbf{x}_2, E) = \langle x_1 | \frac{1}{p\cdot\gamma - m} | x_2 \rangle. \tag{35}$$

S_d is a nonrelativistic proton propagator with the reduced mass in the effective proton–neutron potential; ψ, E_ψ and ϕ, E_ϕ are the electron and the proton wave functions and energies, respectively. G_{ij} is defined by

$$G_{ij} = -\frac{1}{k^2}\left(\delta_{ij} - \frac{k^i\, k^j}{\mathbf{k}^2}\right). \tag{36}$$

Since the deuteron radius r_{Ed} is much smaller than the electron Compton wavelength λ_e, we perform the dipole approximation, which means that we neglect $\mathbf{x}_1'\, \mathbf{x}_2'$ in arguments of the photon propagator. Making use of a relation for the proton matrix element

$$\begin{aligned}\langle\phi| \frac{p^i}{M}\, \frac{1}{E_\phi - \omega - H_d}\, \frac{p^j}{M} |\phi\rangle \\ = \delta^{ij}\, \frac{1}{3} w^2\, \langle\phi| r^k\, \frac{1}{E_\phi - \omega - H_d}\, r^k |\phi\rangle\end{aligned} \tag{37}$$

and replacing $\psi(r)$ by $\psi(0)$ we arrive at the expression for the energy shift

$$\begin{aligned}\Delta E = i\, e^4 \int \frac{d\omega}{2\pi}\, f(\omega)\, \frac{1}{3} w^2\, \langle\phi| r^k \\ \times \frac{1}{E_\phi - \omega - H_d}\, r^k |\phi\rangle,\end{aligned} \tag{38}$$

where

$$\begin{aligned}f(\omega) = \int \frac{d^3k}{(2\pi)^3}\, \frac{1}{(\omega^2 - \mathbf{k}^2)^2} \left(\delta_{ij} - \frac{k^i\, k^j}{\mathbf{k}^2}\right) \\ \times \mathrm{Tr}\left[\gamma^i \left(\frac{1}{\not p - \not k - m} + \frac{1}{\not p + \not k - m}\right) \right. \\ \left. \times \gamma^j\, \frac{(\gamma^0 + I)}{4}\right]\end{aligned} \tag{39}$$

$$= \frac{1}{8\pi\,\Omega\,\omega}\, [2\,\omega + \Omega\, (X' - X)] \tag{40}$$

and

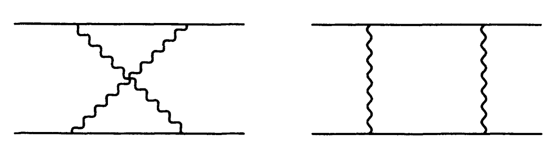

FIG. 1. Feynman diagrams representing the exchange of a virtual transversal photon between the deuteron and electron.

$$\Omega = \sqrt{-\omega^2}\,,$$
$$X = \sqrt{2\,\omega - \omega^2}\,,$$
$$X' = \sqrt{-2\,\omega - \omega^2}\,. \qquad (41)$$

For the final ω integration, we change the Feynman contour in such a way that it encircles the positive real axis. On this axis we have branch cuts only from Ω, X, X'. We may thus rewrite (38) in the form

$$\Delta E = e^4 \int_0^\infty \frac{d\omega}{2\pi i}\, f(\omega + i\,\epsilon)\, \frac{\omega^2}{3} \times \langle\phi| r^k \frac{1}{H_d - E_\phi + \omega} r^k |\phi\rangle + \text{c.c.} \qquad (42)$$

For the part of the contour above the postitive real axis we have

$$\Omega = -i\,\omega\,, \qquad (43)$$
$$X = -i\,\sqrt{\omega^2 - 2\,\omega}\,\Theta(\omega - 2) + \sqrt{2\,\omega - \omega^2}\,\Theta(2 - \omega)\,, \qquad (44)$$
$$X' = -i\,\sqrt{\omega^2 + 2\,\omega}\,. \qquad (45)$$

After performing the ω integration and expanding in the ratio

$$\frac{m}{H_d - E_\phi} \leq \frac{1}{5}\,, \qquad (46)$$

we obtain

$$\Delta E = -2\,m\,\alpha\,\phi(0)^2\,\frac{2}{3}\,\alpha\langle\phi|\mathbf{x}\frac{1}{H_d - E_\phi}\left(-\frac{5}{12} + \frac{1}{2}\ln\left[2(H_d - E_\phi)\right]\right)\mathbf{x}|\phi\rangle$$
$$= -m\,\alpha\,\phi(0)^2\,\alpha_d\left(-\frac{5}{6} + \ln(2\,\bar{E})\right) = -2.3\ \text{kHz}\,. \qquad (47)$$

The terms from the Coulomb and transversal photon exchange sum to

$$E_{\rm pol} = -m\,\alpha\,\phi(0)^2\,\alpha_d\left(\frac{19}{6} + 5\,\ln(2\,\bar{E})\right)\,. \qquad (48)$$

The main uncertainty in $E_{\rm pol}$ comes from the determination of α_d and expansion in $m/(H-E_d)$ ratio. For the latter, the next-to-leading term in (31) is $[m/(H_d - E_d)]^2 < 1/25$, which gives an error of the order of 1 kHz for the $1S$ state. For α_d the different models ([10] and references therein) give results in the range 0.62–0.64, and the experimental determinations give 0.70(5) and 0.61(4). Thus, we can assume the uncertainty in $\alpha_d = 0.635$ to be 0.030, which gives an error of 1 kHz. As a final uncertainty for the $1S$-energy shift we have a value of 2 kHz. For the $2S$-$1S$ difference we obtain

$$\Delta E_{\rm pol} = 19(2)\ \text{kHz}\,. \qquad (49)$$

The sum of all contributions is

$$\Delta E = \Delta E_{\rm RM} + \Delta E_{\rm QED} + \Delta E_{\rm RS} + \Delta E_{\rm RR} + \Delta E_{\rm RE} + \Delta E_{\rm FS} + \Delta E_{\rm pol} = 670\,994\,445(33)\ \text{kHz}\,. \qquad (50)$$

III. CONCLUSIONS

The difference between the new theory and the measurement of reference [1] is

$$\nu_{\rm theo} - \nu_{\rm expt} = 108(33)(22)\ \text{kHz}\,, \qquad (51)$$

where the first error comes from the electron–proton mass ratio and uncertainty in rms radius difference, and the second from the experiment [1]. This surprisingly large difference is probably caused by an incorrect value of the deuteron matter radius r_{Ed}. To determine r_{Ed} from electron-scattering-data experimental data, a model potential for the deuteron has to be assumed. As was stated in Ref. [9], such models, when fitted to the radius, give inconsistent results for low energy neutron–proton effective-range parameters. This suggests that more experimental and theoretical work is neccesary for a reliable determination of r_{Ed} from the electron–deuteron scattering. A very recent analysis of an electron–deuteron scattering experiment in Saclay [11] suggests a higher value for the deuteron structure radius, although this experiment has been performed at too high momentum transfer to extract a precise value for this radius.

From the experimental value of the hydrogen-deuterium isotope shift of $1S$-$2S$ we could determine the difference in mean-square charge radius between the deuteron and proton

$$r_{\rm ch}^2 - r_p^2 = 3.807(26)\,, \qquad (52)$$

which also gives a higher value for the deuteron charge radius [cf. (29)].

A new and more precise experiment in Garching for the $1S$-$2S$ isotope shift should reduce the second error in (51) to as low as 1 kHz, leaving the determination of the proton and deuteron radii as the main obstacle to achieving high precision Lamb shift tests of QED. Alternatively, one could regard such an experiment as a measurement of the nuclear radius. After evaluation of all remaining two-loop binding corrections to the Lamb shift, such a radius determination will be available from precise measurements of the $2S$-$2P$ transition, and two-photon transitions in hydrogen and deuterium for different S states.

Comparison of these results with the directly measured charge square nuclear radius may be regarded as a way to test the compatibility of high- and low-energy experimental results.

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