RAPID COMMUNICATIONS

PHYSICAL REVIEW A

ATOMIC, MOLECULAR, AND OPTICAL PHYSICS

THIRD SERIES, VOLUME 48, NUMBER 1 JULY 1993

RAPID COMMUNICATIONS

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Nuclear-structure correction to the Lamb shift

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(Received 9 March 1993)

In this paper the second-order nuclear-structure correction to the energy of hydrogenlike systems is estimated and previous results are corrected. Both deuterium and hydrogen are considered. In the case of deuterium the correction is proportional to the nuclear polarizability and amounts to about −19 kHz for the $1S$ state. For hydrogen the resulting energy shift is about −60 Hz.

PACS number(s): 32.30.Jc, 12.20.Ds

Recent advances in the experimental precision of laser spectroscopy on atomic hydrogen and deuterium [1–3] make it possible to compare theory and measured values up to an accuracy where effects that have been neglected so far start to play a role. The isotope shift of the $1S$-$2S$ transition in atomic hydrogen and deuterium was directly measured [2] with the help of a novel ultrafast electro-optic modulator [4]. The result of 670 994.337(22) MHz has an uncertainty 25 times smaller than the previous best experimental value [5]. It is comparable to the precision of the theoretical value of 670 994.414(18) MHz (without the nuclear-structure contribution) that is limited by the uncertainty in the charge radii difference.

In this paper the second-order energy correction due to the nuclear structure, which is expected to explain the difference in theoretical and experimental results, is estimated, and it is pointed out that the experimental accuracy needed to resolve these corrections in an isotope shift measurement is on the horizon, provided the quadratic charge radii are better known. There is a proposal of Taqqu [7] to improve the accuracy of these values by measurements with muonic atoms. If this is done, the nuclear properties could be measured by high-resolution spectroscopy in a domain of relative momentum of nucleus and electron that is intrinsically inaccessible to collider experiments.

The second-order nuclear-structure correction for light atoms has been analyzed in detail in the context of the hydrogen hyperfine structure, but there is no similar analysis for the Lamb- or isotope-shift problem, mainly due to the smallness of this effect. One paper [8] on this problem gives an incorrect estimation, as was noticed by Sapirstein [9], because the *crossed graph* [the second term in Eq. (15)] was not included. In another paper [10] only the heavy atoms are considered.

We start from the nonrelativistic treatment of the deuterium structure correction, to show that the relativistic electron momentum dominates in the sum over intermediate states. The second-order correction to the energy is given by the formula [11]

$$\Delta E^{(2)} = -\left\langle \psi\phi \left| V \frac{1}{H_d + H_e - E_d^0 - E_e^0} V \right| \phi\psi \right\rangle , \qquad (1)$$

where H_d is the internal deuteron Hamiltonian, H_e is the electron Hamiltonian in the pointlike source of the Coulomb field,

$$H_e = \frac{p^2}{2m} - \frac{\alpha}{r} , \qquad (2)$$

and E_d^0, E_e^0, ψ, ϕ are ground-state energies and wave functions of the deuteron and the electron, respectively. For simplicity we put $\hbar = c = 1$. The interaction Hamiltonian V has the form

$$V = -\alpha \left(\frac{1}{r} - \frac{1}{|\frac{1}{2}\mathbf{R} - \mathbf{r}|} \right) , \qquad (3)$$

where R is the distance between the proton and the neutron in the deuteron. In other words, R describes the actual position of the charge because the proton is treated as a pointlike particle. The recoil effects are partially included in the definition of p and r as relative electron coordinates with respect to the center of deuterium mass, and of m as a reduced electron mass. As the first step the electron matrix element P is considered. Denoting the difference

$$H_d - E_d^0 = \Lambda , \qquad (4)$$

one has

$$P=\left\langle\phi\left|V\frac{1}{\Lambda+H_e-E_e^0}V\right|\phi\right\rangle$$
$$=\alpha^2\left\langle\phi\left|\left(\frac{1}{r}-\frac{1}{|\frac{1}{2}\mathbf{R}-\mathbf{r}|}\right)\frac{1}{\Lambda+H_e-E_e^0}\left(\frac{1}{r}-\frac{1}{|\frac{1}{2}\mathbf{R}'-\mathbf{r}|}\right)\right|\phi\right\rangle . \tag{5}$$

This matrix element depends on α. Since α is small we expand in it and take only the leading term. This expansion is equivalent to the following replacements:

$$\phi(r)\to\phi(0)\,, \tag{6}$$
$$H_e\to\frac{p^2}{2m}\,, \tag{7}$$
$$E_e^0\to 0\,. \tag{8}$$

After these replacements P becomes,

$$P=\alpha^2\phi(0)^2\int\frac{d^3q}{(2\pi)^3}\left(\frac{4\pi}{q^2}\right)^2\frac{1}{\Lambda+q^2/(2m)}\left(1-e^{\frac{i}{2}\mathbf{q}\cdot\mathbf{R}}\right)\left(1-e^{-\frac{i}{2}\mathbf{q}\cdot\mathbf{R}'}\right) . \tag{9}$$

Because the electron is treated nonrelativistically its momentum should be somehow limited. The simplest way is the condition $|\mathbf{q}|<m$. This inequality implies

$$\mathbf{q}\cdot\mathbf{R}\approx mR_d=5.5\times10^{-3}\ll 1, \tag{10}$$

where $R_d=2.12$ fm is the deuteron radius; hence one can apply the dipole approximation. Since the lowest value of Λ is the binding energy E_B [cf. (26)]

$$m/\Lambda<0.2\ll 1, \tag{11}$$

one obtains for the electron matrix element P

$$P=\alpha^2\phi(0)^2\frac{1}{\Lambda}\int^m\frac{d^3q}{(2\pi)^3}\left(\frac{4\pi}{q^2}\right)^2\frac{\mathbf{q}\cdot\mathbf{R}}{2}\,\frac{\mathbf{q}\cdot\mathbf{R}'}{2}$$
$$=\frac{2}{3}\alpha^2\phi(0)^2m\frac{\mathbf{R}\cdot\mathbf{R}'}{\Lambda}\,. \tag{12}$$

Inserting this expression into (1), ΔE becomes

$$\Delta E=-\frac{2}{3}\left\langle\psi\left|\mathbf{R}\frac{1}{H_d-E_d^0}\mathbf{R}\right|\psi\right\rangle m\alpha^2\phi(0)^2$$
$$=-4\,m\,\alpha\,\phi(0)^2\,\alpha_d\,, \tag{13}$$

where α_d denotes the deuterium polarizability and will be calculated later.

From this nonrelativistic consideration, one sees that the relativistic electron momentum plays the dominant role in the energy shift, because without a cutoff the integral in (9) will strongly diverge. Thus one should treat the electron in a relativistic manner. The correction to the energy shift is now given by the formula

$$\Delta E=\sum_{n,m}\frac{|\langle\psi\phi|V\gamma_0|\phi_n\psi_m\rangle|^2}{E_e^0-E_n^+-\Lambda_m}+\frac{|\langle\psi\phi|V\gamma_0|\phi_n\psi_m\rangle|^2}{E_e^0-E_n^-+\Lambda_m} \tag{14}$$
$$=\sum_m\langle\psi\phi|V\gamma_0\,S^+(E_e^0-\Lambda_m)V\gamma_0|\phi\psi\rangle$$
$$+\langle\psi\phi|V\gamma_0\,S^-(E_e^0+\Lambda_m)V\gamma_0|\phi\psi\rangle\,, \tag{15}$$

where Λ_m is the deuteron energy level with respect to the ground state and E_n^+ and E_n^- are positive and negative eigenvalues of the Dirac Hamiltonian, respectively. In the lowest order in α one can replace $\phi(r)$ by $\phi(0)$ and neglect α in the Coulomb-Dirac Hamiltonian; thus $H=\boldsymbol{\alpha}\cdot\mathbf{p}+\beta m$ and

$$S^+(E)=\frac{E_q+H}{2E_q}\frac{1}{E-E_q}\gamma_0\,, \tag{16}$$
$$S^-(E)=\frac{E_q-H}{2E_q}\frac{1}{E+E_q}\gamma_0\,, \tag{17}$$

with $E_q=\sqrt{q^2+m^2}$.

Hence for the electron matrix element P one obtains

$$P=\langle\phi|V\gamma_0\left(S^+(E_e^0-\Lambda)+S^-(E_e^0+\Lambda)\right)V\gamma_0|\phi\rangle$$
$$=\alpha^2\phi(0)^2\int\frac{d^3q}{(2\pi)^3}\left(\frac{4\pi}{q^2}\right)^2\left(1-e^{\frac{i}{2}\mathbf{q}\cdot\mathbf{R}}\right)\left(1-e^{-\frac{i}{2}\mathbf{q}\cdot\mathbf{R}'}\right)\left(\frac{E_q+m}{2\,E_q}\frac{1}{m-\Lambda-E_q}+\frac{E_q-m}{2\,E_q}\frac{1}{m+\Lambda+E_q}\right) . \tag{18}$$

Among the arguments of P, R^{-1} is much larger than m and Λ; thus one can expand in R, and it is equivalent to the dipole approximation

$$P=\alpha^2\,\phi(0)^2\frac{\mathbf{R}\cdot\mathbf{R}'}{12}\int\frac{d^3q}{(2\pi)^3}\frac{(4\pi)^2}{q^2}\left(\frac{E_q+m}{2\,E_q}\frac{1}{m-\Lambda-E_q}+\frac{E_q-m}{2\,E_q}\frac{1}{m+\Lambda+E_q}\right) . \tag{19}$$

Since (11) holds, one also expands in m/Λ and obtains for P

$$P=-\alpha^2\phi(0)^2\,\frac{2}{3}\frac{m}{\Lambda}\left[1+\ln\left(2\frac{\Lambda}{m}\right)\right]\mathbf{R}\cdot\mathbf{R}'\,. \tag{20}$$

Hence for the energy shift one has

$$\Delta E = -m\,\alpha^2\phi(0)^2\,\frac{2}{3}\left\langle\psi\left|\mathbf{R}\,\frac{1}{H-E_0}\left[1+\ln\left(2\frac{(H-E_0)}{m}\right)\right]\mathbf{R}\right|\psi\right\rangle . \tag{21}$$

The first term in square brackets in the above expression reproduces the previously obtained nonrelativistic result.

If we replace the energy difference in the logarithm by the average energy $\overline{E} = H - E_0$, the energy shift becomes

$$\Delta E = -4\,m\,\alpha\,\phi(0)^2\,\alpha_d\left[1+\ln\left(2\frac{\overline{E}}{m}\right)\right], \tag{22}$$

where α_d was defined previously and denotes the deuteron polarizability

$$\alpha_d = \frac{2}{3}\,\alpha\left\langle\psi\left|\frac{1}{2}\mathbf{R}\,\frac{1}{H-E_0}\,\frac{1}{2}\mathbf{R}\right|\psi\right\rangle . \tag{23}$$

To calculate α_d and $\overline{E}$ one needs to know something about the deuteron Hamiltonian H. We choose the simplest, with a square well potential for the neutron-proton interaction,

$$H = \frac{p^2}{2\,M} + V(r), \tag{24}$$

$$V = \begin{cases} -V_0 & \text{for } |\mathbf{r}| < R_0, \\ 0 & \text{for } |\mathbf{r}| > R_0, \end{cases} \tag{25}$$

where M here is a reduced proton-neutron mass. The values for E_0, R_0, V_0 are taken to be consistent with the measured values of [12]

$$E_B \equiv -E_0 = 2.226\ \text{MeV}, \tag{26}$$

$$R_0 = 2.04\ \text{fm}, \tag{27}$$

$$V_0 = 35.411\ \text{MeV}. \tag{28}$$

In calculating the polarizability we first find the ground-state wave function

$$\phi^{\text{in}} = A\,e^{-\beta R_0}\,\frac{\sin(\alpha r)}{r}, \tag{29}$$

$$\phi^{\text{out}} = A\,\sin(\alpha R_0)\,\frac{e^{-\beta r}}{r}, \tag{30}$$

and then the eigenstate from the continuum spectrum with the angular momentum $l = 1$:

$$\psi_k^{\text{in}} = B\,j_1(k' r), \tag{31}$$

$$\psi_k^{\text{out}} = 2\,k\,[\cos(\phi)\,j_1(k r) - \sin(\phi)\,n_1(k r)], \tag{32}$$

where $\alpha = \sqrt{2M(V_0 - E_B)}$, $\beta = \sqrt{2ME_B}$, $k' = \sqrt{2\,M\,(E+V_0)}$, $k \equiv \sqrt{2\,M\,E}$, and j_1 and n_1 are the Bessel functions

$$j_1(x) = \frac{\sin(x)}{x^2} - \frac{\cos(x)}{x}, \tag{33}$$

$$n_1(x) = -\frac{\cos(x)}{x^2} - \frac{\sin(x)}{x}. \tag{34}$$

The coefficients A, B, and ϕ are determined by the normalization and continuity conditions. The polarizability and the average energy are then given by the integral

$$\alpha_d = \frac{\alpha}{6}\int_0^\infty \frac{dk}{2\pi}\langle\phi|r|\psi_k\rangle^2\,\frac{1}{E+E_B}, \tag{35}$$

$$\ln\left(2\frac{\overline{E}+E_B}{m}\right) = \frac{\alpha}{6\,\alpha_d}\int_0^\infty \frac{dk}{2\pi}\langle\phi|r|\psi_k\rangle^2\,\frac{1}{E+E_B} \times \ln\left(2\frac{E+E_B}{m}\right). \tag{36}$$

Our calculation gives

$$\alpha_d = 0.635\ \text{fm}^3, \tag{37}$$

$$\overline{E} = 4.915\ \text{MeV} \approx 2\,E_B. \tag{38}$$

The result for α_d coincides with those listed in [13] and is close to the measured value of $\alpha_d = 0.70(5)\ \text{fm}^3$ [14]. Finally, for the second-order nuclear structure correction to the deuterium energy, we obtain

$$\Delta E = -19.45\ \text{kHz}. \tag{39}$$

We would like to stress that this value is only a rough estimation. We performed a quite strong approximation; e.g., we assumed that the proton and neutron were point-like particles, although the proton size $R_p = 0.87$ fm was not much smaller than the deuteron size $R_d = 2.12$ fm [6]. Furthermore we also took a rather crude interaction Hamiltonian and we neglected the electric quadrupole moment of the deuteron.

We now turn to the case of the hydrogen atom. The energy shift can be expressed as

$$\Delta E = \Delta E_r + \Delta E_p, \tag{40}$$

where the first term is a rigid term, i.e., Λ in the denominator in (5) is equal to zero and the second term is a polarizability term. The interaction Hamiltonian V is

$$V = -\alpha\left(\frac{1}{r} - \frac{1}{|\mathbf{R}-\mathbf{r}|}\right), \tag{41}$$

where $\mathbf{R}$ describes the local position of proton charge density. The electron matrix element P for the rigid contribution reads

$$P_r = \alpha^2\,\phi(0)^2\int\frac{d^3q}{(2\pi)^3}\,\frac{(4\pi)^2}{q^4}\,\left(1-e^{i\mathbf{q}\cdot\mathbf{R}}\right)\left(1-e^{-i\mathbf{q}\cdot\mathbf{R}'}\right)\left(\frac{E_q+m}{2\,E_q}\,\frac{1}{m-E_q}+\frac{E_q-m}{2\,E_q}\,\frac{1}{m+E_q}\right)$$
$$= -2\,m\,\alpha^2\,\phi(0)^2\int\frac{d^3q}{(2\pi)^3}\,\frac{(4\pi)^2}{q^6}\,\left(1-e^{i\mathbf{q}\cdot\mathbf{R}}\right)\left(1-e^{-i\mathbf{q}\cdot\mathbf{R}'}\right). \tag{42}$$

After inserting this into (1) the rigid contribution to the energy becomes

$$\Delta E_r = -16 m\alpha^2\,\phi(0)^2 \int_0^\infty dq\,\frac{1}{q^4}[1-F_1(q^2)]^2\,, \tag{43}$$

where F_1 is a proton form factor. We can roughly estimate the value of the above integral by assuming that a proton is a charged sphere with the radius R_p:

$$\Delta E_r = -\frac{2\pi}{5}\,m\alpha^2\phi^2(0)\,R_p^3 \approx -11.25\,\text{Hz}. \tag{44}$$

There is another term from the first-order nuclear size contribution that is of the same order, namely (for the $1S$ state)

$$\Delta E' = \int d^3r\phi^2(0)(-2\,m\alpha\,r)V(r)$$
$$= -\frac{2\pi}{3}\,m\alpha^2\phi^2(0)\,R_p^3 \approx -18.75\,\text{Hz}. \tag{45}$$

The polarizability contribution consists of the sum over the excited states of the proton. All other energies can be neglected with respect to the proton excitation energy Λ. Thus the electron matrix element becomes

$$P_p = \alpha^2\,\phi(0)^2 \int \frac{d^3q}{(2\pi)^3}\left(\frac{4\pi}{q^2}\right)^2 (1-e^{i\mathbf{q}\cdot\mathbf{R}})$$
$$\times(1-e^{-i\mathbf{q}\cdot\mathbf{R}'})\left(-\frac{m}{2E_q\Lambda}\right). \tag{46}$$

The integral over q in the leading order in $m\,R_p$ ($mR_p \approx 5.3\times10^{-3} \ll 1$) is the following:

$$m^2\int d^3q\,\frac{1}{q^4E_q}\left(1-e^{i\mathbf{q}\cdot\mathbf{R}}\right)\left(1-e^{-i\mathbf{q}\cdot\mathbf{R}'}\right)$$
$$= -4\pi\left\{\left(\frac{11}{8}+\frac{C}{3}\right)\mathbf{R}\cdot\mathbf{R}' + \frac{1}{3}\ln\left(\frac{m|\mathbf{R}-\mathbf{R}'|}{2}\right) - \frac{1}{6}R^2\ln\left(\frac{|\mathbf{R}-\mathbf{R}'|}{R}\right) - \frac{1}{6}R'^2\ln\left(\frac{|\mathbf{R}-\mathbf{R}'|}{R'}\right)\right\}. \tag{47}$$

If we neglect the weak logarithmic dependence $\ln|\mathbf{R}-\mathbf{R}'|$ and replace it by $\ln(R_p)$, the R^2 and R'^2 terms in the above equation give no contribution and we obtain for the energy shift,

$$\Delta E_p = 2\alpha\,\phi(0)^2\alpha_p \ln\left(\frac{mR_p}{2}\right), \tag{48}$$

where α_p is the proton polarizability. α_p was recently measured [15] and amounts to $\alpha_p = 10.8(1)\times10^{-4}\,\text{fm}^3$. This contribution gives a correction of about -30 Hz. The sum of second-order contributions $\Delta E'+\Delta E_r+\Delta E_p$ is about -60 Hz, and thus is below experimental observability.

In conclusion the second-order nuclear-structure correction to the energy level can be observable not only for heavy atoms but also for the light ones. In deuterium this correction is mainly governed by the nuclear polarizability, and amounts to about -19 kHz. Because the energy corrections for the deuterium $2S$ state and those for the $1S$ and $2S$ states in hydrogen are much smaller than the latter value, a measurement of the $1S$-$2S$ isotope shift difference between these atoms is mainly sensitive to the $1S$ nuclear-structure correction to the deuterium energy. The present experimental resolution of 22 kHz is nearly sufficient to measure that contribution. So precision spectroscopy is now on the horizon for a new application field, namely to measure nuclear properties and thus complement the hyperfine-structure and collider measurements.

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