# Nuclear-structure corrections to the hyperfine splitting in muonic deuterium

Marcin Kalinowski[∗](#page-0-0) and Krzysztof Pachucki[†](#page-0-1)

Faculty of Physics, University of Warsaw, Pasteura 5, 02-093 Warsaw, Poland

Vladimir A. Yerokhin

Center for Advanced Studies, Peter the Great St. Petersburg Polytechnic University, 195251 St. Petersburg, Russia

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Nuclear structure corrections of orders  $Z \alpha E_F$  and  $(Z \alpha)^2 E_F$  are calculated for the hyperfine splitting of the muonic deuterium. The obtained results disagree with previous calculations and lead to a  $5\sigma$  disagreement with the current experimental value of the 2S hyperfine splitting in  $\mu$ D.

## I. INTRODUCTION

Nuclear structure effects represent the main limitation for precise theoretical description of atomic energy levels. These effects are particularly important for muonic atoms, where the Compton wavelength of the bound muon ∼2 fm is of the same order as the nuclear size. It is, therefore, not surprising that the uncertainty of modern theoretical predictions of energy levels of light muonic atoms is dominated by the uncertainty of nuclearstructure effects. Specifically, the current theoretical value of the hyperfine splitting (hfs) of the 2S state of muonuic deuterium  $(\mu D)$  is [\[1\]](#page-9-0)

<span id="page-0-2"></span>
$$
E_{\rm hfs}(2S)_{\rm theo} = 6.2791(50) \,\text{meV} \,, \tag{1}
$$

where the uncertainty comes almost exclusively from the deuteron polarizability  $(\pm 0.0049 \text{ meV})$ . The theoretical value [\(1\)](#page-0-2) was obtained in Ref. [\[1\]](#page-9-0) by compiling two independent calculations, by Borie [\[2\]](#page-9-1) and by Faustov et al. [\[3\]](#page-9-2). The theoretical result is in good agreement with the experimental value [\[4\]](#page-10-0):

<span id="page-0-3"></span>
$$
E_{\rm hfs}(2S)_{\rm exp} = 6.2747(70)_{\rm stat}(20)_{\rm syst} \text{ meV} \,. \tag{2}
$$

In this work we will demonstrate that the deuteron structure corrections to hfs in  $\mu$ D were previously treated incorrectly and that the good agreement with the experimental value was probably accidental. Specifically, the calculation by Borie [\[2\]](#page-9-1) included only the elastic part of the nuclear structure, which does not reproduce even the correct sign of the total nuclear structure effect. Faustov and coworkers [\[3\]](#page-9-2) included both the Zemach and the Low corrections at the same time, which is inconsistent, and, moreover, used an incorrect formula for the nuclear polarizability.

In the present work we derive the nuclear-structure corrections in  $\mu$ D induced by the two- and three-photon exchange between the bound muon and the nucleus and analyze discrepancies with the previous calculation [\[3\]](#page-9-2) and the experimental result [\[4\]](#page-10-0).

The leading-order hfs of atomic levels of light atoms is independent of nuclear structure and is given (for the  $nS$ states) by the Fermi contact term,

$$
E_F = \frac{4g_N m_r^3}{3m_p m n^3} (Z\alpha)^4 \langle \vec{s}_N \cdot \vec{s}_\mu \rangle , \qquad (3)
$$

where  $n$  is the principal quantum number,  $Z$  is the nuclear charge number,  $\alpha$  is the fine-structure constant, m and  $m_p$  are masses of the lepton and the proton, respectively,  $m_r$  is the reduced mass of the atom,  $\vec{s}_{\mu}$  and  $\vec{s}_{N}$  are the spin operators of the lepton and the nucleus, respectively,  $g_N$  is the 'modified' g-factor of the nucleus defined by

$$
\vec{\mu}_N = \frac{Ze\,g_N}{2\,m_p}\,\vec{s}_N\,,\tag{4}
$$

 $\vec{\mu}_N$  is the nuclear magnetic moment operator and e is the elementary charge. Numerical values of  $E_F$  for the ground and the first excited state of muonic deuterium are

$$
E_F = \begin{cases} 49.0875 \,\text{meV}, & \text{for the } 1S \text{ state}, \\ 6.135 \,94 \,\text{meV}, & \text{for the } 2S \text{ state}. \end{cases} \tag{5}
$$

If we assume the point nuclear model and account for all known QED corrections, the theoretical result for the 2S state is [\[1\]](#page-9-0)

<span id="page-0-4"></span>
$$
E_{\rm hfs}(\text{point}) = 6.178\,15(20)\,\text{meV}\,,\tag{6}
$$

which corresponds to the sum of entries  $h_1 + h_2 + h_4 +$  $h_5 + h_7 + h_8 + h_9 + h_{9b} + h_{12} + h_{13} + h_{14} + h_{18}$  from Table IV of Ref. [\[1\]](#page-9-0). The deviation of the experimental value [\(2\)](#page-0-3) from the theoretical point-nucleus result [\(6\)](#page-0-4) can be regarded as the "experimental value" of the nuclearstructure correction,

<span id="page-0-5"></span>
$$
\delta E_{\text{nucl}} = E_{\text{hfs}}(\exp) - E_{\text{hfs}}(\text{point}) = 0.0966(73) \,\text{meV} \,. (7)
$$

From the theoretical side the nuclear-structure correction for light atoms can be described within the  $Z \alpha$  expansion,

<span id="page-0-6"></span>
$$
\delta E_{\text{nucl}} = \delta^{(1)} E_{\text{nucl}} + \delta^{(2)} E_{\text{nucl}} + \dots \tag{8}
$$

where  $\delta^{(1)}E_{\text{nucl}}$  is the two-photon exchange correction of order  $(Z \alpha) E_F$ ,  $\delta^{(2)} E_{\text{nucl}}$  is the three-photon exchange

<span id="page-0-0"></span><sup>∗</sup>[mj.kalinowski@student.uw.edu.pl](mailto:mj.kalinowski@student.uw.edu.pl)

<span id="page-0-1"></span><sup>†</sup><www.fuw.edu.pl/~krp>

correction of order  $(Z \alpha)^2 E_F$ , and ... denotes smaller contributions due to exchange of larger number of photons and radiative corrections. In the following discussion, we calculate the two-photon and the three-photon exchange nuclear-structure corrections for the hfs of  $nS$ states of muonic deuterium. Relativistic units ( $\hbar = c$  = 1) are employed throughout.

# II. TWO-PHOTON EXCHANGE NUCLEAR **STRUCTURE**

The most straightforward way of including the nuclear effects is to assume that the nucleus is described by some elastic electric and magnetic formfactors. This leads to the so-called elastic, or finite-nuclear-size (fns) corrections. The leading fns correction originates from the twophoton exchange. It was derived long ago by Zemach [\[5\]](#page-10-1) and is given by

$$
\delta E_{\text{Zem}} = -2 m_r Z \alpha r_Z E_F,\tag{9}
$$

where  $r_Z$  is the Zemach radius defined by

$$
r_Z = \int d^3 r_1 \int d^3 r_2 \, \rho_M(r_1) \, \rho_E(r_2) \, |\vec{r}_1 - \vec{r}_2| \,. \tag{10}
$$

(Note that the subscript  $Z$  in  $r_Z$  is not related to the nuclear charge.) In the above equation,  $\rho_E$  and  $\rho_M$  are the charge and the magnetic-moment distributions of the nucleus, respectively, i.e., the Fourier transform of the corresponding formfactors. The numerical value of the Zemach correction for the  $2S$  state of  $\mu$ D, in the nonrecoil limit, with  $r_Z = 2.593(16)$  fm [\[6\]](#page-10-2), is

$$
\delta E_{\text{Zem}} = -0.1177(33) \,\text{meV} \,. \tag{11}
$$

We note the opposite sign of the Zemach correction as compared to the experimental value of the total nuclear structure [\(7\)](#page-0-5). This demonstrates that the description of the nucleus only through the elastic formfactors is not adequate.

Various hfs corrections arise from excitations of the nucleus by the bound lepton, usually referred to as the inelastic nuclear-structure corrections. In the case of the proton, the inelastic contribution can be obtained from the experimentally accessible spin-dependent structure functions by using dispersion relations [\[7–](#page-10-3)[10\]](#page-10-4). For other nuclei, including deuteron, the inelastic spin-dependent structure functions are unknown, and one has to rely on theoretical calculations.

In our calculations we consider the elastic and inelastic contributions together, and use a perturbation expansion over a small parameter, namely, the ratio of the average nucleon binding energy over the nucleon mass. Specifically, the two-photon exchange correction can be represented as

<span id="page-1-4"></span>
$$
\delta^{(1)}E_{\text{nucl}} = \delta E_{\text{Low}} + \delta E_{\text{nucl}} + \delta E_{\text{pol}} + \dots \tag{12}
$$

The leading-order term  $\delta E_{\text{Low}}$  was first derived by Low [\[11\]](#page-10-5). For the particular case of an  $nS$  state in  $\mu$ D, the numerical value of Low's correction in the point-nucleon model is

<span id="page-1-0"></span>
$$
\delta E_{\text{Low}} \approx -2 \, m_r \, \alpha \, E_F \, \frac{g_n}{g_d} \langle R \rangle = \frac{2.640}{n^3} \, \text{meV} \,. \tag{13}
$$

Here,  $R$  is the distance of the proton from the center of mass. Its expectation value was calculated using the AV18 potential [\[12\]](#page-10-6) as  $\langle R \rangle = 1.629$  fm.

A more detailed calculation of the leading-order term was performed by Friar and Payne [\[13,](#page-10-7) [14\]](#page-10-8), with inclusion of the finite nucleon size and meson exchange currents. Their result was reported for the  $1S$  state of ordinary (electronic) deuterium,  $\delta E_{\text{Low}}(eD) = 87.3 \text{ kHz}$ . Rescaling it to the  $nS$  states of  $\mu$ D one gets

<span id="page-1-3"></span>
$$
\delta E_{\text{Low}} = \frac{m_r^4(\mu D)}{m_r^4(eD)} \frac{m(e)}{m(\mu)} \frac{1}{n^3} \delta E_{\text{Low}}(eD) = \frac{2.566}{n^3} \text{ meV},\tag{14}
$$

in good agreement with the approximate result of Eq. [\(13\)](#page-1-0).

 $\delta E_{\text{1nucl}}$  is the contribution induced by individual nucleons. It is given by the individual nucleon Zemach corrections,

<span id="page-1-2"></span>
$$
\delta E_{\text{Inucl}} = -\frac{8\,\alpha^2}{3\,n^3}\,\frac{m_r^3}{m_p + m}\,\vec{s}_\mu \cdot \langle \sum_a g_a \,\vec{s}_a \, r_{aZ} \rangle. \tag{15}
$$

where  $r_{aZ}$  is the effective radius of the nucleon a. If only the elastic part is included, the result for the proton is  $r_{pZ} = 1.086(12)$  fm [\[6\]](#page-10-2) and for the neutron,  $r_{nZ} =$ −0.042 fm [\[14\]](#page-10-8). The result for the proton effective radius that includes the recoil and polarizability contributions can be obtained from the 1S muonic hydrogen correction  $\delta E_{\text{nucl}}(\mu H) = -1.131(24) \,\text{meV}$  obtained by Tomalak in Ref. [\[15\]](#page-10-9), namely  $r_{pZ} = 0.883(19)$  fm, and for the neutron from Ref. [\[16\]](#page-10-10),  $r_{nZ} = 0.06(1)$  fm.

 $\delta E_{\text{pol}}$  is the contribution of the nuclear vector polarizability. It has been studied for ordinary atoms by Khriplovich and Milstein [\[17\]](#page-10-11) and later by one of us (Pachucki) [\[18\]](#page-10-12). Results of Ref. [\[17\]](#page-10-11) obtained in the logarithmic approximation were shown in Ref. [\[18\]](#page-10-12) to be incorrect, because the coefficient of logarithm for an arbitrary chosen cutoff vanishes completely. Moreover, the derivation of Ref. [\[17\]](#page-10-11) is applicable only for the 'electronic' atoms but not for the muonic ones. Nevertheless, the result of Ref. [\[17\]](#page-10-11) was later used by Faustov et al. in their calculations of the nuclear structure in  $\mu$ D [\[3\]](#page-9-2). In the present work we derive the nuclear vector polarizability correction  $\delta E_{\text{pol}}$  for muonic deuterium.

Following the method of Ref. [\[18\]](#page-10-12), we obtain the vector polarizability corrections to hfs in  $\mu$ D in the form

<span id="page-1-1"></span>
$$
\delta E_{\rm pol} = -e^2 \psi^2(0) \int \frac{d\omega}{2\pi} \int \frac{d^3k}{(2\pi)^3} \qquad (16)
$$

$$
\times \frac{(\omega^2 \epsilon^{klj} + k^i k^k \epsilon^{lij} - k^i k^l \epsilon^{kij}) \sigma^j \alpha^{kl}}{\omega (\omega^2 + 2m\omega - k^2) (\omega^2 - 2m\omega - k^2) (\omega^2 - k^2)},
$$

where  $\alpha^{kl}$  is the antisymmetric part of the scattering amplitude tensor  $T^{kl}$ . In the simplest case of the electric dipole coupling  $-\vec{D}\cdot\vec{E}$ ,  $\alpha^{kl}$  takes the form

$$
\alpha^{kl} = \omega^2 \left\langle D^k \frac{1}{E_N - \tilde{H}_N - \omega} D^l + D^l \frac{1}{E_N - \tilde{H}_N + \omega} D^k \right\rangle, \tag{17}
$$

where  $\tilde{H}_N = H_N + k^2/(2 M)$ ,  $H_N$  is the nuclear internal Hamiltonian,  $E_N = \langle H_N \rangle$ ,  $\vec{D} = \sum_a e_a \vec{R}_a$ , and  $\vec{R}_a$  is the nucleon position with respect to the mass center. After integration over  $\omega$  and k, and expansion in the small parameter

$$
X = \sqrt{\frac{2(H_N - E_N)}{m_r}},\tag{18}
$$

we obtain the dipole polarizability correction as

$$
\delta E_{\text{pol}0} = -\frac{i e^2}{12\pi} \psi^2(0) \left(\frac{m_r}{m}\right)^2 \epsilon^{ijk} \sigma^k \left\langle D^i X D^j \right\rangle. \tag{19}
$$

 $\delta E_{\text{pol}}$  vanishes in the nonrelativistic limit and its numerical contribution is expected to be small, because it requires the presence of both the spin-orbit and the quadrupole-spin interactions between nucleons.

There are, however, other polarizability corrections that yield significant numerical contributions. The first one is the correction due to the magnetic quadrupole interaction,

<span id="page-2-2"></span>
$$
\delta H = -\sum_{a} \frac{e g_a}{2 m_p} R_a^i \, s_a^j \, B_{,i}^j \,. \tag{20}
$$

The corresponding contribution to the scattering tensor is

$$
\delta \alpha^{kl} = i \omega \sum_{a} \frac{e g_a}{2 m_p} \left\langle \vec{R}_a \vec{k} \left( \vec{s}_a \times \vec{k} \right)^k \frac{1}{E_N - \tilde{H}_N - \omega} D^l \right. \\ + D^l \frac{1}{E_N - \tilde{H}_N + \omega} \vec{R}_a \vec{k} \left( \vec{s}_a \times \vec{k} \right)^k - (k \leftrightarrow l, \omega \to -\omega) \right\rangle. \tag{21}
$$

The first term in the small- $X$  expansion gives the following correction to the hyperfine splitting of  $\mu$ D

$$
\delta E_{\text{pol1}} = -\frac{2\alpha}{3} \frac{g_p - g_n}{g_d} E_F m_r^2 \left\langle \vec{R} \, X \, \vec{R} \right\rangle. \tag{22}
$$

The second correction of the same order in  $X$  comes from the magnetic dipole interaction, which is enhanced by the factor of  $(g_p - g_n)^2$ ,

$$
\delta H = -\frac{e}{2\,m_p} \left[ \sum_a g_a \,\vec{s}_a - g_d \,\vec{s}_d \right] \vec{B} = -(\vec{\mu} - \langle \vec{\mu} \rangle) \,\vec{B}.\tag{23}
$$

The corresponding contribution to the scattering tensor is

$$
\delta \alpha^{kl} = \left\langle \left[ (\vec{\mu} - \langle \vec{\mu} \rangle) \times \vec{k} \right]^k \frac{1}{E_N - \tilde{H}_N - \omega} \left[ (\vec{\mu} - \langle \vec{\mu} \rangle) \times \vec{k} \right]^l \right. \\ \left. + (k \leftrightarrow l, \omega \to -\omega) \right\rangle, \tag{24}
$$

which gives the following correction to the hyperfine splitting in  $\mu$ D

$$
\delta E_{\text{pol2}} = -\frac{\alpha}{16} \frac{m_r^2}{m_p m} \frac{(g_p - g_n)^2}{g_d} E_F \left\langle \left(\vec{s}_p - \vec{s}_n\right) X \left(\vec{s}_p - \vec{s}_n\right) \right\rangle. \tag{25}
$$

Further corrections are of higher order in X. The  $X^2$ terms vanish, as shown in Ref. [\[18\]](#page-10-12), and the next-order nonvanishing terms are proportional to  $X<sup>3</sup>$ . Namely, the next-order (in  $X$ ) term of the correction coming from  $\delta \alpha^{kl}$  in Eq. [\(21\)](#page-2-0) is

$$
\delta E_{\text{pol3}} = \frac{\alpha}{4} \frac{g_p - g_n}{g_d} E_F \frac{5m_r - 2m}{3m^3} m_r^4 \left\langle \vec{R} X^3 \vec{R} \right\rangle. \tag{26}
$$

Another  $X^3$  correction,  $\delta E_{\text{pol}4}$ , comes from the following spin dependent coupling to the electric field [\[18\]](#page-10-12),

<span id="page-2-4"></span><span id="page-2-3"></span>
$$
\delta H = -\vec{T} \cdot \frac{\partial \vec{E}}{\partial t},\qquad(27)
$$

where  $\vec{T}$  is defined as

$$
\vec{T} = \sum_{a} \left( \frac{e_a}{2m_p} (g_a - 1) - \frac{Ze}{2M} \right) \vec{s}_a \times \vec{x}_a \,. \tag{28}
$$

The corresponding vector polarizability correction is

$$
\delta \alpha^{kl} = i \omega^3 \left\langle D^k \frac{1}{E_N - \tilde{H}_N - \omega} T^l + T^l \frac{1}{E_N - \tilde{H}_N + \omega} D^k - (k \leftrightarrow l, \omega \to -\omega) \right\rangle, \tag{29}
$$

<span id="page-2-0"></span>and the contribution to the hyperfine splitting of  $\mu$ D is

<span id="page-2-5"></span>
$$
\delta E_{\text{pol}4} = -\frac{\alpha}{3} \frac{g_p - g_n - 1}{g_d} E_F \frac{m_r^4}{m^2} \left\langle \vec{R} \, X^3 \, \vec{R} \right\rangle. \tag{30}
$$

<span id="page-2-1"></span>The last nuclear polarizability correction  $\delta E_{\text{pol}5}$  comes from the fourth-order terms of the expansion of the vector polarizability  $\delta \alpha^{kl}$  in the small parameter  $\vec{k} \cdot \vec{R}$ . In order to derive this correction, we rewrite Eq. [\(16\)](#page-1-1) by using  $k^i T^{ik} = \omega T^{0k}$  and apply the nonrelativistic approximation. The result is

$$
\delta E_{\rm hfs} = -e^2 \psi^2(0) \int \frac{d\omega}{2\pi} \int \frac{d^3k}{(2\pi)^3} \frac{(\vec{k} \times \vec{\sigma})^i (T^{0i} - T^{i0})}{k^2 (2m\omega - k^2)(2m\omega + k^2)} \n= \frac{e^4}{m} \psi^2(0) \int \frac{d^3k}{(2\pi)^3} i \frac{(\vec{\sigma} \times \vec{k})^i}{k^4} \sum_{a,b} \left\langle j_a^0 e^{i \vec{k} \cdot \vec{R}_a} \frac{1}{H_N - E_N + \frac{k^2}{2m_r}} j_b^i e^{-i \vec{k} \cdot \vec{R}_b} \right\rangle,
$$
\n(31)

where, in the nonrelativistic approximation,  $j_a^0 = 1$  and  $j_b^i = -i \vec{\sigma}_b \times \vec{k} g_b/(4 m_p)$ . By neglecting  $H_N - E_N$  in the above expression one obtains the Low correction given by Eq. [\(13\)](#page-1-0). The quadratic terms of the expansion of Eq. [\(31\)](#page-3-0) in  $\vec{k} \cdot \vec{R}_a$  gives  $\delta E_{\text{pol}}$ . We now consider the fourth power of  $\vec{k} \cdot \vec{R}_a$  and obtain for  $\mu$ D the following correction

$$
\delta E_{\text{pol}5} = \frac{\alpha}{15} E_F m_r^4 \left\{ \frac{5}{6} \frac{g_p + g_n}{g_d} \left\langle R^2 X^3 R^2 \right\rangle - 2 \frac{g_p - g_n}{g_d} \left\langle R^2 \vec{R} X^3 \vec{R} \right\rangle \right.+ \frac{g_p + g_n}{g_d} \left\langle \left(R^i R^j - R^2 \delta^{ij}/3\right) X^3 \left(R^i R^j - R^2 \delta^{ij}/3\right) \right\rangle \right\}.
$$
 (32)

We are not aware of any further significant contributions, therefore we write the nuclear vector polarizability correction as

<span id="page-3-5"></span>
$$
\delta E_{\rm pol} = \sum_{i=1}^{5} \delta E_{\rm pol\,i} \,, \tag{33}
$$

and assume a 5% uncertainty due to omitted  $\delta E_{\text{pol}}$  and higher-order (in  $X$ ) corrections. Our result disagrees with the result by Faustov and Martynenko [\[3\]](#page-9-2), because they used incorrect formula for the polarizability correction derived for electronic atoms and included in addition the Low correction.

The nuclear vector polarizability is presently the main source of the theoretical uncertainty of the total nuclearstructure correction. This means that in the future, detailed investigations should reanalyze all possible contributions to the nuclear vector polarizability.

#### III. THREE-PHOTON-EXCHANGE ELASTIC **CORRECTION**

The  $(Z\alpha)^2 E_F$  elastic contribution to the hyperfine splitting  $\delta^{(2)}E_{\text{fns}}$  can be derived by following the approach developed earlier for the case of the Lamb shift in Ref. [\[19\]](#page-10-13). Instead of a direct use of the Dirac equation, which is possible but tedious, we shall split the total correction into low-energy  $\delta E_L$  and high-energy  $\delta E_H$  parts. Both these parts are separately divergent, so we employ dimensional regularization with  $d = 3-2\epsilon$  (see Appendix [A](#page-9-3) for details) and cancel singularities  $\sim 1/\epsilon$  in the sum  $\delta^{(2)}E_{\text{fns}} = \delta E_L + \delta E_H$ . For convenience we assume lepton mass  $m = 1$  from now on and restore it only in the final expression from dimensional analysis.

## <span id="page-3-4"></span><span id="page-3-0"></span>A. Low-energy part

In the low-energy part, where  $p \sim Z\alpha$ , the nonrelativistic approximation is valid. The nonrelativistic Hamiltonian  $H$  with the nuclear electric  $G_E$  and magnetic  $G_M$  formfactors (with their respective Fourier transforms  $\rho_E, \rho_M$ ), here normalized to unity, is given by

$$
H = \frac{p^2}{2} + V(r) + \frac{4\pi Z\alpha}{dm_p} g_p(\vec{s}_p \cdot \vec{s}_\mu)_\epsilon \rho_M(r) ,\qquad(34)
$$

where the potential  $V$  is defined by its Fourier transform

<span id="page-3-1"></span>
$$
V(p) = -G_E(p^2) \frac{4\pi Z\alpha}{p^2}
$$
\n(35)

and where  $(\vec{s}_p \cdot \vec{s}_\mu)_{\epsilon}$  is defined in [\(A3\)](#page-9-4).

Because the characteristic momentum  $p$  is much smaller than the inverse of the nuclear size, the nuclear formfactors can be expanded in  $p^2$ . We thus obtain

<span id="page-3-3"></span><span id="page-3-2"></span>
$$
H = H_0 + H_{\text{hfs}} + \delta V + \delta H_{\text{hfs}}\,,\tag{36}
$$

where

$$
H_0 = \frac{p^2}{2} - Z\alpha \left[\frac{1}{r}\right]_{\epsilon},\tag{37}
$$

$$
H_{\text{hfs}} = \frac{4\pi Z\alpha}{dm_p} g_p(\vec{s}_p \cdot \vec{s}_\mu)_\epsilon \delta^{(d)}(\vec{r}), \qquad (38)
$$

$$
\delta V = -4\pi Z \alpha G_E'(0) \delta^{(d)}(\vec{r}), \qquad (39)
$$

$$
\delta H_{\text{hfs}} = -\frac{4\pi Z\alpha}{dm_p} g_p(\vec{s}_p \cdot \vec{s}_\mu)_\epsilon G'_M(0) \nabla^2 \delta^{(d)}(\vec{r}). \tag{40}
$$

and where  $[1/r]_{\epsilon}$  denotes a d-dimensional generalization of the  $1/r$  potential. The corresponding correction to the hyperfine splitting of order  $(Z\alpha)^6$  is

$$
\delta E_L = 2 \left\langle \delta V \frac{1}{(E_0 - H_0)'} H_{\text{hfs}} \right\rangle + \langle \delta H_{\text{hfs}} \rangle. \tag{41}
$$

Calculating matrix elements in  $d$  dimensions and using  $G'_E(0) = -r_p^2/6$ ,  $G'_M(0) = -r_m^2/6$ , with  $r_p$  and  $r_m$  being charge and magnetic radius of the nucleus, respectively, we obtain the following expression for the lowenergy part,

$$
\delta E_L = \frac{4}{d} (r_p Z \alpha)^2 E_F \left[ -\frac{1}{4\epsilon} - \frac{1}{n} - \frac{1}{2} + \gamma - \ln \frac{n}{2} + \right. \\
\left. + \Psi(n) + \ln(Z\alpha) + \frac{r_m^2}{4r_p^2 n^2} \right].\n\tag{42}
$$

The singularity  $\sim 1/\epsilon$  in the above equation will cancel out with  $\delta E_H$ .

# B. High-energy part

In the high-energy part  $\delta E_H$ , the lepton momentum is of the order of the inverse of the nuclear size, so one can employ the scattering approximation. Specifically,  $\delta E_H$ is given by the forward three-photon exchange amplitude, which can be represented by the three diagrams shown in Fig. [1.](#page-5-0) The resulting expression is

$$
\delta E_H = \delta E_{H1} + \delta E_{H2} + \delta E_{H3} \qquad (43)
$$
  
\n
$$
\delta E_{H1} = \psi^2(0) \int \frac{d^d p}{(2\pi)^d} \int \frac{d^d q}{(2\pi)^d} \langle \bar{t} | e \vec{\gamma} \cdot \vec{A} (-\vec{p}) \rangle
$$
  
\n
$$
\times \frac{1}{\not{p} - 1} \gamma^0 V(\vec{p} - \vec{q}) \frac{1}{\not{q} - 1} \gamma^0 V(\vec{q}) | t \rangle ,
$$
  
\n
$$
\delta E_{H2} = \psi^2(0) \int \frac{d^d p}{(2\pi)^d} \int \frac{d^d q}{(2\pi)^d} \langle \bar{t} | \gamma^0 V (-\vec{p}) \rangle
$$
  
\n
$$
\times \frac{1}{\not{p} - 1} \gamma^0 V(\vec{p} - \vec{q}) \frac{1}{\not{q} - 1} e \vec{\gamma} \cdot \vec{A}(\vec{q}) | t \rangle ,
$$
  
\n
$$
\delta E_{H3} = \psi^2(0) \int \frac{d^d p}{(2\pi)^d} \int \frac{d^d q}{(2\pi)^d} \langle \bar{t} | \gamma^0 V (-\vec{p}) \rangle
$$
  
\n
$$
\times \frac{1}{\not{p} - 1} e \vec{\gamma} \cdot \vec{A} (\vec{p} - \vec{q}) \frac{1}{\not{q} - 1} \gamma^0 V(\vec{q}) | t \rangle ,
$$

where  $t = (1, \vec{0}), \not\equiv (1, \vec{p})^{\nu} \gamma_{\nu}$ , and

<span id="page-4-0"></span>
$$
A^{i}(q) = \frac{i Z e g_p}{4 m_p} \sigma_p^{ik} \frac{q^k}{q^2} G_M(q^2).
$$
 (44)

After performing Dirac algebra,  $\delta E_H$  can be expressed in the coordinate representation as

<span id="page-4-4"></span>
$$
\delta E_H = \frac{8\psi^2(0)}{dm_p} (Z\alpha)^3 g_p \langle \vec{s}_p \cdot \vec{s}_\mu \rangle_\epsilon
$$
  
 
$$
\times \int d^d r \left( 2\pi \rho_M(r) [\mathcal{V}_E^{(2)}]^2 + \mathcal{V}_M \mathcal{V}_E \mathcal{V}_E^{(2)} \right) (45)
$$

where d-dimensional potentials  $\mathcal{V}_E$  and  $\mathcal{V}_M$  are defined in Appendix [A.](#page-9-3) The first term under the integral sign is convergent due to the presence of  $\rho_M$  and thus can be evaluated in three dimensions. The second term, however, contains a singularity  $\sim 1/\epsilon$ , which has to be separated out. This is achieved by splitting the domain of integration into  $(0, \Lambda)$  and  $(\Lambda, \infty)$ . The integral over  $(\Lambda, \infty)$  is evaluated by using the asymptotic form of the potentials in d dimensions. The final result for the high-energy part is

$$
\delta E_H = \frac{4}{d} (r_p Z \alpha)^2 E_F \left[ \frac{1}{4\epsilon} + \ln r_{pp} + \frac{1}{2} + \gamma \right]. \tag{46}
$$

<span id="page-4-3"></span>Here,  $r_{pp}$  is the effective radius defined by

<span id="page-4-5"></span>
$$
\ln \frac{r_{pp}}{r_p} = \frac{1}{G_E'(0)} \int_0^\infty dr \ln \frac{r}{r_p} \frac{d}{dr} r^3 \left\{ 2\pi \rho_M(r) [V_E^{(2)}]^2 + V_M V_E V_E^{(2)} + \frac{1}{r^2} \left( \frac{r}{2} - \frac{G_E'(0)}{r} \right) \right\}, \quad (47)
$$

where  $V_{E(M)}$  are three-dimensional versions of potentials  $\mathcal{V}_{E(M)}$ , which depend on electric and magnetic formfactors, and are presented in Appendix [A.](#page-9-3)

The final result for the elastic three-photon exchange correction,  $\delta^{(2)} E_{\text{fns}} = \delta E_L + \delta E_H$ , with m restored from dimensional analysis, is

$$
\delta^{(2)} E_{\text{fns}} = \frac{4}{3} E_F (mr_p Z \alpha)^2 \left[ -\frac{1}{n} + 2\gamma - \ln \frac{n}{2} + \Psi(n) + \ln(mr_{pp} Z \alpha) + \frac{r_m^2}{4r_p^2 n^2} \right].
$$
\n(48)

This expression is valid for any nucleus, both for muonic and electronic atoms.

For the dipole parametrization of the nuclear formfactors

<span id="page-4-2"></span><span id="page-4-1"></span>
$$
G_E(q) = G_M(q) = \frac{1}{(1 + q^2/\Lambda^2)^2},
$$
\n(49)

one easily obtains the following results

$$
r_m = r_p
$$
,  $r_Z/r_p = \frac{35}{16\sqrt{3}}$ ,  $r_{pp}/r_p = 5.274565...$ , (50)

which are independent of parameter  $\Lambda$  and thus valid for any nucleus. Numerical values of the elastic  $(Z\alpha)^2 E_F$ correction for the  $1S$  and  $2S$  states of muonic hydrogen are

$$
\delta^{(2)} E_{\text{fns}}(\mu \text{H}) = \begin{cases}\n-0.0093 \,\text{meV}, & \text{for the } 1S \text{ state}, \\
-0.00096 \,\text{meV}, & \text{for the } 2S \text{ state}.\n\end{cases}
$$
\n(51)

The above result for the 2S state deviates from the value of −0.00065 meV calculated by Indelicato [\[20\]](#page-10-14) and quoted by Antognini et al. [\[21\]](#page-10-15) (entry h21 in Table III of that work). One of possible reasons could be the inclusion of the reduced mass in Indelicato's calculation, while our result is obtained in the nonrecoil limit. We claim that the recoil effect on this relativistic correction cannot be accounted for in terms of the reduced mass. Our analytic result is verified by a numerical calculation in the following subsection.



<span id="page-5-0"></span>FIG. 1: Three diagrams representing contributions to the high-energy part  $\delta E_H$ . Wavy lines represent magnetic photons carrying potential [\(44\)](#page-4-0), and dashed lines are electric photons carrying potential [\(35\)](#page-3-1).

#### C. Numerical verification

The analytical expression [\(48\)](#page-4-1) for the fns correction of order  $(Z\alpha)^2 E_F$  has been verified by comparison with the numerical evaluation of the fns correction to all orders in  $Z\alpha$ . Specifically, the numerical all-order fns correction was obtained by evaluating the expectation value of the Fermi-Breit operator  $H_{\mu}$  with solutions of the Dirac equation with an extended nucleus and subtracting the point-nucleus result. The (extended-nucleus) Fermi-Breit operator is

$$
H_{\mu} = \frac{|e|}{4\pi} \frac{\alpha \cdot [\mu \times r]}{r^3} F(r) , \qquad (52)
$$

where  $\mu$  is the nuclear magnetic moment operator,  $\alpha$ is the vector of Dirac matrices, and  $F(r)$  describes the radial distribution of the magnetic moment,  $F(r) \approx 1$ outside of the nucleus. For the dipole parametrization [\(49\)](#page-4-2), the distribution function is given by

$$
F(r) = 1 - e^{-\lambda r} \left( 1 + \lambda r + \frac{1}{2} (\lambda r)^2 \right),\tag{53}
$$

where  $\lambda = 2\sqrt{3}/r_m$ .

We define the relativistic fns correction that contains orders  $(Z\alpha)^2 E_F$  and higher by subtracting the Zemach contribution from the numerical fns correction,

<span id="page-5-2"></span>
$$
\delta^{(2+)}E_{\text{fns}} = E_{\text{fns},\text{num}} - \delta E_{\text{Zem}}. \tag{54}
$$

Results for the relativistic fns correction are presented in Fig. [2,](#page-5-1) which demonstrates agreement between the numerical and analytical approaches for  $Z = 0$ . The difference between the numerical and analytical results scales linearly with Z, representing the contribution of orders  $(Z\alpha)^3 E_F$  and higher.

# IV. THREE-PHOTON EXCHANGE NUCLEAR STRUCTURE CORRECTION

In this section we address the inelastic three-photon exchange nuclear-structure correction  $\sim (Z \alpha)^2 E_F$  to the



<span id="page-5-1"></span>FIG. 2: Numerical and analytical results for the fns correction normalized by the factor of  $E_F(Z\alpha)^2$ , for the 1S state of muonic hydrogen-like ions with the nuclear root-mean-square radius 1 fm, as a function of nuclear charge Z. Solid line and dots (red) represent numerical results [\(54\)](#page-5-2); dashed line (green) shows analytical results [\(48\)](#page-4-1); dotted line and triangles (blue) show the difference.

hyperfine splitting, which has not been studied in the literature so far. We will perform an approximate treatment of this correction and evaluate the largest contribution, namely that due to the electric dipole polarizability. Furthermore, we will demonstrate partial cancellations occurring between the elastic and inelastic parts for the case of muonic deuterium,  $\mu$ D.

The nuclear-structure correction  $\delta^{(2)}E_{\text{nucl}}$  can be represented as a sum of several contributions,

<span id="page-5-3"></span>
$$
\delta^{(2)}E_{\text{nucl}} = \delta E_{\text{DP}} + \delta E_L(D) + \delta E_H(p) + \delta E_H(pn) \tag{55}
$$

where  $\delta E_{\rm DP}$  is the low-energy dipole polarizability contribution,  $\delta E_L(D)$  is the elastic low-energy part, and  $\delta E_H(p)$  and  $\delta E_H(pn)$  are the high-energy corrections.

It is convenient to introduce the common factor

$$
\mathcal{E} = \frac{4\pi\,\alpha}{3m_p}\,\psi^2(0)\,,\tag{56}
$$

which will frequently appear in formulas below.

## A. Elastic low-energy contribution

The elastic low-energy part  $\delta E_L(D)$  can be obtained from Eq. [\(42\)](#page-4-3) by replacing the proton charge  $r_p$  and magnetic  $r_m$  radii with their deuteron counterparts  $r_d$  and  $r_{md}$ , because at low energies muon sees the nucleon as a whole. The resulting expression is

$$
\delta E_L(D) = \frac{4}{d} (r_d \alpha)^2 \mathcal{E} \left[ -\frac{1}{4\epsilon} - \frac{1}{n} - \frac{1}{2} + \gamma - \ln \frac{n}{2} + \Psi(n) + \ln \alpha + \frac{r_{md}^2}{4r_d^2 n^2} \right] g_d \langle \vec{s}_d \cdot \vec{s}_\mu \rangle_\epsilon, \quad (57)
$$

where  $\langle \vec{s}_d \cdot \vec{s}_\mu \rangle_\epsilon$  is defined in Eq. [\(A3\)](#page-9-4).

## B. Polarizability contribution

We derive here the leading dipole polarizability correction  $\delta E_{\rm DP}$  and represent it as a sum of two terms

$$
\delta E_{\rm DP} = \delta E_{\rm DP1} + \delta E_{\rm DP2} \tag{58}
$$

The first one  $\delta E_{\text{DP1}}$  is obtained by taking the secondorder matrix element with dipole interaction in the nonrelativistic approximation and perturbing it with the magnetic dipole-dipole interaction  $H_{\text{hfs}}$ . The result is

$$
\delta E_{\rm DP1} = \alpha^2 \delta_{\rm hfs} \left\langle \psi \phi_N \middle| \vec{R} \cdot \vec{\nabla} \left[ \frac{1}{r} \right]_{\epsilon} \right\rangle
$$
\n
$$
\times \frac{1}{E_N + E_0 - H_N - H_0} \vec{R} \cdot \vec{\nabla} \left[ \frac{1}{r} \right]_{\epsilon} \left| \psi \phi_N \right\rangle.
$$
\n(59)

Here,  $\vec{R}$  is the proton position with respect to the deuteron mass center and  $\delta_{\rm hfs}$  denotes the first-order perturbation due to the hyperfine interaction  $H_{\text{hfs}}$  which is an analog of  $H_{\text{hfs}}$  in Eq. [\(38\)](#page-3-2) for the deuterium

$$
H_{\text{hfs}} = \frac{4\pi\alpha}{dm_p} \delta^{(d)}(\vec{r}) g_d(\vec{s}_d \cdot \vec{s}_\mu)_\epsilon,\tag{60}
$$

where  $H_N$  is the nuclear Hamiltonian and  $H_0$  is the nonrelativistic muon Hamiltonian defined in Eq. [\(37\)](#page-3-3). The perturbative treatment of  $H_{\text{hfs}}$  means that the polarizability correction is expressed as a sum of two terms, originating from perturbations of the denominator and the wave function. However, the first term vanishes and  $\delta E_{\rm DP1}$  becomes

$$
\delta E_{\rm DP1} = 2\alpha^2 \left\langle \psi \phi_N \left| \vec{R} \cdot \vec{\nabla} \left[ \frac{1}{r} \right]_{\epsilon} \frac{1}{E_0 + E_N - H_0 - H_N} \vec{R} \cdot \vec{\nabla} \left[ \frac{1}{r} \right]_{\epsilon} \frac{1}{(E_0 - H_0)'} H_{\rm hfs} \right| \psi \phi_N \right\rangle, \tag{61}
$$

Because we are interested in the leading correction only, we neglect the D-wave in the ground deuteron state and neglect the Coulomb corrections, so

$$
\delta E_{\rm DP1} = \frac{12}{d^2} \alpha^2 \mathcal{E} \sum_{\Lambda} \left\langle \phi_N \right| \vec{R} \left| \Lambda \right\rangle \left\langle \Lambda \right| \vec{R} \left| \phi_N \right\rangle g_d \left\langle \vec{s}_d \cdot \vec{s}_\mu \right\rangle_\epsilon \int \frac{d^d p}{(2\pi)^d} \frac{d^d q}{(2\pi)^d} \frac{4\pi}{p^2} \frac{4\pi}{q^2} \frac{\vec{p} \cdot \vec{q}}{(\vec{p} - \vec{q})^2} \frac{2}{p^2 + 2\Lambda} . \tag{62}
$$

After integration we obtain the following expression for the polarizability correction

$$
\delta E_{\rm DP1} = \frac{4}{d} (r_s \alpha)^2 \mathcal{E} \left( \frac{1}{4\epsilon} + \frac{2}{3} - \frac{1}{2} \ln 2 \bar{E} \right) \langle g_d \vec{s}_d \cdot \vec{s}_\mu \rangle_\epsilon \,, \tag{63}
$$

where  $\bar{E}$  is the mean excitation energy defined by

<span id="page-6-0"></span>
$$
\ln \frac{\bar{E}}{m} = \frac{1}{r_s^2} \left\langle \phi_N \left| \vec{R} \ln \left[ \frac{(H_N - E_N)}{m} \right] \vec{R} \right| \phi_N \right\rangle. \tag{64}
$$

and  $r_s$  is the deuteron structure radius

$$
r_s = \sqrt{\langle R^2 \rangle} \,. \tag{65}
$$

The mean excitation energy [\(64\)](#page-6-0) was calculated in Ref. [\[19\]](#page-10-13) using the AV18 potential [\[12\]](#page-10-6), with the result

$$
\bar{E} = 7.37(7) \,\text{MeV}.\tag{66}
$$

The pion-less EFT in the next-to-leading order [\[22\]](#page-10-16) reproduces this result with 2 % accuracy.

The second dipole polarizability contribution  $\delta E_{\text{DP2}}$ is the Coulomb distortion correction to the leading twophoton exchange contribution  $\delta E_{\text{pol1}}$  in Eq. [\(22\)](#page-2-1). We derive it by considering the nonrelativistic formula for the second order correction to energy that comes from the electric dipole interaction and the magnetic quadrupole term in Eq.  $(20)$ 

$$
\delta E_{\rm DP2} = 4\pi \alpha^2 \frac{g_p - g_n}{dm_p} \langle \vec{s}_d \cdot \vec{s}_\mu \rangle_\epsilon \delta_C \left\langle \psi \phi_N | \vec{R} \cdot \vec{\nabla} \left[ \frac{1}{r} \right]_\epsilon \frac{1}{H_0 + H_N - E_0 - E_N} \vec{R} \cdot \vec{\nabla} \delta(\vec{r}) | \psi \phi_N \right\rangle, \tag{67}
$$

where  $\delta_C$  denotes the Coulomb correction, namely that beyond  $E_{\text{pol1}}$  in Eq. [\(22\)](#page-2-1). This Coulomb correction is the forward scattering three-photon exchange amplitude, which takes the following form in the momentum representation

$$
\delta E_{\rm DP2} = \frac{3\alpha^2}{d} \frac{g_p - g_n}{g_d} E_F \sum_{\Lambda'} \langle \phi_N | R^k | \Lambda \rangle \langle \Lambda | R^i | \phi_N \rangle \int \frac{d^d p}{(2\pi)^d} \frac{d^d q}{(2\pi)^d} \frac{4\pi p^k}{p^2} \frac{4\pi q^i}{\frac{q^2}{2} + \Lambda} \left[ \frac{1}{\frac{p^2}{2} + \Lambda} \frac{1}{|\vec{p} - \vec{q}|^2} + \frac{2}{|\vec{p} - \vec{q}|^4} \right]. \tag{68}
$$

After integration we obtain for  $\delta E_{\text{DP2}}$ 

$$
\delta E_{\rm DP2} = \frac{4}{3} (\alpha r_s)^2 \frac{g_p - g_n}{g_d} E_F \left( \frac{3}{4} - \ln 2 \right) \tag{69}
$$

Its value is heavily suppressed by the numerical factor in the parentheses.

#### C. High-energy contribution  $\delta E_H(pn)$

When muon momentum is of the order of the inverse of internucleon distance, the muon sees different positions of the proton and the neutron inside the nucleus, and effectively one can discern which photon interacts with which nucleon in the three-photon exchange. Because one can neglect the nuclear excitation energy in comparison to the muon kinetic energy, the high-energy contribution can be represented as an expectation value of the effective interaction potential,

$$
\delta E_H(pn) = \langle \phi_N | \delta V_H | \phi_N \rangle \,, \tag{70}
$$

where

$$
\delta V_H = \psi^2(0) \int \frac{d^d p}{(2\pi)^d} \int \frac{d^d q}{(2\pi)^d} \left[ \delta V_{H1} + \delta V_{H2} + \delta V_{H2} \right],\tag{71}
$$

and

$$
\delta V_{H1} = \langle \bar{t} | e \vec{\gamma} \cdot \vec{A}_a (-\vec{p}) e^{i \vec{p} \cdot \vec{R}_a} \frac{1}{\not p - 1} \gamma^0 V_b (\vec{p} - \vec{q}) e^{i (\vec{q} - \vec{p}) \cdot \vec{R}_b} \frac{1}{\not q - 1} \gamma^0 e^{-i \vec{q} \cdot \vec{R}_c} V_c(\vec{q}) | t \rangle ,
$$
  
\n
$$
\delta V_{H2} = \langle \bar{t} | \gamma^0 V_c (-\vec{p}) e^{i \vec{p} \cdot \vec{R}_c} \frac{1}{\not p - 1} \gamma^0 V_b (\vec{p} - \vec{q}) e^{i (\vec{q} - \vec{p}) \cdot \vec{R}_b} \frac{1}{\not q - 1} e^{-i \vec{q} \cdot \vec{R}_a} e \vec{\gamma} \cdot \vec{A}_a(\vec{q}) | t \rangle ,
$$
  
\n
$$
\delta V_{H3} = \langle \bar{t} | \gamma^0 V_b (-\vec{p}) e^{i \vec{p} \cdot \vec{R}_b} \frac{1}{\not p - 1} e \vec{\gamma} \cdot \vec{A}_a (\vec{p} - \vec{q}) e^{i (\vec{q} - \vec{p}) \cdot \vec{R}_a} \frac{1}{\not q - 1} \gamma^0 e^{-i \vec{q} \cdot \vec{R}_c} V_c(\vec{q}) | t \rangle .
$$

 $\sqrt{ }$ 

Indices  $(a, b, c) \in \{p, n\}$  discern whether the interacting nucleon is the proton or the neutron. We neglect all the contributions where the electric photon interacts with the neutron  $(b = c = p)$  and thus are left with two cases. We first consider the case when the magnetic photon hits the neutron  $(a = n)$ . This gives the following correction

$$
\delta E_H(pn) = \frac{8\psi^2(0)}{dm_p} \alpha^3 g_n \langle \vec{s}_n \cdot \vec{s}_\mu \rangle_\epsilon \qquad (72)
$$

$$
\times \left\langle \phi_N \middle| \int d^d r \left( 2\pi \rho_M (\vec{r} + 2 \vec{R}) \left[ \mathcal{V}_E^{(2)} \right]^2 \right. \right.
$$

$$
+ \mathcal{V}_M (\vec{r} + 2 \vec{R}) \mathcal{V}_E \mathcal{V}_E^{(2)} \left. \middle| \phi_N \right\rangle,
$$

which is almost the same as Eq. [\(45\)](#page-4-4), but has magnetic terms shifted by the proton-neutron distance. All the potentials in Eq.  $(72)$  are functions of r, unless explicitly written and magnetic potentials refer to the neutron formfactor, while electric ones to the proton one, both through definitions [\(A5\)](#page-9-5). The treatment of Eq. [\(72\)](#page-7-0) follows the same pattern as that of Eq. [\(45\)](#page-4-4). The only difference is that magnetic factors are shifted by  $2 \vec{R}$ , which leads to additional terms. The result is

<span id="page-7-0"></span>
$$
\delta E_H(pn) = \frac{4}{d} (r_p \alpha)^2 \mathcal{E} g_n \langle \vec{s}_n \cdot \vec{s}_\mu \rangle_\epsilon
$$
  
 
$$
\times \left( \frac{1}{4\epsilon} + \gamma - \frac{1}{2} + \frac{3r_{pn}^2 + 2r_s^2}{r_p^2} + \ln 2r_l \right), \quad (73)
$$

where  $r_l$  is defined as

<span id="page-7-2"></span><span id="page-7-1"></span>
$$
\ln(2mr_l) = \langle \phi_N | \ln(2mR) | \phi_N \rangle \tag{74}
$$

and its value can be found in Table [I.](#page-8-0) The effective

proton-neutron radius  $r_{pn}$  in Eq. [\(73\)](#page-7-1) is defined as

$$
2\pi r_{pn}^2 = \left\langle \phi_N \right| \int d^3r \left( 2\pi \rho_M (\vec{r} + 2\,\vec{R}) [V_E^{(2)}]^2 \right) \tag{75}
$$

$$
~~+V_M(\vec{r}+2\,\vec{R})\,V_E\,V_E^{(2)}+\frac{1}{|\vec{r}+2\,\vec{R}|}\left(\frac{1}{2}-\frac{G_E'(0)}{r^2}\right)\Bigg)\Bigg|\phi_N\Bigg>
$$

.

where  $\rho_M$  and  $V_M$  correspond to the neutron, while  $G_E$ and  $V_E$  correspond to the proton. It is worth noting that in the point-nucleon limit the proton-neutron effective radius  $r_{pn}$ , given by Eq. [\(75\)](#page-8-1), is equal to the deuteron structure radius  $(r_{pn} \rightarrow r_s)$ .

#### D. High-energy contribution  $\delta E_H(p)$

In the case when all three photons interact with the proton, one should use the complete four-vector current, as in the two-photon case. We are not able to perform such a calculation at present, and thus we assume that the dominating contribution comes from the elastic part in the nonrecoil limit,

$$
\delta E_H(p) = \frac{4}{d} (r_p \alpha)^2 \mathcal{E} \left[ \frac{1}{4\epsilon} + \ln r_{pp} + \frac{1}{2} + \gamma \right] g_p \left\langle \vec{s}_p \cdot \vec{s}_\mu \right\rangle_\epsilon. \tag{76}
$$

#### E. Total three-photon exchange correction

Summing all contributions in Eq. [\(55\)](#page-5-3) and restoring  $m$ 's from dimensional analysis, we obtain the threephoton nuclear-structure correction of order  $(Z \alpha)^2 E_F$ for  $\mu D$ ,

$$
\delta^{(2)}E_{\text{nucl}} = \frac{4}{3}(m\alpha)^{2}E_{F}\left[r_{pn}^{2}\frac{3g_{n}}{2g_{d}} + r_{md}^{2}\frac{1}{4n^{2}} + r_{s}^{2}\left(\frac{g_{n}}{g_{d}} - \gamma\right) + \frac{g_{p} - g_{n}}{g_{d}}\left(\frac{3}{4} - \ln 2\right) + \frac{1}{6} - \frac{1}{2}\ln\frac{2\bar{E}}{m}\right) + r_{d}^{2}\left(2\gamma - \frac{1}{n} - \ln\frac{n}{2} + \Psi(n) + \ln\alpha\right) + r_{p}^{2}\left(g_{p}\ln(mr_{pp}) + g_{n}\ln(2mr_{l}) - g_{n}\right)\frac{1}{2g_{d}}\right].
$$
\n(77)

In deriving this final formula we made use of an approximate identity  $\langle g_d\vec{s}_d\rangle \approx \langle g_p\vec{s}_p + g_n\vec{s}_n\rangle /$  to cancel out the  $\epsilon$  singularity and  $\langle \vec{s}_p \rangle = \langle \vec{s}_n \rangle = \langle \vec{s}_d \rangle /2$  for further simplifications. Numerical values for all parameters in the final formula are listed in Table [I.](#page-8-0)

Our final results for the three-photon exchange deuteron structure correction  $\delta^{(2)}E_{\text{nucl}}$  are presented in Table [II.](#page-9-6) We assume a 25 % uncertainty of these results, due to neglect of the polarizability corrections beyond the electric dipole contribution and of the unknown inelastic proton contribution, although we must admit that we can not well justify this uncertainty estimate.

<span id="page-8-1"></span><span id="page-8-0"></span>TABLE I: Effective radii and g-factors for the three-photon nuclear-structure correction for  $\mu$ D, given by Eq. [\(77\)](#page-8-2). Proton-neutron radius  $r_{pn}$  is taken in the point-nucleon limit  $(r_{pn} = r_s)$  and  $r_l$  is obtained with the AV18 potential [\[12\]](#page-10-6)

Variable	Value	Units	Source
$r_p$	0.84087(39)	fm	Ref. [23]
$r_d$	2.1256(8)	fm	Ref. [24]
$r_s$	1.954661(79)	fm	Ref. [19]
$r_{md}$	2.312(10)	fm	Ref. [25]
$r_{pp}$	4.435	fm	Eq. $(47)$
$r_{pn}$	1.955	fm	Eq. (75)
$r_{pZ}$	0.883(19)	fm	Ref. [15]
$r_{nZ}$	0.06(1)	fm	Ref. [16]
$r_l$	1.339	fm	Eq. (74)
$g_p$	5.585694702(17)		Ref. [26]
$g_d$	0.8574382311(48)		Ref. [26]
$g_n$	$-3.82608545(90)$		Ref. [26]

Our results for the three-photon exchange structure correction disagree with corresponding formulas obtained by Faustov *et al.* [\[3\]](#page-9-2) (given by Eqs.  $(55)$ ,  $(58)$ , and (59) of that work). The reason for this disagreement is two-fold. First, Faustov et al. considered only the lowenergy part of the nuclear-structure correction, omitting completely the high-energy part. Second, the term proportional to the deuteron magnetic radius  $r_{md}$  in their calculation contains an additional factor of  $1/n^3$ , due to a mistake in evaluation of the matrix element presented in Eq. [\(A8\)](#page-9-7).

### V. SUMMARY

<span id="page-8-2"></span>A summary of all known nuclear-structure contributions to the hyperfine splitting of the 1S and 2S states in  $\mu$ D is presented in Table [II.](#page-9-6) We find that the total theoretical result for the deuteron structure correction for the 2S state differs from the experimental value by about  $5\sigma$ . A possible reason for this discrepancy might be our insufficient knowledge of the spin-dependent coupling of nucleus to the electromagnetic field, in particular the unknown corrections to the nonrelativistic current in Eq. [\(31\)](#page-3-0). Another possible reason could be a mistake in calculations of QED effects for the point nucleus, although it looks much less probable since these calculations were performed independently by two groups [\[2,](#page-9-1) [3\]](#page-9-2).

Summarizing, in the present work we have calculated the two- and three-photon exchange nuclear structure corrections to the hyperfine splitting of the  $nS$  states in  $\mu$ D. The obtained results disagree with the previous theoretical calculation [\[3\]](#page-9-2) and with the experimental result [\[4\]](#page-10-0).

<span id="page-9-6"></span>TABLE II: Nuclear structure corrections for hyperfine splitting of the 1S and 2S states of muonic deuterium, in meV. Numerical results are obtained with the AV18 potential [\[12\]](#page-10-6).

Correction	1S	2S	Source
$\delta E_{\rm{pol1}}$	$-1.1007$	$-0.1376$	Eq. $(22)$
$\delta E_{\rm pol2}$	$-0.0823$	$-0.0103$	Eq. (25)
$\delta E_{\rm pol3}$	0.1513	0.0189	Eq. $(26)$
$\delta E_{\rm pol4}$	$-0.1979$	$-0.0283$	Eq. $(30)$
$\delta E_{\rm{pol}5}$	$-0.0327$	$-0.0041$	Eq. $(32)$
$\delta E_{\rm pol}$	$-1.2623(631)$	$-0.1578(79)$	Eq. $(33)$
$\delta E_{\rm 1nucl}$	$-0.9450(224)$	$-0.1181(28)$	Eq. (15)
$\delta E_{\rm Low}$	2.566	0.3208	Eq. (14)
$\delta^{(1)}E_{\text{nucl}}$	0.3587(670)	0.0448(84)	Eq. $(12)$
$\delta^{(2)}E_{\rm nucl}$	$-0.0547(137)$	$-0.0065(16)$	Eq. (77)
$\delta E_{\text{nucl,theo}}$	0.304(68)	0.0383(86)	Eq. (8)
$\delta E_{\rm nucl,exp}$		0.0966(73)	Eq. (7)
difference		0.0583(113)	

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# <span id="page-9-3"></span>Appendix A: Dimensional regularization

In order to extend spin  $\frac{1}{2}$  into d dimensions, we define antisymmetric tensor

$$
\sigma^{ij} = \frac{i}{2} [\gamma^i, \gamma^j], \qquad (A1)
$$

that in the three-dimensional limit simplifies to

$$
\sigma^{ij} \stackrel{d \to 3}{=} 2\varepsilon^{ijk} s^k. \tag{A2}
$$

Additionally, for the deuteron we define  $\sigma_d^{ij} = \sigma_p^{ij} + \sigma_n^{ij}$ and use the following convenient notation

$$
(\vec{s}_a \cdot \vec{s}_b)_\epsilon = \frac{1}{8} \sigma_a^{ij} \sigma_b^{ij} \tag{A3}
$$

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Throughout our calculations we extensively used the following result for the general d-dimensional integral,

$$
\int \frac{d^d p}{(2\pi)^d} \frac{4\pi}{p^n} e^{i\vec{p}\cdot\vec{r}} = 2^{2-n}\pi^{1-d/2} \frac{\Gamma\left(\frac{d-n}{2}\right)}{\Gamma\left(\frac{n}{2}\right)} r^{n-d}.
$$
 (A4)  
Two special cases are of particular importance (with  $d =$ 

 $3 - 2\epsilon$ :

<span id="page-9-5"></span>
$$
\mathcal{V}(r) = \int \frac{d^d p}{(2\pi)^d} \frac{4\pi}{p^2} e^{i\vec{p}\cdot\vec{r}} = \pi^{\epsilon-1/2} \Gamma(1/2 - \epsilon) \frac{1}{r^{1-2\epsilon}},
$$
  

$$
\mathcal{V}^{(2)}(r) = \int \frac{d^d p}{(2\pi)^d} \frac{4\pi}{p^4} e^{i\vec{p}\cdot\vec{r}} = \frac{1}{4} \pi^{\epsilon-1/2} \Gamma(-1/2 - \epsilon) r^{1+2\epsilon}.
$$

We define also the associated potentials:

$$
\mathcal{V}_X = 4\pi \int \frac{d^d p}{(2\pi)^d} \frac{G_X(p^2)}{p^2} e^{i\vec{p}\cdot\vec{r}},
$$
  

$$
\mathcal{V}_X^{(2)} = 4\pi \int \frac{d^d p}{(2\pi)^d} \frac{G_X(p^2)}{p^4} e^{i\vec{p}\cdot\vec{r}},
$$
 (A5)

where  $X \in \{E, M\}$ . Asymptotic forms of these potentials at  $r \to \infty$  are:

$$
\mathcal{V}_X \rightarrow \mathcal{V} + \text{local terms},
$$
  

$$
\mathcal{V}_X^{(2)} \rightarrow \mathcal{V}^{(2)} + G'_X(0)\mathcal{V} + \text{local terms}.
$$

The corresponding three-dimensional potentials are

$$
V_X = 4\pi \int \frac{d^3 p}{(2\pi)^3} \frac{G_X(p^2)}{p^2} e^{i\vec{p}\cdot\vec{r}},
$$
  

$$
V_X^{(2)} = 4\pi \int \frac{d^3 p}{(2\pi)^3} \frac{[G_X(p^2) - 1]}{p^4} e^{i\vec{p}\cdot\vec{r}},
$$
 (A6)

with the asymptotic form

$$
V_X \rightarrow \frac{1}{r} + \text{local terms},
$$
  

$$
V_X^{(2)} \rightarrow -\frac{r}{2} + \frac{G'_X(0)}{r} + \text{local terms}. \tag{A7}
$$

Furthermore, we point out that in the framework of dimensional regularization the following matrix element vanishes

<span id="page-9-7"></span>
$$
\langle \vec{p} \; \delta^{(d)}(\vec{r}) \; \vec{p} \rangle = 0. \tag{A8}
$$

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