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CORRECTIONS TO THE DEUTERIUM HYPERFINE STRUCTURE DUE TO DEUTERON EXCITATIONS

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We consider corrections to the deuterium hyperfine structure originating from the two-photon exchange between the electron and the deuteron, with the deuteron excitations in intermediate states. In particular, the motion of the two intermediate nucleons as a whole is taken into account. The problem is solved in the zero-range approximation. The result is in good agreement with the experimental value of the deuterium hyperfine splitting.

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1. INTRODUCTION

The hyperfine splitting in the deuterium ground state has been measured with high accuracy. The most precise experimental result, obtained with an atomic deuterium maser, is given by [1]

$$\nu_{exp} = 327\,384.352\,522\,2(17)\,\mathrm{kHz}. \tag{1}$$

On the other hand, theoretical calculation including higher-order pure QED corrections gives

$$\nu_{QED} = 327\,339.27(7)\,\mathrm{kHz}. \tag{2}$$

This value was obtained by using the theoretical result for the hydrogen hyperfine splitting in Ref. [2],

$$1\,420\,451.95(14)\,\mathrm{kHz},$$

which does not include the proton structure and recoil radiative correction, and by further combining it with the theoretical ratio of the hyperfine constants in hydrogen and deuterium in [3],

$$4.339\,387\,6(8),$$

based on the ratio of the nuclear magnetic moments and including the reduced mass effect in $|\psi(0)|^2$.

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It was recognized long ago that the discrepancy

$$\nu_{exp} - \nu_{QED} = 45\,\mathrm{kHz} \tag{3}$$

is due to the effects caused by the finite size of the deuteron. Such effects are obviously much larger in deuterium than in hydrogen. The corresponding contributions to the deuterium hyperfine splitting were discussed long ago with some intuitive arguments [4], and then in more detail in Refs. [5–7].

We believe that in the past, the most systematic treatment of such effects, which are due to the electron–deuteron interaction of the second order in α, was performed in Ref. [8]. The effective Hamiltonian of the hyperfine interaction of the second order in $\alpha = e^2/4\pi$ was derived therein from the elastic forward scattering amplitude of virtual photons off the deuteron.

In particular, the low-energy theorem for forward Compton scattering [9–12] was generalized in [8] to the case of virtual photons and a target with an arbitrary spin. The corresponding contribution of the momentum transfers k, bounded from above by the inverse deuteron size $\varkappa = 45.7$ MeV, to the relative correction to the deuterium hyperfine structure is

$$\Delta^d_{el} = \frac{3\alpha}{8\pi}\left(\mu_d - 2 - \frac{3}{\mu_d}\right)\frac{m_e}{m_p}\ln\frac{\varkappa}{m_e}. \tag{4}$$

Here, m_e and m_p are the electron and proton masses respectively and $\mu_d = 0.857$ is the deuteron magnetic moment. The relative corrections Δ are defined here and below as the ratios of the corresponding contributions to the electron–deuteron scattering amplitude to the spin-dependent Born term in this amplitude,

$$T_0 = -\frac{2\pi\alpha}{3m_e m_p}\,\mu_d\,(\boldsymbol{\sigma}\cdot\mathbf{s}), \tag{5}$$

where $\mathbf{s}$ is the deuteron spin.

At larger momentum transfers, $k > \varkappa$, the amplitude of the Compton scattering on a deuteron is just the coherent sum of those amplitudes on the free proton and neutron. This correction is given by

$$\Delta^{pn}_{in} = \frac{3\alpha}{4\pi}\,\frac{1}{\mu_d}\,(\,\mu_p^2 - 2\,\mu_p - 3 + \mu_n^2\,)\,\frac{m_e}{m_p}\,\ln\frac{m_\rho}{\varkappa}, \tag{6}$$

where $\mu_p = 2.79$ and $\mu_n = -1.91$ are the proton and neutron magnetic moments and $m_\rho = 770$ MeV is the usual hadronic scale.

Strong numerical cancellation between Δ_{el} and Δ_{in} is worth mentioning.

The next correction to the deuterium hyperfine structure, obtained in Ref. [8], is induced by the deuteron virtual excitations due to spin currents only. It is given by

$$\Delta^{(1)}_{in} = \frac{3\alpha}{8\pi}\,\frac{(\mu_p-\mu_n)^2}{\mu_d}\,\frac{m_e}{m_p}\,\ln\frac{m_p}{\varkappa}. \tag{7}$$

There is also a correction due to a finite distribution of the deuteron charge and magnetic moment[1)]. In the zero-range approximation used in Ref. [8], this correction is

$$\Delta_f = -\alpha\,\frac{m_e}{3\,\varkappa}\,(1 + 2\ln 2). \tag{8}$$

2. LEADING INELASTIC NUCLEAR CORRECTION TO THE DEUTERIUM HYPERFINE STRUCTURE

The leading inelastic nuclear correction is of the relative order $\alpha\, m_e/\varkappa$ (as well as the Zemach correction (8)). The corresponding effect calculated in Ref. [8] is additionally enhanced by the large factor

$$\mu_p - \mu_n = 4.7.$$

In the present paper, we consider two more effects of the same order $\alpha\, m_e/\varkappa$. Although both of them are proportional to

$$\mu_p + \mu_n = 0.88$$

(and are therefore essentially smaller numerically than the effect considered in [8]), we believe that their investigation is worth being considered.

We use the gauge $A_0 = 0$, where the photon propagator is given by

$$\begin{gathered} D_{im}(\omega,\mathbf{k}) = \frac{d_{im}}{\omega^2 - \mathbf{k}^2}, \\ d_{im} = \delta_{im} - \frac{k_i k_m}{\omega^2}, \quad D_{00} = D_{0m} = 0. \end{gathered} \tag{9}$$

The electron–deuteron nuclear-spin-dependent scattering amplitude generated by the two-photon exchange is

$$T = 4\pi\alpha i\int\frac{d^4k}{(2\pi)^4}\,\frac{d_{im}d_{jn}}{k^4}\,\frac{\gamma_i(\hat{l}-\hat{k}+m_e)\gamma_j}{k^2-2lk}M_{mn}, \tag{10}$$

where $l_\mu = (m_e, 0, 0, 0)$ is the electron momentum. The structure $\gamma_i(\hat{l}-\hat{k}+m_e)\gamma_j$ reduces to $-i\omega\epsilon_{ijl}\sigma_l$, where $\boldsymbol{\sigma}$ is the electron spin. We calculate the nuclear matrix elements entering the deuteron Compton amplitude M_{mn} in the zero-range approximation, which allows us to obtain all the results in a closed analytical form.

The inelastic $1/\varkappa$ contribution to the hyperfine structure is induced by the combined action of the convection and spin currents. Because the convection current is spin-independent, all the intermediate states are triplet ones, as is the ground state. Therefore, the spin current operator

$$\frac{e}{2m_p} i\mathbf{k}\times[\mu_p\boldsymbol{\sigma}_p\exp(i\mathbf{k}\cdot\mathbf{r}_p) + \mu_n\boldsymbol{\sigma}_n\exp(i\mathbf{k}\cdot\mathbf{r}_n)]$$

simplifies to

$$\frac{e}{2m_p}\,i[\mathbf{k}\times\mathbf{s}]\,[\mu_p\exp(i\mathbf{k}\cdot\mathbf{r}_p) + \mu_n\exp(i\mathbf{k}\cdot\mathbf{r}_n)]. \tag{11}$$

In the initial state $|0\rangle$, the deuteron is at rest. But in the excited state, the system of nucleons moves as a whole with the momentum $\mathbf{k}$, and its wave function is therefore given by $|n\rangle\exp(i\mathbf{k}\cdot\mathbf{R})$, where $|n\rangle$ refers to the deuteron internal degrees of freedom and is a function of $\mathbf{r} = \mathbf{r}_p - \mathbf{r}_n$ and $\mathbf{R} = (\mathbf{r}_p + \mathbf{r}_n)/2$ is the deuteron centre-of-mass coordinate. Thus, a typical matrix element of the spin current can be written as

$$\begin{aligned} &\frac{e}{2m_p}\,i\mathbf{k}\times\langle n|\exp(-i\mathbf{k}\cdot\mathbf{R})\mathbf{s}[\mu_p\exp(i\mathbf{k}\cdot\mathbf{r}_p) + \\ &\qquad + \mu_n\exp(i\mathbf{k}\cdot\mathbf{r}_n)]|0\rangle = \\ &= \frac{e}{2m_p}\,i\mathbf{k}\times\langle n|\mathbf{s}[\mu_p\exp(i\mathbf{k}\cdot\mathbf{r}/2) + \\ &\qquad + \mu_n\exp(-i\mathbf{k}\cdot\mathbf{r}/2)]|0\rangle. \end{aligned} \tag{12}$$

1) In the case of hydrogen, this problem was considered many years ago by Zemach [13].

A typical matrix element of the convection current transforms as

$$\frac{e}{2m_p}\langle n|\exp(-i\mathbf{k}\cdot\mathbf{R})\hat{\mathbf{p}}_p\exp(i\mathbf{k}\cdot\mathbf{r}_p)+ \\ +\exp(i\mathbf{k}\cdot\mathbf{r}_p)\hat{\mathbf{p}}_p|0\rangle = \\ =\frac{e}{2m_p}\langle n|\left(\hat{\mathbf{p}}+\frac{\mathbf{k}}{2}\right)\exp(i\mathbf{k}\cdot\mathbf{r}/2)+\exp(i\mathbf{k}\cdot\mathbf{r}/2)\hat{\mathbf{p}}|0\rangle = \\ =\frac{e}{m_p}\langle n|\hat{\mathbf{p}}\exp(i\mathbf{k}\cdot\mathbf{r}/2)|0\rangle, \quad (13)$$

where $\hat{\mathbf{p}}$ acts on the relative coordinate $\mathbf{r}$.

We first take the intermediate states $|n\rangle$ in the corresponding nuclear Compton amplitude to be just plane waves, eigenstates of $\hat{\mathbf{p}}$. We thus take into account all the states with $l \neq 0$, which are free in our zero-range approximation, and in addition the $^3S_1$ wave function in the free form

$$\psi_p(r)=\frac{\sin(pr)}{pr}$$

(the deviation of the $^3S_1$ wave function from the free one is considered below). Then, with the zero-range-approximation deuteron wave function

$$\psi_0(r)=\sqrt{\frac{\varkappa}{2\pi}}\,\frac{\exp(-\varkappa r)}{r}, \quad (14)$$

the only matrix element entering the amplitude is

$$\langle\psi_0\,|\exp(\pm i\mathbf{k}\cdot\mathbf{r}/2)|\mathbf{p}\rangle=\frac{\sqrt{8\pi\varkappa}}{(\mathbf{p}\pm\mathbf{k}/2)^2+\varkappa^2}. \quad (15)$$

Thus the amplitude simplifies to

$$M^{(2)}_{mn}=\left(\frac{e}{2m_p}\right)^2 2\varkappa\omega\int\frac{d\mathbf{p}}{\pi^2}\left\{\frac{\mu_p}{[(\mathbf{p}-\mathbf{k}/2)^2+\varkappa^2]^2}+ \right. \\ \left. +\frac{\mu_n}{[(\mathbf{p}-\mathbf{k}/2)^2+\varkappa^2][(\mathbf{p}+\mathbf{k}/2)^2+\varkappa^2]}\right\}\times \\ \times\frac{2p_m\,i\,\epsilon_{nrs}k_rs_s-2p_n\,i\,\epsilon_{mrs}k_rs_s}{\omega^2-(p^2+k^2/4+\varkappa^2)^2/m_p^2}. \quad (16)$$

Because the motion of the system as a whole is taken into account in the intermediate states, this expression differs from the corresponding one in our previous paper [8] in two respects. First, in [8], the operator $\hat{\mathbf{p}}_p$ in (13) was identified with $\mathbf{p}$, and instead of $2p_{m,n}$ we therefore obtained $(2p-k/2)_{m,n}$ in the analogue of the present formula (16). At present, the term proportional to μ_n in (16) is an odd function of $\mathbf{p}$, and therefore vanishes after integration over $d\mathbf{p}$. Second, the energy difference in the denominator has acquired the contribution $k^2/4m_p$, which is the kinetic energy of the proton–neutron system as a whole, and hence

$$\frac{p^2+\varkappa^2}{m_p}$$

has transformed into

$$\frac{p^2+k^2/4+\varkappa^2}{m_p}.$$

We now substitute (16) in (10) and take the integral over ω under the condition $\omega \gg \varkappa^2/m$. For the relative correction to the hyperfine structure, we obtain

$$\Delta^{(2)}_{in}=\frac{2\alpha\varkappa\mu_p m_e}{\pi^4\mu_d m_p}\iint\frac{d\mathbf{p}\,d\mathbf{k}}{k^4}\times \\ \times\frac{\mathbf{pk}}{[(\mathbf{p}-\mathbf{k}/2)^2+\varkappa^2]^2}\left[\frac{m_p}{p^2+k^2/4+\varkappa^2}-\frac{3}{2k}\right]. \quad (17)$$

The result of integration over $\mathbf{p}$ and then over $\mathbf{k}$ is given by

$$\Delta^{(2)}_{in}=\alpha\,\frac{\mu_p}{\mu_d}\,\frac{m_e}{\varkappa}-\frac{6\alpha}{\pi}\,\frac{\mu_p}{\mu_d}\,\frac{m_e}{m_p}\ln\frac{m_p}{\varkappa}. \quad (18)$$

The logarithmic contribution here originates from integration of the term $3/2k$ in the square brackets in (17) over the range

$$\varkappa^2/m_p \ll k \ll \varkappa.$$

The result (18) differs from the corresponding one in [8] by a term proportional to $\mu_p+\mu_n$, which is relatively small numerically. It is only natural that our present account of the motion of the proton–neutron system as a whole in the intermediate states results in a correction proportional to $\mu_p+\mu_n$.

We now calculate the correction $\Delta^{(3)}_{in}$ corresponding to the effect of deviation of the intermediate $^3S_1$ wave function $\Psi_p(r)$ from the free one. In the zero-range approximation, $\Psi_p(r)$ is given by

$$\Psi_p(r)=\frac{\sin(pr)}{pr}-\frac{1}{\varkappa+ip}\,\frac{\exp(ipr)}{r}= \\ =\frac{\varkappa\sin(pr)-p\cos(pr)}{pr(\varkappa+ip)}. \quad (19)$$

This follows, for instance, from the orthogonality to deuteron wave function (14). Below, we use the function

$$\rho_p(r_1,r_2)=\Psi_p(r_1)\Psi^*_p(r_2)-\psi_p(r_1)\psi^*_p(r_2)= \\ =\frac{p\cos(p(r_1+r_2))-\varkappa\sin(p(r_1+r_2))}{(\varkappa^2+p^2)pr_1r_2}. \quad (20)$$

After integration over ω, the expression for $\Delta_{in}^{(3)}$ becomes

$$\Delta_{in}^{(3)} = \frac{4\alpha(\mu_p+\mu_n)m_e}{\pi^3\mu_d m_p}\iint dk\,dp\,p^2 \times \\ \times \iint d\mathbf{r}_1 d\mathbf{r}_2\,\psi_0(r_1)\psi_0(r_2)\,\rho_p(r_1,r_2)\frac{\sin(kr_1)}{kr_1}\times \\ \times\left[\frac{\sin(kr_2)}{kr_2} - \frac{(1+\varkappa r_2)}{(kr_2)^2}\left(\frac{\sin(kr_2)}{kr_2} - \cos(kr_2)\right)\right]\times \\ \times\left[\frac{m_p}{p^2+k^2/4+\varkappa^2} - \frac{3}{2k}\right]. \quad (21)$$

The integral over p is

$$\int_0^\infty dp\,\frac{p^2\,\rho_p(r_1,r_2)}{p^2+k^2/4+\varkappa^2} = \frac{2\pi}{r_1 r_2 k^2}\times \\ \times\left[(Q+\varkappa)\exp[-Q(r_1+r_2)] - \right. \\ \left. -2\varkappa\exp[-\kappa(r_1+r_2)]\right], \quad (22)$$

where

$$Q = \sqrt{\varkappa^2+k^2/4}.$$

We now integrate (21) over r_1 and r_2 and then over k. The final result for the discussed correction is given by

$$\Delta_{in}^{(3)} = -\alpha\,\frac{\mu_p+\mu_n}{\mu_d}\,\frac{m_e}{\varkappa}\,\frac{1}{3}\,(2-2\ln 2) + \\ + \frac{3\alpha}{\pi}\,\frac{\mu_p+\mu_n}{\mu_d}\,\frac{m_e}{m_p}\ln\frac{m_p}{\varkappa}. \quad (23)$$

Again, it is only natural that due to common selection rules, the contribution of the ${}^3S_1$ intermediate state is proportional to $\mu_p+\mu_n$. We also note that the first term in (23) is additionally suppressed by the small numerical factor

$$\frac{2-2\ln 2}{3} = 0.20.$$

We finally return to the effect due to a finite distribution of the deuteron charge and magnetic moment. The Zemach correction Δ_f in Eq. (8) can also be easily derived in the present approach. Using the identity

$$\langle\psi_0\,|\hat{\mathbf{p}}\exp(i\mathbf{k}\cdot\mathbf{r}/2)|\psi_0\rangle = \frac{\mathbf{k}}{4}\langle\psi_0|\exp(i\mathbf{k}\cdot\mathbf{r}/2)|\psi_0\rangle,$$

we obtain the corresponding amplitude

$$M_{mn}^f = \left(\frac{e}{2m_p}\right)^2(\mu_p+\mu_n)\,\omega\left[F^2(k)-1\right]\times \\ \times\frac{k_m\,i\,\epsilon_{nrs}k_r s_s - k_n\,i\,\epsilon_{mrs}k_r s_s}{\omega^2-(p^2+k^2/4+\varkappa^2)^2/m_p^2}, \quad (24)$$

where

$$F(k) = \langle\psi_0\,|\exp(i\mathbf{k}\cdot\mathbf{r}/2)|\psi_0\rangle = \frac{4\varkappa}{k}\,\mathrm{arctg}\,\frac{k}{4\varkappa} \quad (25)$$

is the deuteron form factor in the zero-range approximation. We note that in our approximation, the electric and magnetic form factors, which in the present case enter the convection current and spin current matrix elements respectively, coincide and are equal to $F(k)$.

Integration over ω leads to the following result for the relative correction Δ_f:

$$\Delta_f = \frac{8\alpha(\mu_p+\mu_n)m_e}{\pi\mu_d}\int_0^\infty\frac{dk}{k^2}[F^2(k)-1] = \\ = -\alpha\frac{\mu_p+\mu_n}{\mu_d}\,\frac{m_e}{\varkappa}\,\frac{1}{3}\,(1+2\ln 2). \quad (26)$$

There is no logarithmic term in Δ_f because

$$F^2(k)-1 \sim k^2 \quad \text{for} \quad k \ll \varkappa.$$

In fact, result (26) agrees with (8) because $\mu_p+\mu_n=\mu_d$ within our accuracy.

The corrections in (18), (23), and (26) combine into the compact result

$$\Delta_c = -\alpha\,\frac{\mu_n}{\mu_d}\,\frac{m_e}{\varkappa} - \frac{3\alpha}{\pi}\,\frac{\mu_p-\mu_n}{\mu_d}\,\frac{m_e}{m_p}\ln\frac{m_p}{\varkappa}. \quad (27)$$

We note that the logarithmic part of Δ_c coincides with the corresponding logarithmic term in [8] (see Eq. (27) therein). This is quite natural: the logarithmic contribution is dominated by small k, and cannot therefore be influenced by an extra power of k arising from the recoil of the proton–neutron system as a whole.

The leading term in (27) coincides with the result in Ref. [5][2)]. However, we could not find any correspondence between our arguments and those in Ref. [5]. In particular, it is stated explicitly in Ref. [5] that the motion of the intermediate proton–neutron system as a whole is there neglected.

3. DISCUSSION OF THE RESULTS

Our total result for the nuclear-structure corrections to the deuterium hyperfine structure, comprising all the contributions in Eqs. (4), (6), (7), and (27), is

2) We are sorry for misquoting the result of Ref. [5] in our paper [8].

$$\Delta = -\alpha \frac{\mu_n}{\mu_d}\frac{m_e}{\varkappa} - \frac{3\alpha}{\pi}\frac{\mu_p-\mu_n}{\mu_d}\frac{m_e}{m_p}\ln\frac{m_p}{\varkappa} + \\ + \frac{3\alpha}{8\pi}\frac{(\mu_p-\mu_n)^2}{\mu_d}\frac{m_e}{m_p}\ln\frac{m_p}{\varkappa} + \\ + \frac{3\alpha}{8\pi}\frac{1}{\mu_d}(\mu_d^2 - 2\mu_d - 3)\frac{m_e}{m_p}\ln\frac{\varkappa}{m_e} + \\ + \frac{3\alpha}{4\pi}\frac{1}{\mu_d}(\mu_p^2 - 2\mu_p - 3 + \mu_n^2)\frac{m_e}{m_p}\ln\frac{m_\rho}{\varkappa}. \quad (28)$$

Numerically, this correction to the hyperfine splitting in deuterium is given by

$$\Delta\nu = 50\,\mathrm{kHz}. \quad (29)$$

It should be compared with the lacking 45 kHz (see (3)). We believe that the agreement is quite satisfactory if we recall the crude nuclear model (zero-range approximation) used here; in particular, the deuteron form factors calculated in the zero-range approximation are certainly harder than the real ones, and the negative Zemach correction is therefore underestimated in that approximation.

We mention here that in a recent paper [14], elastic contributions and the Zemach effect were considered in a quite different theoretical technique, but with some phenomenological desription of the deuteron form factors. The result is smaller than the corresponding part of ours by 13 kHz.

Clearly, the nuclear effects discussed are responsible for the bulk of the difference between the pure QED calculations and the experimental value of the deuterium hyperfine splitting. Calculation of this correction, including accurate treatment of nuclear effects, would serve as one more sensitive check of detailed models of the deuteron structure.

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