Corrections to Deuterium Hyperfine Structure Due to Deuteron Excitations

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Abstract

We consider the corrections to deuterium hyperfine structure originating from the two-photon exchange between electron and deuteron, with the deuteron excitations in the 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 (hf) splitting in deuterium ground state has been measured with high accuracy. The most precise experimental result for it was obtained with an atomic deuterium maser and constitutes \[ \nu_{\text{exp}} = 327,384,352,522 \pm 17 \text{ kHz}. \] (1)

Meanwhile the theoretical calculation including higher order pure QED corrections gives \[ \nu_{\text{QED}} = 327,339,27(7) \text{ kHz}. \] (2)

The last number was obtained by using the theoretical result for the hydrogen hf splitting from Ref. [2]

\[ 1,420,451,95(14) \text{ kHz} \]

which does not include proton structure and recoil radiative correction, and combining it with the theoretical ratio of the hf constants in hydrogen and deuterium from Ref. [3]

\[ \frac{4,339,387,6(8)}{\mu_d} \]

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

It was recognized long ago that the discrepancy \[ \nu_{\text{exp}} - \nu_{\text{QED}} = 45 \text{ kHz} \] (3)

is due to the effects caused by the finite size of deuteron. Such effects are obviously much larger in deuterium than in hydrogen. Corresponding contributions to the deuterium hf splitting were discussed long ago with some intuitive arguments [4], and then in more detail in Refs. [5, 6, 7].

We believe that in the past the most systematic treatment of such effects, which are due to the electron-deuteron interaction of second order in \( \alpha \), was performed in Ref. [8]. The effective Hamiltonian of the hf interaction of 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, 10, 11, 12] was generalized in [8] to the case of virtual photons and a target with arbitrary spin. The corresponding contribution of the momentum transfers \( k \), bounded from above by the inverse deuteron size \( \kappa = 45.7 \text{ MeV} \), to the relative correction to the deuterium hyperfine structure is

\[ \Delta_{el} = \frac{3\alpha}{8\pi} \left( \mu_d - 2 - \frac{3}{\mu_d} \right) \frac{m_e}{m_p} \ln \frac{\kappa}{m_e}. \] (4)

Here \( m_e \) and \( m_p \) are the electron and proton masses, respectively, \( \mu_d = 0.857 \) is the deuteron magnetic moment. The relative corrections \( \Delta \)'s are defined here and below as the ratios of the corresponding contributions to the ed scattering amplitude to the spin-dependent Born term in this amplitude, \[ T_0 = -\frac{2\pi\alpha}{3m_em_p} \mu_d (\sigma \cdot s), \] (5)

where \( s \) is the deuteron spin.

At larger momentum transfers, \( k > \kappa \), the amplitude of the Compton scattering on a deuteron is just the coherent sum of those amplitudes on free proton and neutron. This correction equals \[ \Delta_{\text{pn}}^m = \frac{3\alpha}{4\pi} \frac{1}{\mu_d} \left( \mu_p^2 - 2\mu_p - 3 + \mu_n^2 \right) \frac{m_e}{m_p} \ln \frac{m_p}{m_e}. \] (6)
Here \( \mu_p = 2.79 \) and \( \mu_n = -1.91 \) are the proton and neutron magnetic moments; \( m_p = 770 \) MeV is the usual hadronic scale.

Strong numerical cancellation between \( \Delta_{el} \) and \( \Delta_{in} \) is worth mentioning.

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

\[
\Delta^{(1)}_m = \frac{3\alpha}{8\pi} \frac{(\mu_p - \mu_n)^2}{\mu_d} \frac{m_e}{m_p} \ln \frac{m_p}{\kappa}.
\] (7)

There is also a correction due to a finite distribution of the deuteron charge and magnetic moment\(^3\). In the zero-range approximation used in Ref. [8] this correction is

\[
\Delta_f = -\alpha \frac{m_e}{3\kappa} (1 + 2\ln 2).
\] (8)

2 Leading inelastic nuclear correction to deuterium hyperfine structure

Leading inelastic nuclear correction is on the relative order \( \alpha m_e/\kappa \) (as well as the Zemach correction \([8]\)). The corresponding effect calculated in Ref. [8] is additionally enhanced by a large factor \( \mu_p - \mu_n = 4.7 \). In the present paper we consider two more effects on the same order \( \alpha m_e/\kappa \). Though both of them are proportional to \( \mu_p + \mu_n = 0.88 \) (and thus are essentially smaller numerically than that considered in [8]), we believe that their investigation is worth attention.

We use the gauge \( A_0 = 0 \) where the photon propagator is

\[
D_{im}(\omega, \vec{k}) = \frac{d_{im}}{\omega^2 - \vec{k}^2}; \quad d_{im} = \delta_{im} - \frac{k_i k_m}{\omega^2}; \quad D_{00} = D_{0m} = 0.
\] (9)

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

\[
T = 4\pi\alpha i \int \frac{d^4k}{(2\pi)^4} \frac{d_{im} d_{jm}}{k^4} \frac{\gamma_i(\hat{l} - \hat{k} + m_e)\gamma_j}{k^2 - 2\ell k} M_{mn}.
\] (10)

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

The inelastic \( 1/\kappa \) contribution to hfs is induced by the combined action of the convection and spin currents. Since the convection current is spin-independent, all the intermediate states are triplet ones, as well as the ground state. Therefore, here the spin current operator

\[
\frac{e}{2m_p} i[\vec{k} \times [\mu_p \sigma_p \exp(i\vec{k}r_p) + \mu_n \sigma_n \exp(i\vec{k}r_n)]
\]

simplifies to

\[
\frac{e}{2m_p} i[\vec{k} \times \vec{s}] [\mu_p \exp(i\vec{k}r_p) + \mu_n \exp(i\vec{k}r_n)].
\] (11)

\(^3\)In the case of hydrogen this problem was considered many years ago by Zemach [13].
In the initial state \(|0\rangle\) the deuteron is at rest. But in the excited state the system of nucleons as a whole moves with the momentum \(k\), so that its wave function is \(|n⟩\exp(ikR)\), where \(|n⟩\) refers to the deuteron internal degrees of freedom and is a function of \(r = r_p - r_n; R = (r_p + r_n)/2\) is the deuteron centre of mass coordinate. Thus, a typical matrix element of the spin current can be written as

\[
\frac{e}{2m_p} i \mathbf{k} \times \langle n | \exp(-i k \mathbf{R}) s [\mu_p \exp(i k r_p) + \mu_n \exp(i k r_n)] |0\rangle
\]

\[
= \frac{e}{2m_p} i \mathbf{k} \times \langle n | s [\mu_p \exp(i k r_p/2) + \mu_n \exp(-i k r_p/2)] |0\rangle. \tag{12}
\]

As to a typical matrix element of the convection current, it transforms now as follows:

\[
\frac{e}{2m_p} \langle n | \exp(-i k \mathbf{R}) \hat{p}_p \exp(i k r_p) + \exp(i k r_p) \hat{p}_p |0\rangle
\]

\[
= \frac{e}{2m_p} \langle n | (\hat{p} + \frac{\mathbf{k}}{2}) \exp(i k r_p/2) + \exp(i k r_p/2) \hat{p} |0\rangle = \frac{e}{m_p} \langle n | \hat{p} \exp(i k r_p/2) |0\rangle; \tag{13}
\]

here \(\hat{p}\) acts on the relative coordinate \(r\).

At first let us take as intermediate states \(|n⟩\) in the corresponding nuclear Compton amplitude just plane waves, eigenstates of \(\hat{p}\). In this way we take into account all the states with \(l \neq 0\), which are free ones in our zero range approximation, and in addition the \(^3S_1\) wave function in the free form \(\psi_p(r) = \sin pr/pr\) (the deviation of the \(^3S_1\) wave function from the free one will be considered below). Then, with the zra deuteron wave function

\[
\psi_0(r) = \sqrt{\frac{x}{2\pi}} \exp(-x r)/r, \tag{14}
\]

the only matrix element entering the amplitude is

\[
\langle \psi_0 | \exp(\pm i k r/2) | p \rangle = \frac{\sqrt{8\pi x}}{(p \pm k/2)^2 + x^2}. \tag{15}
\]

In this way the amplitude itself simplifies to

\[
M_{mn}^{(2)} = \left(\frac{e}{2m_p}\right)^2 2x\omega \int \frac{d\mathbf{p}}{π^3} \left\{ \frac{\mu_p}{[(p - k/2)^2 + x^2]^2} + \frac{\mu_n}{[(p - k/2)^2 + x^2][(p + k/2)^2 + x^2]} \right\}
\]

\[
\times \frac{2p_m i \epsilon_{mn r s} k_r s_s - 2p_n i \epsilon_{mn r s} k_r s_s}{ω^2 - (p^2 + k^2/4 + x^2)^2/m_p^2}. \tag{16}
\]

Due to the account for the motion of the system as a whole in the intermediate states, this expression differs from the corresponding one from our previous paper [8] in two respects. First, in [8] the operator \(\mathbf{p}_p\) in [13] was identified with \(\mathbf{p}\). Thus, therein instead of 2\(p_{m,n}\) in the analogue of the present formula (16), we obtained \((2p - k/2)_{m,n}\). At present, in (16) the term proportional to \(\mu_n\) is an odd function of \(\mathbf{p}\), and therefore vanishes after integration over \(d\mathbf{p}\).

Second, in the denominator the energy difference has acquired the contribution \(k^2/4m_p\), which is the kinetic energy of the \(pn\) system as a whole, and thus \((p^2 + x^2)/m_p\) has transformed into \((p^2 + k^2/4 + x^2)/m_p\).

Now we substitute (16) into (14) and take the integral over \(\omega\) under the condition \(\omega \gg x^2/m\). For the relative correction to the hf structure we obtain

\[
\Delta_{mn}^{(2)} = \frac{2\alpha x \mu_p m_e}{π^4 μ_d m_p} \int \frac{d\mathbf{p} d\mathbf{k}}{k^4} \frac{pk}{[(p - k/2)^2 + x^2]^2} \left[ \frac{m_p}{p^2 + k^2/4 + x^2 - \frac{3}{2k}} \right]. \tag{17}
\]
The result of integration over $p$ and then over $k$ reads

$$\Delta_{in}^2 = \frac{\alpha \mu_p m_e}{\mu_d \pi} \frac{6\alpha \mu_p m_e}{\mu_d m_p} \ln \frac{m_p}{\pi}.$$  \hspace{1cm} (18)

The logarithmic contribution here originates from integration of the term $3/2k$ in the square brackets in (17) over the range $\infty/k < k \ll \infty$. The result (18) differs from the corresponding one of [3] by a term proportional to $\mu_p + \mu_n$, which is relatively small numerically. It is only natural that our present account for the motion of the proton-neutron system as a whole in the intermediate states results in the correction proportional to $\mu_p + \mu_n$.

Let us calculate now the correction $\Delta_{in}^{(3)}$ corresponding to the effect of deviation of the intermediate $^3S_1$ wave function $\Psi_p(r)$ from the free one. In the zra $\Psi_p(r)$ reads

$$\Psi_p(r) = \frac{\sin pr}{pr} - \frac{1}{\pi + ip} \frac{\exp(ipr)}{r} = \frac{\pi \sin pr - p \cos pr}{pr(\pi + ip)}.$$  \hspace{1cm} (19)

It follows, for instance, from the orthogonality to the deuteron wave function (14). We use below the function

$$\rho_p(r_1, r_2) = \Psi_p(r_1)\Psi_p^*(r_2) - \psi_p(r_1)\psi_p^*(r_2) = \frac{p \cos p(r_1 + r_2) - \pi \sin p(r_1 + r_2)}{(\pi^2 + p^2)\rho_p(r_1, r_2)}.$$  \hspace{1cm} (20)

Then, after integration over $\omega$ the expression for $\Delta_{in}^{(3)}$ reads

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

The integral over $p$ is

$$\int_0^\infty dp \frac{p^2 \rho_p(r_1, r_2)}{p^2 + k^2/4 + \pi^2} = \frac{2\pi}{2} \frac{r_1 r_2 k^2}{(Q + \pi)(1 - Q(r_1 + r_2))} - 2k \exp[-Q(r_1 + r_2)] - 2\pi \exp[-Q(r_1 + r_2)],$$  \hspace{1cm} (22)

where $Q = \sqrt{\pi^2 + k^2/4}$. Now we integrate (21) over $r_1, r_2$, and then over $k$. The final result for the discussed correction reads:

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

Again, it is only natural that due to common selection rules the contribution of the $^3S_1$ intermediate state is proportional to $\mu_p + \mu_n$. Let us note also that the first term in (23) is additionally suppressed by a small numerical factor $(2 - 2 \ln 2)/3 = 0.20$.

At last, we wish to come back to the effect due to a finite distribution of the deuteron charge and magnetic moment. The Zemach correction $\Delta_f$ [3] can be also easily derived in the present approach. Using the identity

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

we obtain the corresponding amplitude:

$$M_{mn}^f = \left( \frac{e}{2m_p} \right)^2 (\mu_p + \mu_n) \omega \left[ F^2(k) - 1 \right] \frac{k_m i \epsilon_{nrs}k_r s_s - k_n i \epsilon_{mrs}k_r s_s}{\omega^2 - (p^2 + k^2/4 + \pi^2)^2/m_p^2},$$  \hspace{1cm} (24)
where \( F(k) \) is the deuteron form factor in the zero-range approximation

\[
F(k) = \langle \psi_0 | \exp(ikr/2) | \psi_0 \rangle = \frac{4\pi}{k} \arctan \frac{k}{4\pi}.
\]  (25)

Let us note that in our approximation both electric and magnetic form factors, which in the present case enter the convection current and spin current matrix elements respectively, coincide and equal \( F(k) \).

The integration over \( \omega \) leads to the following result for the relative correction \( \Delta_f \)

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

There is no logarithmic term in \( \Delta_f \) since \( F^2(k) - 1 \sim k^2 \) for \( k \ll \pi \). In fact, the result \( (26) \) agrees with \( (8) \) since to our accuracy \( \mu_p + \mu_n = \mu_d \).

The corrections \( (18), (23), (26) \) combine into a compact result

\[
\Delta_c = -\alpha \frac{\mu_n}{\mu_d} \frac{m_e}{\pi \pi} - \frac{3\alpha}{\pi} \frac{\mu_p - \mu_n}{\mu_d} \frac{m_e}{\mu_p} \ln \frac{m_p}{\pi}. \]  (27)

Let us notice that its logarithmic part coincides with the corresponding logarithmic term in \( (8) \) (see formula \( (27) \) therein). This is quite natural: the log is dominated by small \( k \), so that extra power of \( k \), which arises from the recoil of the \( pn \) system as a whole, cannot influence it.

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

3 Discussion of results

Our total result for the nuclear-structure corrections to the deuterium hf structure, comprising all the contributions, \( (4), (6), (7), (27) \), is

\[
\Delta = -\alpha \frac{\mu_n}{\mu_d} \frac{m_e}{\pi} - \frac{3\alpha}{\pi} \frac{\mu_p - \mu_n}{\mu_d} \frac{m_e}{\mu_p} \ln \frac{m_p}{\pi}
\]  + \[ \frac{3\alpha}{8\pi} \frac{(\mu_p - \mu_n)^2}{\mu_d} \frac{m_e}{m_p} \ln \frac{m_p}{\pi} \]  + \[ \frac{3\alpha}{8\pi} \frac{1}{\mu_d} (\mu_d^2 - 2\mu_d - 3) \frac{m_e}{m_p} \ln \frac{m_p}{\pi} + \frac{3\alpha}{4\pi} \frac{1}{\mu_d} (\mu_p^2 - 2\mu_p - 3 + \mu_n^2) \frac{m_e}{m_p} \ln \frac{m_p}{\pi}. \]  (28)

Numerically this correction to the hf splitting in deuterium constitutes

\[
\Delta \nu = 50 \text{ kHz}. \]  (29)

It should be compared with the lacking 45 kHz (see \( (3) \)). We believe that the agreement is quite satisfactory if one recalls the crude nuclear model (zra) used here; in particular the deuteron form factors, as calculated in the zra, are certainly harder than the real ones, and thus in zra the negative Zemach correction is underestimated.

\[ \text{We are sorry for misquoting the result of Ref. \( (5) \) in our paper \( (8) \).} \]
Let us 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 description 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 hf splitting. The calculation of this correction, including accurate treatment of nuclear effects, would serve as one more sensitive check of detailed models of deuteron structure.

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