Nuclear structure corrections in muonic deuterium

Krzysztof Pachucki

Faculty of Physics, University of Warsaw, Hoża 69, 00-681 Warsaw, Poland
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The muonic hydrogen experiment measuring the $2P - 2S$ transition energy [R. Pohl *et al.*, Nature **466**, 213 (2010)] is significantly discrepant with theoretical predictions based on quantum electrodynamics. A possible approach to resolve this conundrum is to compare experimental values with theoretical predictions in another system, muonic deuterium μD. The only correction which might be questioned in μD is that due to the deuteron polarizability. We investigate this effect in detail and observe cancellation with the elastic contribution. The total value obtained for the deuteron structure correction in the $2P - 2S$ transition is 1.680(16) meV.

The determination of electromagnetic properties of nuclei from precise atomic spectroscopy has become possible due to significant progress in atomic structure theory, which in turn is based on quantum electrodynamics (QED). The proton charge radius as obtained from the Lamb shift in hydrogen [1] is more accurate than any determination using electron scattering, including the most recent ones [2, 3], and in agreement with them. The determination of the deuteron charge radius from the measurement of the hydrogen-deuterium isotope shift in the 2S-1S transition frequency [4, 5], apart from being the most accurate, has stimulated reanalysis of the electron scattering data. At present the atomic isotope shift determinations of charge radii for helium, lithium and beryllium atoms are not only the most accurate ones, but also the only ones available for short lived isotopes [6].

It was a great surprise that the proton charge radius r_p determined from the muonic hydrogen Lamb shift [7] gave a result in conflict with the value determined from electronic hydrogen. The $5\,\sigma$ discrepancy in r_p is the first indication that our knowledge of interactions in these simple atomic systems is not complete. While we will not pursue the possible explanations of the proton charge radius discrepancy, we point attention to the critical test which can be performed with muonic deuterium. The electronic H-D isotope shift gives a very accurate difference for the deuteron and proton charge radii. If the results for the difference between μD and μH are consistent with the electronic H-D, this would mean that there is an extra muon-proton interaction, which cancels out in the μH-μD difference. In order to draw these conclusions, all other effects contributing to the isotope shift have to be analyzed. The only correction which goes beyond the standard QED treatment is that due to the nuclear polarizability, and is in general due to the nuclear structure. It is the purpose of this work to study these effects in muonic deuterium.

Before this, however, we note that there is no unique definition of the charge radius for all nuclei. It depends on the nuclear spin, and in particular, there is no established definition for spin 1 nuclei, such as the deuteron. The mean square charge radius $\langle R^2 \rangle$ for an arbitrary spin I particle is defined through the effective interaction with the electromagnetic field

$$
\begin{aligned}
\delta H \; = \; & e\,A^0 - e\,\vec{d}\cdot\vec{E} - e\left(\frac{\langle R^2\rangle}{6} + \frac{\delta_I}{M^2}\right)\vec{\nabla}\cdot\vec{E} \\
& -\frac{e}{2}\,Q\,(I^i\,I^j)^{(2)}\,\nabla^j E^i - \vec{\mu}\cdot\vec{B}
\end{aligned}
\tag{1}
$$

where μ and Q are the magnetic dipole and the electric quadrupole moments. For a scalar particle $\delta_0 = 0$, and for a half-spin particle $\delta_{1/2} = 1/8$. For a vector and higher spin particle we proceed as follows. The most general Lagrangian for particle with spin $I = 1$, which includes terms linear in the electromagnetic field strength F is [8]

$$
\begin{aligned}
\mathcal{L} \; = \; & -\frac{1}{2}\,u^{*\mu\nu}\,u_{\mu\nu} + m^2\,u^{*\mu}\,u_\mu \\
& + \frac{i\,e}{2}\,(g - 1)\,(u_\mu^*\,u_\nu - u_\mu\,u_\nu^*)\,F^{\mu\nu} \\
& + \frac{i\,e}{4}\left(Q + \frac{g-1}{m^2}\right)(u_{\mu\nu}^*\,u_\lambda - u_{\mu\nu}\,u_\lambda^*)\,\partial^\lambda F^{\mu\nu}
\end{aligned}
\tag{2}
$$

where $u_{\mu\nu} = \nabla_\mu u_\nu - \nabla_\nu u_\mu$, $\nabla_\mu = \partial_\mu + i\,e\,A_\mu$, and $F^{\mu\nu} = \partial^\mu A^\nu - \partial^\nu A^\mu$. The effective nonrelativistic Hamiltonian obtained from Eq. (2) gives the $\vec{\nabla}\cdot\vec{E}$ term with the coefficient $e\,Q/6$ [9]. What part of this coefficient should be included in the charge radius, and what in the kinematical term δ_I? The most natural assumption is that $\langle R^2 \rangle = 0$ for a point $I = 1$ particle. One possible choice for a point vector particle is $g = 1$, $Q = 0$, and another one $g = 2$, $Q = -1/m^2$. The second choice has the advantage that it leads to the renormalized QED theory of a charged vector particle, while the first choice leads to the simplest form of the Lagrangian. In this work, following [10], we adopt the first choice, and consequently assume for a vector and a higher spin particle $\delta_I = 0$. This assumption affects the relativistic recoil correction, while the finite nuclear size correction is

$$
E_{FS} = \frac{2\,\pi\,\alpha}{3}\,\phi^2(0)\langle R^2\rangle,
\tag{3}
$$

where $\phi^2(0) = (m_r\,\alpha)^3/(\pi\,n^3)\,\delta_{l0}$, and m_r is the μD reduced mass.

Having defined the leading finite size effect, we proceed to the evaluation of nuclear structure corrections. A nucleus is not a rigid particle, it can be excited by an orbiting electron or muon, which results in the shift of atomic energies. In the following, we derive general formulas for the nuclear polarizability shift with any Hamiltonian for deuterium, using the perturbation expansion in the muon mass m over the deuteron mass m_D, including the so called Coulomb correction. Here, the deuteron binding energy counts as m^2/m_D. With the assumed accuracy relativistic effects for the muon, as well as for the deuteron, can be treated perturbatively and we start derivation from the leading electric dipole excitations. The nonrelativistic formula for the electric dipole nuclear (scalar) polarizability correction is

$$\delta E = \alpha^2 \left\langle \phi \, \phi_D \left| \frac{\vec{d}\cdot\vec{r}}{r^3} \frac{1}{E_D + E_0 - H_D - H_0} \frac{\vec{d}\cdot\vec{r}}{r^3} \right| \phi \, \phi_D \right\rangle \tag{4}$$

where H_0 is the nonrelativistic Coulomb Hamiltonian for the muon with reduced mass m_r. Denoting the nuclear excitation energy by E, the polarizability correction is

$$\delta E = \frac{\alpha^2}{3} \int_{E_T} dE \, |\langle\phi_D|\vec{d}|E\rangle|^2 \left\langle \phi \left| \frac{\vec{r}}{r^3} \frac{1}{E_0 - H_0 - E} \frac{\vec{r}}{r^3} \right| \phi \right\rangle \tag{5}$$

The nuclear excitation energy E is much larger than a typical atomic (muonic deuterium) excitation energy, thus one may perform the large E expansion of the muonic matrix element. The appropriate formula for this expansion is

$$\left\langle \phi \left| \frac{\vec{r}}{r^3} \frac{1}{H_0 - E_0 + E} \frac{\vec{r}}{r^3} \right| \phi \right\rangle$$
$$= 4\pi\,\phi^2(0)\sqrt{\frac{2\,m_r}{E}} + c_1\frac{\alpha^4\,m_r^4}{E} - c_2\frac{\alpha^5\,m_r^4}{E}\sqrt{\frac{2\,m_r}{E}} + \ldots, \tag{6}$$

where

$$c_1(2S) = \frac{1}{8} + \frac{1}{2}\ln\left(\frac{2\,m_r\,\alpha^2}{E}\right), \quad c_2(2S) = \frac{21}{32} + \frac{\pi^2}{12},$$
$$c_1(2P) = \frac{1}{24}, \qquad\qquad c_2(2P) = \frac{1}{16}. \tag{7}$$

From this expansion, the leading electric dipole polarizability correction is [12]

$$\delta_0 E = -\frac{4\pi\,\alpha^2}{3}\,\phi^2(0)\int_{E_T} dE\,\sqrt{\frac{2\,m_r}{E}}\,|\langle\phi_D|\vec{d}|E\rangle|^2, \tag{8}$$

while the leading Coulomb correction, written explicitly for $2P-2S$ transition, is

$$\delta_{C1} E = \frac{\alpha^6\,m_r^4}{6}\int_{E_T}\frac{dE}{E}\,|\langle\phi_D|\vec{d}|E\rangle|^2\left[\frac{1}{6}+\ln\left(\frac{2\,m_r\,\alpha^2}{E}\right)\right]$$
$$= \frac{\alpha^5\,m_r^4}{4}\,\alpha_E\left[\frac{1}{6}+\ln\left(\frac{2\,m_r\,\alpha^2}{\bar{E}}\right)\right] \tag{9}$$

where α_E is the electric dipole polarizability of a nucleus

$$\alpha_E = \frac{2\,\alpha}{3}\int_{E_T}\frac{dE}{E}\,|\langle\phi_D|\vec{d}|E\rangle|^2 \tag{10}$$

and $\bar{E}$ is the mean excitation energy. Both of them have already been accurately calculated for the deuteron, namely $\alpha_E = 0.6330(13)$ fm^3 and $\bar{E} = 4.94$ MeV [11]. Our numerical results obtained in this work are in an agreement with them. We shall mention that the formula for the leading Coulomb correction in $1S$ and $2S$ states was first obtained by Friar in [12].

The next to leading Coulomb correction, which has not been considered so far, written explicitly for $2P-2S$ transition, is

$$\delta_{C2} E = -\frac{1}{6}\left(\frac{19}{32}+\frac{\pi^2}{12}\right)\alpha^7 m_r^3\int_{E_T} dE\left(\frac{2\,m_r}{E}\right)^{3/2}|\langle\phi_D|\vec{d}|E\rangle|^2 \tag{11}$$

The dipole operator $\vec{d}$ is the position $\vec{R}$ of the proton with respect to the deuteron mass center. It is thus assumed that there are no corrections to the electric dipole operator, and for example mass center of the proton coincides with the charge center of the proton within the nucleus. The uncertainty introduced by this approximation is unknown. This is due to the fact that the underlying QCD theory is nonperturbative and the resulting exact theory of nuclear forces is not yet known.

In the evaluation of further corrections we take the infinite nuclear mass limit, thus neglecting nuclear recoil. The relativistic corrections to the electric dipole polarizability effects can be obtained from the two-photon exchange amplitude [13]

$$\delta E = i\,e^4\,\phi^2(0)\frac{1}{3}\int_{E_T} dE\langle\phi_D|\vec{d}|E\rangle^2\int\frac{d\omega}{2\pi}$$
$$\int\frac{d^3k}{(2\pi)^3}\frac{1}{E+\omega}\left(1+\frac{2\omega^4}{(\omega^2-k^2)^2}\right)$$
$$\times\frac{4}{(\omega^2+2\,m\,\omega-k^2)(\omega^2-2\,m\,\omega-k^2)}. \tag{12}$$

The nuclear excitation energy E is much smaller than the muon mass m and the nonrelativistic contribution comes from the region $\omega \approx E$ and $k \approx \sqrt{2\,m\,E}$. Thus to obtain it one neglects ω^2 and ω^4. The leading nonrelativistic term agrees with that in Eq. (8), with the reduced mass m_r replaced by a muon mass m. Relativistic correction comes from the next terms in the small E expansion, namely

$$\delta_R E = i\,e^4\,\phi^2(0)\frac{1}{3}\int_{E_T} dE\langle\phi_D|\vec{d}|E\rangle^2\int\frac{d\omega}{2\pi}$$
$$\int\frac{d^3k}{(2\pi)^3}\frac{1}{E+\omega}\frac{8\omega^2\,k^2}{(k^2-2\,m\,\omega)^2(k^2+2\,m\,\omega)^2}$$
$$= \frac{2\pi\,\alpha^2}{3}\,\phi^2(0)\int_{E_T} dE\,\sqrt{\frac{E}{2\,m}}\,|\langle\phi_D|\vec{d}|E\rangle|^2. \tag{13}$$

This is the only relativistic correction which is not negligible at our level of accuracy.

The corrections due to higher multipole polarizabilities and higher order corrections due to the finite deuteron size can be treated together, and we show that they cancel each other at the leading order. Let us consider at first the related muonic matrix element P for the nonrelativistic two-photon exchange

$$P = \left\langle \phi \left| \frac{\alpha}{|\vec{r} - \vec{R}|} \frac{1}{(H_0 - E_0 + E)} \frac{\alpha}{|\vec{r} - \vec{R}'|} \right| \phi \right\rangle, \quad (14)$$

where H_0 is the nonrelativistic Hamiltonian for the muon in the nonrecoil limit, and $\vec{R}$ is a position of proton with respect to the nuclear mass center. Using on mass shell approximation with subtractions of the leading Coulomb interaction, the finite size, and the electric dipole polarizability, it becomes

$$P = \alpha^2 \phi^2(0) \int \frac{d^3 q}{(2\pi)^3} \left(\frac{4\pi}{q^2} \right)^2 \left(E + \frac{q^2}{2m} \right)^{-1}$$
$$\left[e^{i\vec{q}\cdot(\vec{R} - \vec{R}')} - 1 + \frac{q^2}{6}(\vec{R} - \vec{R}')^2 \right] \quad (15)$$
$$\approx \frac{\pi}{3} m \alpha^2 \phi^2(0) |\vec{R} - \vec{R}'|^3 \left(1 - \frac{\sqrt{2mE}}{5} |\vec{R} - \vec{R}'| \right),$$

where we performed expansion in the small parameter $\sqrt{2mE}|\vec{R} - \vec{R}'|$. The corresponding correction to atomic energy is

$$\delta_Q E = - \sum\!\!\!\!\!\!\int dE \int d^3 R \, d^3 R' \, \phi_D^*(\vec{R}) \, \phi_E(\vec{R}) \, \phi_D(\vec{R}') \, \phi_E^*(\vec{R}) \, P \quad (16)$$

Consider now the first E-independent term. When $\phi_E = \phi_D$, it will be the elastic part know as a Zemach correction [14], but the inclusion of all excited states leads to $\delta(\vec{R} - \vec{R}')$ and the $|\vec{R} - \vec{R}'|^3$ term vanishes completely. As a result, there is no Zemach [elastic $O(\alpha^5)$] correction for muonic deuterium. From Eq. (15) only the second term remains, which gives

$$\delta_Q E = \frac{2\pi}{15} m^2 \alpha^2 \phi^2(0) \int_{E_T} dE \sqrt{\frac{E}{2m}} \int d^3 R \, d^3 R' \quad (17)$$
$$\phi_D^*(\vec{R}) \, \phi_E(\vec{R}) \, \phi_D(\vec{R}') \, \phi_E^*(\vec{R}') \, [(\vec{R} - \vec{R}')^2]^2.$$

These corrections are due to the electric dipole, the quadrupole and the monopole nuclear excitations, namely

$$\delta_Q E = \frac{2\pi}{15} m^2 \alpha^2 \phi^2(0) \int_{E_T} dE \sqrt{\frac{E}{2m}}$$
$$\left[\frac{10}{3} \langle \phi_D | R^2 | E \rangle^2 - 8 \langle \phi_D | R^i | E \rangle \langle E | R^2 R^i | \phi_D \rangle \right.$$
$$\left. + 4 \langle \phi_D | (R^i R^j - \delta^{ij} R^2/3) | E \rangle^2 \right] \quad (18)$$
$$= \delta_{Q0} E + \delta_{Q1} E + \delta_{Q2} E.$$

As we assumed at the beginning, all corrections of order $\alpha^5 m^2/m_D$ are neglected. However, due to the large magnetic moment anomaly of the proton and the neutron, we make an exception and consider the magnetic dipole polarizability correction. It comes from

$$H_{M1} = -\vec{\mu} \cdot \vec{B} = -\frac{e}{2m_p}(g_p \vec{s}_p + g_n \vec{s}_n) \cdot \vec{B}$$
$$\approx -\frac{e(g_p - g_n)}{2m_p} \frac{(\vec{s}_p - \vec{s}_n)}{2} \cdot \vec{B}, \quad (19)$$

where $g_p = 5.586$, and $g_n = -3.826$. We use the analogous two-photon exchange formula as for the electric dipole transitions

$$\delta_M E = i e^2 \phi^2(0) \int \frac{d\omega}{2\pi} \int \frac{d^3 k}{(2\pi)^3} \frac{\delta^{ik}}{\omega^2 - k^2} \frac{\delta^{jl}}{\omega^2 - k^2}$$
$$\times \mathrm{Tr} \left[\left(\gamma^j \frac{1}{\not{p} - \not{k} - m} \gamma^i + \gamma^i \frac{1}{\not{p} + \not{k} - m} \gamma^j \right) \frac{(\gamma^0 + I)}{4} \right]$$
$$\times \left\langle \phi_D \left| (\vec{\mu} \times \vec{k})^k \frac{1}{E_D - H_D - \omega} (\vec{\mu} \times \vec{k})^l \right| \phi_D \right\rangle \quad (20)$$

and perform the nonrelativistic approximation:

$$\delta_M E = \frac{8\pi\alpha^2}{3} \phi^2(0) \left(\frac{g_p - g_n}{4m_p} \right)^2$$
$$\times \int_{E_T} dE \sqrt{\frac{E}{2m}} \langle \phi_D | \vec{s}_p - \vec{s}_n | E \rangle^2 \quad (21)$$

Corrections due to the intrinsic proton polarizability and the proton Zemach moment are to a good approximation the same as in muonic hydrogen. Therefore, we use a recent result of very thorough calculations [15] $\Delta E(2S) = -36.9(2.4)\,\mu\mathrm{eV}$ and scale it by a factor

$$\delta_P E = -\Delta E(2S) \, m_{rD}^3 / m_{rH}^3. \quad (22)$$

The final expression for the nuclear polarizability combined with the elastic contribution is

$$\Delta E = \delta_0 E + \delta_C E + \delta_R E + \delta_Q E + \delta_M E + \delta_P E. \quad (23)$$

Numerical calculation of deuteron matrix elements are performed using the discrete variable representation (DVR) [16] method. In the DVR method, the Hamiltonian is represented as a symmetric matrix, which can be diagonalized and all formulas represented as a finite sum over the spectrum. Numerical results using the modern nucleon-nucleon AV18 potential from Argonne National Laboratory [17], are presented in Table I. We have checked numerics by the calculation of the electric dipole polarizability, and our result $\alpha_d = 0.634$ fm^3 is close to the recommended value from [11]. The difference of about 0.001 fm^3 comes from the fact that we take into account a small neutron-proton mass difference in the electric dipole operator.

Surprisingly, the total value ΔE is close to the nonrelativistic electric dipole polarizability contribution $\delta_0 E +$

TABLE I: Nuclear structure corrections in muonic deuterium for $2P - 2S$ transition.

correction	value in meV
$\delta_0 E$	1.910
$\delta_{C1} E$	-0.255
$\delta_{C2} E$	-0.006
$\delta_R E$	-0.035
$\delta_{Q0} E$	-0.045
$\delta_{Q1} E$	0.151
$\delta_{Q2} E$	-0.066
$\delta_M E$	-0.016
$\delta_P E$	0.043(3)
ΔE	1.680(16)

$\delta_{C1} E + \delta_{C2} E = 1.649$ meV. This means that relativistic and higher multipole corrections, although individually not small, tend to cancel between themselves. For the final uncertainty, we assume 50% of these higher order corrections. We can not at this moment give a more reliable estimate of uncertainty, but note that it is about 20 times smaller than the discrepancy in muonic hydrogen.

Our result for the nuclear structure correction ΔE is not in good agreement with former calculations. Leidemann and Rosenfelder in [18] obtained for the polarizability correction of 2S state the result $-1.500(25)$ meV. This should be combined with the elastic contribution obtained by Martynenko [19] of -0.37 meV and the Coulomb correction of 0.26 meV, which totals to $-1.61(3)$ meV. This is 2σ away from our result, shown in Table I. The difference may come from three sources. The first one is lack of clear separation between the elastic contribution from [19] and the inelastic one from [18], thus some terms might be counted twice. The second one

is neglect in [18] of the intrinsic proton polarizability correction of 0.013 meV [15]. The third source is the extra coefficient $R_\mu = 0.9778$ used in [18] for the polarizability correction, which reflects the fact that probability of finding muon within the deuteron is not exactly $\phi^2(0)$ but $R_\mu \phi^2(0)$. To verify this coefficient one has to investigate three photon exchange correction, details are beyond the scope of this work but we claim lack of such coefficient.

In order to shed light on the proton charge radius discrepancy, we consider the difference $E_D(2P - 2S) - E_H(2P - 2S)\, m_{rD}^3/m_{rH}^3$, where the proton size and the proton polarizability cancel out. This difference is sensitive to the deuteron structure radius, which is known from a very accurate H-D$(2S - 1S)$ isotope shift [5]. If agreement between experiment and theoretical predictions based on QED calculations [20, 21] including nuclear polarizability correction calculated in this work is observed, this may mean that the muonic hydrogen discrepancy is caused by a local ($\sim$ fm) muon-proton interaction or by a 5σ shift in the Rydberg constants [7]. There could be as well a different source of the discrepancy, a long-range type interaction ($\sim$ 200 fm), and this will not cancel out in the H-D difference, and a small discrepancy in μD will persist in this case.

In summary, we have demonstrated in this work that accurate predictions for muonic deuterium are feasible, the non-QED corrections have been here accurately calculated, and comparison with experimental transitions in μD will give hints on a possible source of discrepancies in the proton charge radius.

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