Hyperfine structure of P states in muonic deuterium

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On the basis of the quasipotential approach to the bound-state problem in quantum electrodynamics we calculate hyperfine structure intervals $\Delta E^{\rm HFS}(2P_{1/2})$ and $\Delta E^{\rm HFS}(2P_{3/2})$ for P states in muonic deuterium. The tensor method of projection operators for the calculation of the hyperfine structure of P states with definite quantum numbers of total atomic momentum F and total muon momentum j in muonic deuterium is formulated. We take into account vacuum polarization, relativistic, quadrupole, and structure corrections of orders α^4, α^5, and α^6. The obtained numerical values of hyperfine splittings are useful for the analysis of experimental data of the CREMA collaboration regarding muonic deuterium.

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I. INTRODUCTION

The investigation of energy spectrum of light muonic atoms (muonic hydrogen, muonic deuterium, ions of muonic helium) has reached a new level at present. This is due to experimental results obtained by the CREMA Collaboration in [1–3]. On the one side these results open a possibility to obtain new values of a number of fundamental physical constants such as nuclear charge radii. While experimental data on atomic transitions have become very precise, our knowledge of the charge radii, which are part of theoretical predictions, is not as accurate as we would like. On the other hand, they call us to look again at the formulation of the theory of bound states in quantum electrodynamics (QED) and possibly revise some of its previous aspects. The second position was proved important after a series of experiments in [1,3] which revealed essential disagreement between two values of the proton charge radius obtained in experiments with electronic and muonic atoms [1,3,4]. An analysis of the situation and determining the causes of discrepancies are investigated in several directions, which are widely discussed in [2,5–13]. It is possible that the publication of new experimental data on the structure of the energy levels of muonic deuterium which is planned in near future will help clarify the problem. A comparison of the theory and experiment for the transition frequencies $\nu(2^{2F+1}P_j–2^{2F'+1}S_{j'})$ in muonic deuterium demands careful consideration of different contributions to the energy P levels. The calculations of fine and hyperfine structure of the energy spectrum of light muonic atoms were made in a series of papers [14–16]. The results of these studies are a reliable benchmark for a comparison with experimental data and provide a starting point for further research. Whereas the calculation of separate contributions to the hyperfine structure of S states of the muonic deuterium, even with a very specific kind, was the subject of intense study, the hyperfine structure of P states was much less investigated. Therefore, in this study we aim to partly fill this gap. In this work we perform an analysis of different corrections to hyperfine splittings of P states which allow us to obtain more accurate results important for a comparison with experimental data. Another aim of our study is to develop a method of projection operators in the investigation of the energy structure of P states. The method of projection operators on the bound states with definite spins was used previously in [17,18] for the construction of particle interaction operator for the hyperfine structure of S states.

II. GENERAL FORMALISM

Let us begin our consideration with basic contributions to hyperfine structure of P states of order α^4. Our approach to the calculation of hyperfine splittings is based on the quasipotential method in quantum electrodynamics in which the two-particle bound state is described by the Schrödinger equation [19–21]. The quasipotential V entering this equation is constructed in QED perturbation theory by means of off-shell two-particle scattering amplitude T projected onto the positive frequency states at zero relative energies of the particles:

$$\begin{aligned} V &= V^{(1)} + V^{(2)} + V^{(3)} + \dots, \\ T &= T^{(1)} + T^{(2)} + T^{(3)} + \dots, \end{aligned} \tag{1}$$

$$V^{(1)} = T^{(1)}, \;\; V^{(2)} = T^{(2)} - T^{(1)} G^f T^{(1)}, \dots, \tag{2}$$

where G^f is a free two-particle Green's function entering into iteration terms of the quasipotential. The leading-order contribution to the quasipotential (the Breit Hamiltonian) is determined by the amplitude of one-photon interaction which we denote below $T_{1\gamma}$. The hyperfine part of the Breit Hamiltonian $\Delta V_B^{\rm HFS}$ is written explicitly in Appendix A in coordinate representation.

In this work we develop another approach to the calculation of hyperfine structure of muonic deuterium based on the tensor

representation of P-wave projection operators describing muonic deuterium states. First we show in an example of calculating the leading-order contributions how a tensor formalism helps investigate the hyperfine structure of the spectrum. It is useful to work in momentum representation where we can write the wave function of the muonic deuterium $2P$ state in the tensor form:

$$\psi_{2P}(\mathbf{p}) = (\varepsilon n_p) R_{21}(p), \tag{3}$$

where ε_δ is the polarization vector of orbital motion, $n_p = (0,\mathbf{p}/p)$, $R_{21}(p)$ is the radial wave function in momentum space. Then the energy shifts are presented in integral form:

$$\Delta E^{\rm HFS} = \int (\varepsilon^* n_q) R_{21}(q) \frac{d\mathbf{q}}{(2\pi)^{3/2}} \times \int (\varepsilon n_p) R_{21}(p) \frac{d\mathbf{p}}{(2\pi)^{3/2}} \Delta V^{\rm HFS}(\mathbf{p},\mathbf{q}). \tag{4}$$

In the leading order the hyperfine potential $\Delta V^{\rm HFS}$ is constructed by means of one-photon interaction amplitude $T_{1\gamma}$. Writing the amplitude $T_{1\gamma}$ we refer to it a part of the bound-state wave function related to orbital motion:

$$T_{1\gamma}(\mathbf{p},\mathbf{q}) = 4\pi Z\alpha(\varepsilon^* n_q)\left[\bar u(q_1)\left(\frac{p_{1,\mu}+q_{1,\mu}}{2m_1} + (1+a_\mu)\sigma_{\mu\epsilon}\frac{k_\epsilon}{2m_1}\right)u(p_1)\right](\varepsilon n_p) D_{\mu\nu}(k) \times \varepsilon^*_{d,\rho}(q_2)\left\{g_{\rho\sigma}\frac{(p_2+q_2)_\nu}{2m_2}F_1(k^2) - \frac{(p_2+q_2)_\nu}{2m_2}\frac{k_\rho k_\sigma}{2m_2^2}F_2(k^2) + (g_{\rho\lambda}g_{\sigma\mu} - g_{\rho\mu}g_{\sigma\lambda})\frac{k_\lambda}{2m_2}F_3(k^2)\right\}\varepsilon_{d,\sigma}(p_2), \tag{5}$$

where $p_{1,2} = \frac{m_{1,2}}{(m_1+m_2)}P \pm p$ are four-momenta of initial muon and deuteron, $q_{1,2} = \frac{m_{1,2}}{(m_1+m_2)}Q \pm q$ are four-momenta of final muon and deuteron. They are expressed in terms of total two-particle momenta P,Q and relative momenta p,q. $D_{\mu\nu}(k)$ is the photon propagator which is taken to be in the Coulomb gauge. Explicit expression of the deuteron wave function $\varepsilon_{d,\sigma}(p)$ has the form

$$\varepsilon_{d,\sigma}(p_2) = \varepsilon_{d,\sigma}(0) - \frac{p_{2,\sigma} + g_{0\sigma}m_2}{\epsilon_2(p)+m_2}\frac{[\varepsilon_{d,\sigma}(0)p_2]}{m_2}. \tag{6}$$

It should be noted that the amplitude (5) has been studied in detail in [22] excepting quadrupole correction. In the center-of-mass rest frame $P = Q = Mv, v = (1,0)$. The form factors $F_{1,2,3}(k^2)$ are related to the charge, magnetic, and quadrupole deuteron form factors as ($\eta = k^2/4m_2^2$) [23,24]

$$\begin{aligned} F_C &= F_1 + \tfrac{2}{3}\eta[F_1 + (1+\eta)F_2 - F_3], \\ F_M &= F_3, \quad F_Q = F_1 + (1+\eta)F_2 - F_3. \end{aligned} \tag{7}$$

We consider (5) as a starting point for a composition of orbital $\mathbf{L}$ momentum, the deuteron spin $\mathbf{s}_2$ (note that the spin of the nucleus is usually denoted by $\mathbf{I}$), and muon spin $\mathbf{s}_1$. In the first scheme of momentum composition we add first momenta $\mathbf{L}$ and $\mathbf{s}_1$ obtaining two muon states with angular momenta $j = 1/2$ and $j = 3/2$. In the Rarita-Schwinger formalism the wave function of the state with half-integer spin $3/2$ is described by

$$\psi_{\mu,\alpha}(\mathbf{p},\sigma) = \sum_{\lambda,\omega}\left\langle \frac{1}{2}\omega; 1\lambda \middle| \frac{3}{2}\sigma\right\rangle \varepsilon_\mu(\mathbf{p},\lambda) u_\alpha(\mathbf{p},\omega), \tag{8}$$

where $\langle \frac{1}{2}\omega; 1\lambda \,|\, \frac{3}{2}\sigma\rangle$ are the Clebsch-Gordon coefficients. Another sequence of angular momentum addition is that in the beginning we add the orbital and intrinsic angular momentum of the deuteron and then the muon spin. When we combine the $L = 1$ and $s_2 = 1$ we get three states with the deuteron momenta $2,1,0$. The deuteron wave function has in this case the form

$$\phi_{\mu\nu}(\mathbf{p},\gamma) = \sum_{\lambda_1,\lambda_2}\langle 1\lambda_1; 1\lambda_2 \,|\, 2\gamma\rangle \varepsilon_\mu(\mathbf{p},\lambda_1)\varepsilon_\nu(\mathbf{p},\lambda_1). \tag{9}$$

After combining $\phi_{\mu\nu}$ with the muon spin on the second stage there arise three states with $F = 5/2,3/2,1/2$ which are described by the tensor-spinor field $\Psi_{\mu\nu}$ satisfying to the Dirac equation

$$(\hat v - 1)\Psi_{\mu\nu} = 0, \;\; v^\mu \psi_{\mu\nu} = 0. \tag{10}$$

The field $\Psi_{\mu\nu}$ can be easily decomposed into different parts with definite atomic angular momentum F:

$$F^P = \frac{5}{2}^- : \Psi_{\mu\nu}; \tag{11}$$

$$F^P = \frac{3}{2}^- : \Psi^S_{\mu\nu} = \frac{1}{\sqrt{10}}(\gamma_{\perp\mu}\gamma_5\psi_\nu + \gamma_{\perp\nu}\gamma_5\psi_\mu), \tag{12}$$

$$F^P = \frac{3}{2}^- : \Psi^A_{\mu\nu} = \frac{1}{\sqrt{2}}(\gamma_{\perp\mu}\gamma_5\psi_\nu - \gamma_{\perp\nu}\gamma_5\psi_\mu), \tag{13}$$

$$F^P = \frac{1}{2}^- : \Psi^A_{\mu\nu} = \frac{1}{2\sqrt{6}}[\gamma_{\perp\mu},\gamma_{\perp\nu}], \tag{14}$$

$$F^P = \frac{1}{2}^- : \Psi^S_{\mu\nu} = \frac{1}{\sqrt{3}}(g_{\mu\nu} - v_\mu v_\nu), \tag{15}$$

where $\Psi_{\mu\nu}$ is the usual $5/2$ generalized, symmetric Rarita-Schwinger tensor spinor [25,26]. The negative parity is obvious for physical reasons. Different states with total momentum $F = 1/2$ and $F = 3/2$ are decomposed into symmetric and antisymmetric parts satisfying (10). The tensor-spinor wave functions were used previously in [27] for the bound states of quarks. For further calculations, we note that each field $\Psi^{S,A}_{\mu\nu}$ with $F = 3/2,1/2$ is a superposition of states with muon angular momentum $j = 1/2$ and $j = 3/2$. Introduced in (11)–(15) tensor-spinor fields can be considered as projection operators on the states with a definite value of the total angular momentum. These projectors are very convenient for the calculation of the matrix elements of the interaction potential corresponding to certain quantum numbers. They allow us to avoid direct cumbersome multiplication of different factors in the amplitudes of the interaction of particles and use the computer methods for calculating amplitudes and the energy shifts [28].

To demonstrate this property of $\Psi_{\mu\nu}$ we continue our calculations of the amplitude (5) corresponding to transitions between states with definite values of F. Introducing projectors $\Psi_{\mu\nu}$ in (5) and averaging the amplitude over the projection of the total angular momentum $\mathcal{M}$ we obtain the following basic relation:

$$\begin{aligned}\overline{T_{1\gamma}(\mathbf{p},\mathbf{q})} = {}& \frac{4\pi Z\alpha}{2F+1} n_q^{\delta} n_p^{\omega} \mathrm{Tr}\left\{\left[\sum_{\mathcal{M}=-F}^{F} \Psi^{\mathcal{M}}_{\omega\sigma_1}\bar{\Psi}^{\mathcal{M}}_{\delta\rho_1}\right]\frac{[m_1(\hat{v}+1)-\boldsymbol{\gamma}\mathbf{q}]}{2m_1}\Gamma_\mu\frac{[m_1(\hat{v}+1)-\boldsymbol{\gamma}\mathbf{p}]}{2m_1}\right\}\\ &\times\left\{g_{\rho\sigma}\frac{(p_2+q_2)_\nu}{2m_2}F_1(k^2)-\frac{(p_2+q_2)_\nu}{2m_2}\frac{k_\rho k_\sigma}{2m_2^2}F_2(k^2)+(g_{\rho\lambda}g_{\sigma\mu}-g_{\rho\mu}g_{\sigma\lambda})\frac{k_\lambda}{2m_2}F_3(k^2)\right\}D_{\mu\nu}(k)\\ &\times\left[g_{\rho\rho_1}-\frac{1}{2m_2^2}(m_2v_{\rho_1}-q_{\rho_1})(2m_2v_\rho-q_\rho)\right]\left[g_{\sigma\sigma_1}-\frac{1}{2m_2^2}(m_2v_{\sigma_1}-p_{\sigma_1})(2m_2v_\sigma-p_\sigma)\right],\end{aligned}\tag{16}$$

where the lepton vertex function $\Gamma_\mu=\frac{p_{1,\mu}+q_{1,\mu}}{2m_1}+(1+a_\mu)\sigma_{\mu\epsilon}\frac{k_\epsilon}{2m_1}$, a_μ is the muon anomalous magnetic moment. The Lorentz factors of the Dirac bispinors and transformed Lorentz factors of deuteron wave functions are written explicitly. Inserting in (16) $\Psi_{\mu\nu}$ from (11)–(15), averaging and summing over initial- and final-state polarizations $\mathcal{M}$, and calculating the trace by means of the package Form [28], we find three matrix elements corresponding to $F=\frac{5}{2}$, $F=\frac{3}{2}$, $F=\frac{1}{2}$. The polarization sums for the fields with half-integer spin looks as follows [17,25,26]:

$$\hat{\Pi}_{\mu\nu}(F=3/2)=\sum_{\mathcal{M}=-F}^{F}\Psi^{\mathcal{M}}_{\mu}\bar{\Psi}^{\mathcal{M}}_{\nu}=\frac{(\hat{v}+1)}{2}\left[g_{\mu\nu}-\frac{1}{3}\gamma_\mu\gamma_\nu-\frac{2}{3}v_\mu v_\nu+\frac{1}{3}(v_\mu\gamma_\nu-v_\nu\gamma_\mu)\right],\tag{17}$$

$$\begin{aligned}\hat{\Pi}_{\mu\nu;\rho\sigma}(F=5/2)=\sum_{\mathcal{M}=-F}^{F}\Psi^{\mathcal{M}}_{\mu\nu}\bar{\Psi}^{\mathcal{M}}_{\rho\sigma}={}&\frac{(\hat{v}+1)}{2}\left[\frac{1}{2}\left(P^1_{\mu\rho}P^1_{\nu\sigma}+P^1_{\mu\sigma}P^1_{\nu\rho}\right)-\frac{1}{3}P^1_{\mu\nu}P^1_{\rho\sigma}\right.\\ &\left.-\frac{1}{10}\left(P^1_\mu P^1_\rho P^1_{\nu\sigma}+P^1_\nu P^1_\rho P^1_{\mu\sigma}+P^1_\mu P^1_\sigma P^1_{\nu\rho}+P^1_\nu P^1_\sigma P^1_{\mu\rho}\right)\right],\quad P^1_{\mu\nu}=g_{\mu\nu}-v_\mu v_\nu,\quad P^1_\mu=P^1_{\mu\nu}\gamma_\mu.\end{aligned}\tag{18}$$

Let us construct by this method basic hyperfine splittings of order α^4. We project the amplitude (5) sequentially on states with $j=1/2$, $F=1/2$ and $j=1/2$, $F=3/2$. Corresponding averaged amplitudes are the following:

$$\begin{aligned}\overline{T_{1\gamma}(\mathbf{p},\mathbf{q})}^{F=1/2}_{j=1/2} = {}& \frac{\pi Z\alpha}{9} n_q^{\delta} n_p^{\omega}\mathrm{Tr}\left\{(\hat{v}+1)(\gamma_{\rho_1}-v_{\rho_1})(\gamma_\delta+v_\delta)\frac{[m_1(\hat{v}+1)-\boldsymbol{\gamma}\mathbf{q}]}{2m_1}\right.\\ &\left.\times\Gamma_\mu\frac{[m_1(\hat{v}+1)-\boldsymbol{\gamma}\mathbf{p}]}{2m_1}(\gamma_\omega+v_\omega)(\gamma_{\sigma_1}-v_{\sigma_1})\right\}D_{\mu\nu}(k)\\ &\times\left\{g_{\rho\sigma}\frac{(p_2+q_2)_\nu}{2m_2}F_1(k^2)-\frac{(p_2+q_2)_\nu}{2m_2}\frac{k_\rho k_\sigma}{2m_2^2}F_2(k^2)+(g_{\rho\lambda}g_{\sigma\mu}-g_{\rho\mu}g_{\sigma\lambda})\frac{k_\lambda}{2m_2}F_3(k^2)\right\}\\ &\times\left[g_{\rho\rho_1}-\frac{1}{2m_2^2}(m_2v_{\rho_1}-q_{\rho_1})(2m_2v_\rho-q_\rho)\right]\left[g_{\sigma\sigma_1}-\frac{1}{2m_2^2}(m_2v_{\sigma_1}-p_{\sigma_1})(2m_2v_\sigma-p_\sigma)\right],\end{aligned}\tag{19}$$

$$\begin{aligned}\overline{T_{1\gamma}(\mathbf{p},\mathbf{q})}^{F=3/2}_{j=1/2} = {}& \frac{\pi Z\alpha}{6} n_q^{\delta} n_p^{\omega}\mathrm{Tr}\left\{(\hat{v}+1)\hat{\Pi}_{\sigma_1\rho_1}(F=3/2)(\gamma_\delta-v_\delta)\gamma_5\right.\\ &\left.\times\frac{[m_1(\hat{v}+1)-\boldsymbol{\gamma}\mathbf{q}]}{2m_1}\Gamma_\mu\frac{[m_1(\hat{v}+1)-\boldsymbol{\gamma}\mathbf{p}]}{2m_1}\gamma_5(\gamma_\omega-v_\omega)\right\}D_{\mu\nu}(k)\\ &\times\left\{g_{\rho\sigma}\frac{(p_2+q_2)_\nu}{2m_2}F_1(k^2)-\frac{(p_2+q_2)_\nu}{2m_2}\frac{k_\rho k_\sigma}{2m_2^2}F_2(k^2)+(g_{\rho\lambda}g_{\sigma\mu}-g_{\rho\mu}g_{\sigma\lambda})\frac{k_\lambda}{2m_2}F_3(k^2)\right\}\\ &\times\left[g_{\rho\rho_1}-\frac{1}{2m_2^2}(m_2v_{\rho_1}-q_{\rho_1})(2m_2v_\rho-q_\rho)\right]\left[g_{\sigma\sigma_1}-\frac{1}{2m_2^2}(m_2v_{\sigma_1}-p_{\sigma_1})(2m_2v_\sigma-p_\sigma)\right].\end{aligned}\tag{20}$$

In the quasipotential method each of the amplitudes (19) and (20) determines the interaction operator of particles corresponding to states with selected quantum numbers. In this case, we get not only the contributions of the hyperfine interaction, but also the Coulomb potential and a potential of fine structure. But the difference (19) and (20) allows us to find the hyperfine splitting of state $j=1/2$ which is written as an expression of the output from the Form program:

$$\begin{aligned}\overline{T_{1\gamma}(\mathbf{p},\mathbf{q})}^{\mathrm{HFS}}_{j=1/2}(F=3/2;1/2) = {}& \frac{Z\alpha}{2}\left\{\frac{m_1}{m_2\kappa_d}\left[-\frac{pq}{\mathbf{k}^2}+\frac{(\mathbf{pq})^2}{pq\mathbf{k}^2}\right]+(\kappa_d+1)\left[\frac{2(\mathbf{pq})^2}{pq\mathbf{k}^2}-\frac{(p^2+q^2)(\mathbf{pq})}{pq\mathbf{k}^2}\right]\right.\\ &\left.+2(1+\kappa_d)\left(1+\frac{a_\mu}{2}\right)\left[-\frac{pq}{\mathbf{k}^2}-\frac{(\mathbf{pq})^2}{pq\mathbf{k}^2}+\frac{(p^2+q^2)(\mathbf{pq})}{pq\mathbf{k}^2}\right]\right\},\end{aligned}\tag{21}$$

where $\kappa_d = 0.714\,025\mu_N$ is the deuteron anomalous magnetic moment [29], connected with the deuteron magnetic moment μ_d by the relation $\kappa_d = (\mu_d m_2/m_p - 1)$. In (21) we take electromagnetic form factors at $k^2 = 0$ and omit the quadrupole contribution which is studied in detail in next section. The normalization factor $3/4\pi$ coming from the wave function of orbital motion is taken into account. Two other hyperfine splittings of the $2P_{3/2}$ state looks as follows:

$$\overline{T_{1\gamma}(\mathbf{p},\mathbf{q})}^{\rm HFS}_{j=3/2}(F=3/2;1/2) = \frac{Z\alpha}{2}\left\{\frac{m_1}{m_2\kappa_d}\left[-\frac{1}{2}\frac{pq}{\mathbf{k}^2}+\frac{11}{10}\frac{(\mathbf{pq})^2}{pq\mathbf{k}^2}-\frac{3}{10}\frac{(p^2+q^2)(\mathbf{pq})}{pq\mathbf{k}^2}\right]+(\kappa_d+1)\left[\frac{(\mathbf{pq})^2}{pq\mathbf{k}^2}-\frac{1}{2}\frac{(p^2+q^2)(\mathbf{pq})}{pq\mathbf{k}^2}\right]\right.$$
$$+\frac{2}{5}(1+\kappa_d)\Big(1-\frac{a_\mu}{4}\Big)\left[-\frac{pq}{\mathbf{k}^2}-\frac{(\mathbf{pq})^2}{pq\mathbf{k}^2}+\frac{(p^2+q^2)(\mathbf{pq})}{pq\mathbf{k}^2}\right]$$
$$\left.-\frac{(\mathbf{pq})}{pq}\left[\frac{3}{2}(1+\kappa_d)-\frac{3}{10}\frac{m_1\kappa_d}{m_2}-\frac{6}{5}(1+\kappa_d)\Big(1-\frac{a_\mu}{4}\Big)\right]\right\}, \tag{22}$$

$$\overline{T_{1\gamma}(\mathbf{p},\mathbf{q})}^{\rm HFS}_{j=3/2}(F=5/2;3/2) = \frac{Z\alpha}{2}\left\{\frac{m_1}{m_2\kappa_d}\left[\frac{5}{6}\frac{pq}{\mathbf{k}^2}-\frac{1}{2}\frac{(\mathbf{pq})^2}{pq\mathbf{k}^2}-\frac{1}{6}\frac{(p^2+q^2)(\mathbf{pq})}{pq\mathbf{k}^2}\right]+(\kappa_d+1)\left[-\frac{5}{3}\frac{(\mathbf{pq})^2}{pq\mathbf{k}^2}+\frac{5}{6}\frac{(p^2+q^2)(\mathbf{pq})}{pq\mathbf{k}^2}\right]\right.$$
$$+\frac{2}{3}(1+\kappa_d)\Big(1-\frac{a_\mu}{4}\Big)\left[\frac{pq}{\mathbf{k}^2}+\frac{(\mathbf{pq})^2}{pq\mathbf{k}^2}-\frac{(p^2+q^2)(\mathbf{pq})}{pq\mathbf{k}^2}\right]$$
$$\left.-\frac{(\mathbf{pq})}{pq}\left[-\frac{5}{2}(1+\kappa_d)-\frac{1}{6}\frac{m_1\kappa_d}{m_2}+2(1+\kappa_d)\Big(1-\frac{a_\mu}{4}\Big)\right]\right\}, \tag{23}$$

where the terms proportional to $(\mathbf{pq}/pq)$ vanish as a result of the angular integration. They are important for the correct calculation of the vacuum polarization effects. There are three types of integrals with the radial wave functions which are calculated analytically:

$$J_1 = \int R_{21}(q)\frac{d\mathbf{q}}{(2\pi)^{3/2}}\int R_{21}(p)\frac{d\mathbf{p}}{(2\pi)^{3/2}}\frac{pq}{(\mathbf{p}-\mathbf{q})^2}$$
$$= \left\langle\frac{pq}{(\mathbf{p}-\mathbf{q})^2}\right\rangle = \frac{3}{16},\quad J_2 = \left\langle\frac{(\mathbf{pq})^2}{pq(\mathbf{p}-\mathbf{q})^2}\right\rangle = \frac{5}{48},$$
$$J_3 = \left\langle\frac{(\mathbf{pq})(p^2+q^2)}{pq(\mathbf{p}-\mathbf{q})^2}\right\rangle = \frac{5}{24}. \tag{24}$$

Note that the terms on the right side of the Eqs. (21)–(23) proportional to $(1+\kappa_d)$ disappear after momentum integration and we obtain the following leading-order contributions of diagonal matrix elements to hyperfine splittings of $2P_{1/2}$ and $2P_{3/2}$ states:

$$\Delta E^{\rm HFS}_{j=1/2}(F=3/2;1/2) = \frac{\alpha^4(1+\kappa_d)\mu^3}{12m_1m_2}\left[1+\frac{m_1\kappa_d}{2m_2(1+\kappa_d)}+\frac{a_\mu}{2}\right]$$
$$= 2070.5040\ \mu\text{eV}, \tag{25}$$

$$\Delta E^{\rm HFS}_{j=3/2}(F=3/2;1/2) = \frac{\alpha^4(1+\kappa_d)\mu^3}{24m_1m_2}\left[\frac{2}{5}+\frac{m_1\kappa_d}{2m_2(1+\kappa_d)}-\frac{a_\mu}{10}\right]$$
$$= 420.9426\ \mu\text{eV}, \tag{26}$$

$$\Delta E^{\rm HFS}_{j=3/2}(F=5/2;3/2) = \frac{5\alpha^4(1+\kappa_d)\mu^3}{72m_1m_2}\left[\frac{2}{5}+\frac{m_1\kappa_d}{2m_2(1+\kappa_d)}-\frac{a_\mu}{10}\right]$$
$$= 701.5712\ \mu\text{eV}. \tag{27}$$

Numerical values of hyperfine splittings in (25)–(27) and other corrections which we calculate are presented with the accuracy 0.0001 μeV. Theoretical errors in (25)–(27) which are determined by uncertainties of fundamental physical constants reach a value $2\times10^{-5}\mu$eV. So, we do not write their values exactly in the text and Tables I–III excepting the quadrupole corrections of order α^4 which are large.

Two amplitudes (19) and (20) are constructed combining first the orbital momentum and muon spin. Then the spin of the nucleus is added. We can act slightly differently expressing the states with $j = 1/2$ and $j = 3/2$ directly in terms of introduced symmetrical and antisymmetrical states. This possibility is illustrated hereinafter. In this method we can evaluate also off-diagonal matrix elements. Their calculation is demonstrated in the next section for quadrupole correction. To facilitate a comparison of the method of calculation and obtained contributions to the previous approaches we make Appendix A, which demonstrates the calculation of corrections of order α^4 in the coordinate representation. All basic contributions to hyperfine structure and numerous higher-order corrections are presented in Table I.

III. QUADRUPOLE INTERACTION CORRECTIONS

Quadrupole interaction originates from the not completely spherical shape of the deuteron. If the potential of the muon has also a nonspherical component at the position of the deuteron (only with muon angular momentum $j > 1/2$) then there exists a quadrupole energy shift [30–32]. Ordinary calculation of this contribution to hyperfine structure in muonic deuterium is based on the representation of quadrupole interaction in coordinate space as a scalar product of two irreducible tensor operators of rank 2. After that the matrix elements of tensor operators are expressed in terms of reduced matrix elements using the Wigner-Eckart theorem.

TABLE I. Diagonal matrix elements of hyperfine structure of $2P$-states in muonic deuterium

Contribution	$2\,^2P_{1/2}$ (μeV)	$2\,^4P_{1/2}$ (μeV)	$2\,^2P_{3/2}$ (μeV)	$2\,^4P_{3/2}$ (μeV)	$2\,^6P_{3/2}$ (μeV)
Leading-order α^4 correction	− 1380.3360	690.1680	8162.2889	8583.2315	9284.8027
Quadrupole correction of order α^4	0	0	433.9033 ±0.0455	− 347.1227 ±0.0364	86.7807 ±0.0091
Vacuum polarization correction of order α^5	− 1.0706	0.5353	− 0.2802	− 0.1121	0.1681
Quadrupole and vacuum polarization correction of order α^5	0	0	0.3564	− 0.2851	0.0713
Relativistic correction of order α^6	− 0.1677	0.0838	− 0.0125	− 0.0050	0.0075
Vacuum polarization correction of order α^6	− 0.0011	0.0005	− 0.0014	− 0.0006	0.0008
Structure correction of order α^6	− 0.0011	0.0021	− 0.0006	0.0010	− 0.0016
Summary contribution	− 1381.5765	690.7897	8596.2539 ±0.0455	8235.7070 ±0.0364	9371.8295 ±0.0091

In this work we develop another approach to the calculation of quadrupole interaction based on tensor representation of P-wave projection operators describing muonic deuterium states. In the case of $F = \frac{1}{2}$ and $F = \frac{3}{2}$ we should take the sum of two contributions regarding the symmetric and antisymmetric wave projection function (12)–(15). For completeness, we present two averaged amplitudes corresponding to $\Psi^S_{\mu\nu}(F = \frac{3}{2})$ and $\Psi^A_{\mu\nu}(F = \frac{3}{2})$:

$$\begin{aligned}\overline{T_{1\gamma}(\mathbf{p},\mathbf{q})}^A &= \frac{\pi\alpha}{4} n_q^\delta n_p^\omega D_{\mu\nu}(k)\mathrm{Tr}\Big\{(\hat v+1)\hat\Pi_{\sigma\delta}(\gamma_\rho - v_\rho)\frac{[m_1(1-\hat v)+\boldsymbol{\gamma}\mathbf{q}]}{2m_1}\Gamma_\mu \\ &\times \frac{[m_1(1-\hat v)+\boldsymbol{\gamma}\mathbf{p}]}{2m_1}(\gamma_\omega - v_\omega) + (\rho\to\delta,\omega\to\sigma) - (\omega\to\sigma) - (\rho\to\delta)\Big\} \\ &\times \Big\{g_{\rho\sigma}\frac{(p_2+q_2)_\nu}{2m_2}F_1(k^2) - \frac{(p_2+q_2)_\nu}{2m_2}\frac{k_\rho k_\sigma}{2m_2^2}F_2(k^2) + (g_{\rho\lambda}g_{\sigma\mu} - g_{\rho\mu}g_{\sigma\lambda})\frac{k_\lambda}{2m_2}F_3(k^2)\Big\} \\ &= -\frac{\pi\alpha Q_d}{3}\left[\frac{pq}{(\mathbf{p}-\mathbf{q})^2} - \frac{(\mathbf{pq})\left(\frac{p}{q}+\frac{q}{p}\right)}{(\mathbf{p}-\mathbf{q})^2} + \frac{(\mathbf{pq})^2}{(\mathbf{p}-\mathbf{q})^2} - \frac{1}{3}\frac{(\mathbf{pq})}{pq}\right],\end{aligned} \tag{28}$$

$$\begin{aligned}\overline{T_{1\gamma}(\mathbf{p},\mathbf{q})}^S &= \frac{\pi\alpha}{20} n_q^\delta n_p^\omega D_{\mu\nu}(k)\mathrm{Tr}\Big\{(\hat v+1)\hat\Pi_{\sigma\delta}(\gamma_\rho - v_\rho)\frac{[m_1(1-\hat v)+\boldsymbol{\gamma}\mathbf{q}]}{2m_1}\Gamma_\mu \\ &\times \frac{[m_1(1-\hat v)+\boldsymbol{\gamma}\mathbf{p}]}{2m_1}(\gamma_\omega - v_\omega) + (\rho\to\delta,\omega\to\sigma) + (\omega\to\sigma) + (\rho\to\delta)\Big\} \\ &\times \Big\{g_{\rho\sigma}\frac{(p_2+q_2)_\nu}{2m_2}F_1(k^2) - \frac{(p_2+q_2)_\nu}{2m_2}\frac{k_\rho k_\sigma}{2m_2^2}F_2(k^2) + (g_{\rho\lambda}g_{\sigma\mu} - g_{\rho\mu}g_{\sigma\lambda})\frac{k_\lambda}{2m_2}F_3(k^2)\Big\} \\ &= \frac{\pi\alpha Q_d}{15}\left[\frac{pq}{(\mathbf{p}-\mathbf{q})^2} - \frac{(\mathbf{pq})\left(\frac{p}{q}+\frac{q}{p}\right)}{(\mathbf{p}-\mathbf{q})^2} + \frac{(\mathbf{pq})^2}{(\mathbf{p}-\mathbf{q})^2} - \frac{1}{3}\frac{(\mathbf{pq})}{pq}\right],\end{aligned} \tag{29}$$

where we keep only the contribution of the quadrupole form factor $F_Q(0) = Q_d$. The index replacements designated in brackets of (28) and (29) refer to the written part of the amplitude. Remaining integration with the radial wave functions is carried out analytically:

$$J = \int \frac{d\mathbf{p}}{(2\pi)^{3/2}}R_{12}(p)\int\frac{d\mathbf{q}}{(2\pi)^{3/2}}R_{12}(q)\left[\frac{pq}{(\mathbf{p}-\mathbf{q})^2} - \frac{(\mathbf{pq})\left(\frac{p}{q}+\frac{q}{p}\right)}{(\mathbf{p}-\mathbf{q})^2} + \frac{(\mathbf{pq})^2}{(\mathbf{p}-\mathbf{q})^2}\right] = \frac{\mu^3(Z\alpha)^3}{16\pi}. \tag{30}$$

The sum of (28) and (29) multiplied by the factor (30) gives the contribution to hyperfine splitting $\frac{\alpha Q(\mu Z\alpha)^3}{48}(-\frac{4}{5}\delta_{F3/2})$. Let us present final results for other transitions:

$$\Delta E_Q^{\rm HFS} = \frac{\alpha Q_d(\mu Z\alpha)^3}{48}\left[\delta_{F1/2} - \frac{4}{5}\delta_{F3/2} + \frac{1}{5}\delta_{F5/2}\right]. \quad (31)$$

The quadrupole moment of the deuteron is taken to be $Q_d = 0.285\,783(30)$ fm^2 [33]. The result (31) coincides exactly with previous calculations made by different approaches [16]. As it follows from numerical values of (31) (see Table I) the quadrupole interaction changes the position of levels $2\,^4P_{3/2}$ and $2\,^2P_{3/2}$. We indicate in Tables I–III the error margins for contributions connected with quadrupole corrections of order α^4 which are numerically large. Other error margins are numerically negligible. Let us investigate in addition how the total angular momentum of the muon is changed in such transitions. For this purpose, build again the amplitude of single-photon exchange combining consistently muon spin with the orbital angular momentum and the deuteron spin. To be specific, we consider two diagonal matrix elements which are determined by averaged amplitudes with $j = 1/2$, $F = 1/2$ and $j = 1/2$, $F = 3/2$:

$$\overline{T_{1\gamma}(\mathbf{p},\mathbf{q})}^{F=1/2}_{(1/2)(1/2)} = \frac{\pi\alpha}{9}n_q^\delta n_p^\omega D_{\mu\nu}(k){\rm Tr}\left\{(\hat v+1)(\gamma_\rho - v_\rho)(\gamma_\delta + v_\delta)\frac{[m_1(1+\hat v) - \boldsymbol{\gamma}\mathbf{q}]}{2m_1}\Gamma_\mu\frac{[m_1(1+\hat v) - \boldsymbol{\gamma}\mathbf{p}]}{2m_1}(\gamma_\omega + v_\omega)(\gamma_\sigma - v_\sigma)\right\}$$
$$\times\left\{g_{\rho\sigma}\frac{(p_2+q_2)_\nu}{2m_2}F_1(k^2) - \frac{(p_2+q_2)_\nu}{2m_2}\frac{k_\rho k_\sigma}{2m_2^2}F_2(k^2) + (g_{\rho\lambda}g_{\sigma\mu} - g_{\rho\mu}g_{\sigma\lambda})\frac{k_\lambda}{2m_2}F_3(k^2)\right\} = 0, \quad (32)$$

$$\overline{T_{1\gamma}(\mathbf{p},\mathbf{q})}^{F=3/2}_{(1/2)(1/2)} = \frac{\pi\alpha}{6}n_q^\delta n_p^\omega D_{\mu\nu}(k){\rm Tr}\left\{(\hat v+1)\hat\Pi_{\sigma\rho}(\gamma_\delta - v_\delta)\gamma_5\frac{[m_1(1+\hat v) - \boldsymbol{\gamma}\mathbf{q}]}{2m_1}\Gamma_\mu\frac{[m_1(1+\hat v) - \boldsymbol{\gamma}\mathbf{p}]}{2m_1}\gamma_5(\gamma_\omega - v_\omega)\right\}$$
$$\times\left\{g_{\rho\sigma}\frac{(p_2+q_2)_\nu}{2m_2}F_1(k^2) - \frac{(p_2+q_2)_\nu}{2m_2}\frac{k_\rho k_\sigma}{2m_2^2}F_2(k^2) + (g_{\rho\lambda}g_{\sigma\mu} - g_{\rho\mu}g_{\sigma\lambda})\frac{k_\lambda}{2m_2}F_3(k^2)\right\} = 0, \quad (33)$$

where lower indexes of the amplitude designate the muon total angular momentum. With one side, the obtained expressions (32) and (33) explicitly show that quadrupole interaction does not contribute to diagonal matrix elements with $j = 1/2$. On the other side they demonstrate our choice of the tensor projectors on the state with $j = 1/2$:

$$\Psi^{F=1/2}_{\mu\nu}(j=1/2) = \tfrac{1}{3}\gamma_5(\gamma_\mu - v_\mu)\gamma_5(\gamma_\nu - v_\nu)\Psi, \quad (34)$$

where the spinor Ψ describes the state with total atomic momentum $F = \frac{1}{2}$. Using the Dirac algebra transformations we can expand (34) on the basis $\Psi^S_{\mu\nu}(F=\frac{1}{2})$ and $\Psi^A_{\mu\nu}(F=\frac{1}{2})$:

$$\Psi^{F=1/2}_{\mu\nu}(j=1/2) = \frac{1}{\sqrt{3}}\Psi^S_{\mu\nu}(F=1/2) + \sqrt{\frac{2}{3}}\Psi^A_{\mu\nu}(F=1/2). \quad (35)$$

The same expansion can be performed for the state with $j = 3/2$ and two states with $j = \frac{1}{2}$, $F = \frac{3}{2}$ and $j = \frac{3}{2}$, $F = \frac{3}{2}$. They looks as follows:

$$\Psi^{F=1/2}_{\mu\nu}(j=3/2) = \sqrt{\frac{2}{3}}\Psi^S_{\mu\nu}(F=1/2) - \sqrt{\frac{1}{3}}\Psi^A_{\mu\nu}(F=1/2), \quad (36)$$

$$\Psi^{F=3/2}_{\mu\nu}(j=1/2) = \sqrt{\frac{5}{6}}\Psi^S_{\mu\nu}(F=3/2) - \sqrt{\frac{1}{6}}\Psi^A_{\mu\nu}(F=3/2), \quad (37)$$

$$\Psi^{F=3/2}_{\mu\nu}(j=3/2) = -\sqrt{\frac{1}{6}}\Psi^S_{\mu\nu}(F=3/2) + \sqrt{\frac{5}{6}}\Psi^A_{\mu\nu}(F=3/2). \quad (38)$$

Using (35)–(38) we can investigate off-diagonal matrix elements corresponding to different values of muon angular momentum j. In fact, contributions with symmetric and antisymmetric tensor-spinor fields $\Psi^S_{\mu\nu}(F=\frac{1}{2},\frac{3}{2})$ and $\Psi^A_{\mu\nu}(F=\frac{1}{2},\frac{3}{2})$ are evaluated above in matrix elements (28) and (29). Thus it is necessary to use only the correct coefficients of expansions (35)–(38). As a result we obtain

$$\Delta E_Q^{\rm HFS}(j=1/2; j'=3/2) = \frac{\alpha Q_d(Z\mu\alpha)^3}{48}\left(\sqrt{2}\delta_{F(1/2)} - \frac{1}{\sqrt{5}}\delta_{F(3/2)}\right). \quad (39)$$

Numerically, all quadrupole corrections are large and presented in Tables I and II. Drawing attention to the significant value of the quadrupole corrections, we proceed to the

TABLE II. Off-diagonal matrix elements in the hyperfine structure of P-wave muonic deuterium.

Contribution to HFS	$2\,^2P_{1/2,3/2}$ (μeV)	$2\,^4P_{1/2,3/2}$ (μeV)
Leading-order α^4 correction	−126.0372	−199.2824
Quadrupole correction of order α^4	613.6320 ± 0.0644	-194.0475 ± 0.0204
Vacuum polarization correction of order α^5	−0.1437	−0.2271
Quadrupole and vacuum polarization correction of order α^5	0.0891	−0.0282
Relativistic correction of order α^6	−0.0043	−0.0067
Vacuum polarization correction of order α^6	0.0001	0.0001
Summary contribution	487.5360 ± 0.0644	-393.5918 ± 0.0204

TABLE III. Hyperfine structure of P states in muonic deuterium.

State	Energy (meV) [16]	Energy (meV)
$2\,^2P_{1/2}$	-1.4056	$-1.405\,34 \pm 0.000\,01$
$2\,^4P_{1/2}$	0.6703	$0.670\,31 \pm 0.000\,001$
$2\,^2P_{3/2}$	8.6194	$8.620\,02 \pm 0.000\,05$
$2\,^4P_{3/2}$	8.2560	$8.256\,18 \pm 0.000\,04$
$2\,^6P_{3/2}$	9.3729	$9.371\,83 \pm 0.000\,01$

consideration of other important effects within the formulated framework.

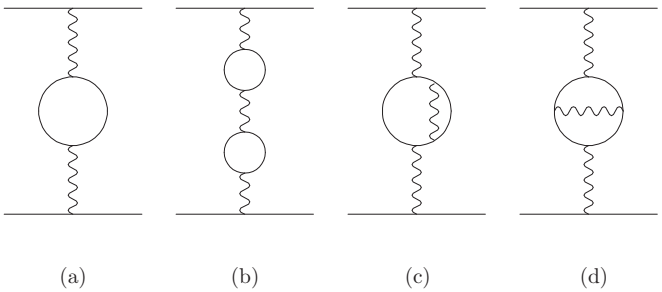

FIG. 1. Vacuum polarization effects in one-photon interaction. The wavy line represents hyperfine part of the interaction.

IV. VACUUM POLARIZATION AND STRUCTURE CORRECTIONS

The above basic formulas for the amplitudes of the muon-deuteron interaction allow us to calculate the various corrections. Next in importance are the corrections to the vacuum polarization (VP) of order α^5. In the formulated framework these effects can be easily studied. In the first-order perturbation theory the one-loop vacuum polarization contribution to hyperfine structure (HFS) is determined by the amplitude in Fig. 1. For its calculation in momentum representation which we use, the following replacement in the photon propagator should be done in (21):

$$\frac{1}{k^2} \to \frac{\alpha}{3\pi}\int_1^\infty \frac{\rho(\xi)d\xi}{k^2+4m_e^2\xi^2},\quad \rho(\xi)=\sqrt{\xi^2-1}(2\xi^2+1)/\xi^4. \tag{40}$$

As a result we find that the vacuum polarization contribution to hyperfine splittings can be expressed in terms of three-momentum integrals which are a generalization of the three integrals discussed earlier in (24):

$$I_1 = \int R_{21}(q)\frac{d\mathbf{q}}{(2\pi)^{3/2}}\int R_{21}(p)\frac{d\mathbf{p}}{(2\pi)^{3/2}}\frac{pq}{(\mathbf{p}-\mathbf{q})^2+4m_e^2\xi^2} = \left\langle\frac{pq}{(\mathbf{p}-\mathbf{q})^2+4m_e^2\xi^2}\right\rangle = \frac{a(3a+8)+6}{2(a+2)^4},\quad a=\frac{4m_e\xi}{\mu\alpha},$$
$$I_2 = \left\langle\frac{(\mathbf{pq})^2}{pq(\mathbf{p}-\mathbf{q})^2+4m_e^2\xi^2}\right\rangle = \frac{a(3a+8)+10}{6(a+2)^4},\quad I_3 = \left\langle\frac{(\mathbf{pq})(p^2+q^2)}{pq(\mathbf{p}-\mathbf{q})^2+4m_e^2\xi^2}\right\rangle = \frac{2(4a+5)}{3(a+2)^4}. \tag{41}$$

Third integration over the spectral parameter ξ also can be carried out analytically, but they are quite cumbersome. So, we present here the necessary VP correction to hyperfine splitting of the $2P_{1/2}$ state only in integral form:

$$\Delta E_{\rm VP}^{\rm HFS}(2P_{1/2}) = \frac{\mu^3\alpha(Z\alpha)^4}{3\pi m_1 m_2}\int_1^\infty \rho(\xi)d\xi\left[\frac{m_1\kappa_d}{2m_2}\frac{(3a+2)}{3(a+2)^3}+(1+\kappa_d)\Big(1+\frac{a_\mu}{2}\Big)\frac{2(3a^2+4a+2)}{3(a+2)^4}-(1+\kappa_d)\frac{a^2}{2(a+2)^4}\right]$$
$$= 1.0718\ \mu\text{eV}. \tag{42}$$

The same calculation can be performed for the $2P_{3/2}$ state. The corresponding results are the following:

$$\Delta E_{\rm VP}^{\rm HFS}(2P_{3/2})(F=3/2;1/2) = \frac{\mu^3\alpha(Z\alpha)^4}{6\pi m_1 m_2}\int_1^\infty \rho(\xi)d\xi\left[\frac{m_1\kappa_d}{2m_2}\frac{(3a+2)}{6(a+2)^3}\right.$$
$$\left.+(1+\kappa_d)\Big(1-\frac{a_\mu}{4}\Big)\frac{(15a^2+8a+4)}{3(a+2)^4}-(1+\kappa_d)\frac{2a^2}{(a+2)^4}\right] = 0.0595\ \mu\text{eV}, \tag{43}$$

$$\Delta E_{\rm VP}^{\rm HFS}(2P_{3/2})(F=5/2;3/2) = \frac{\mu^3\alpha(Z\alpha)^4}{6\pi m_1 m_2}\int_1^\infty \rho(\xi)d\xi\left[\frac{m_1\kappa_d}{2m_2}\frac{5(3a+2)}{18(a+2)^3}\right.$$
$$\left.+(1+\kappa_d)\Big(1-\frac{a_\mu}{4}\Big)\frac{2(15a^2+8a+4)}{9(a+2)^4}-(1+\kappa_d)\frac{10a^2}{3(a+2)^4}\right] = 0.0992\ \mu\text{eV}. \tag{44}$$

Another important VP effect is related to the quadrupole interaction discussed in previous section. Using for its calculation basic expression (21), (22), (23), and (41) we obtain for diagonal and off-diagonal matrix elements

$$\Delta E_{Q,\rm VP} = \frac{\mu^3\alpha(Z\alpha)^4 Q_d}{36\pi}\int_1^\infty \frac{(5a^2+8a+4)}{(a+2)^4}\rho(\xi)d\xi\left[\delta_{F(1/2)}-\frac{4}{5}\delta_{F(3/2)}+\frac{1}{5}\delta_{F(5/2)}\right]$$
$$= \left[\delta_{F(1/2)}-\frac{4}{5}\delta_{F(3/2)}+\frac{1}{5}\delta_{F(5/2)}\right]\times 0.2441\ \mu\text{eV}, \tag{45}$$

$$\Delta E_{Q,\mathrm{VP}}(j=3/2;j'=1/2)=\frac{\mu^3\alpha(Z\alpha)^4Q_d}{72\pi}\int_1^\infty\frac{(5a^2+24a+24)}{3(a+2)^4}\rho(\xi)d\xi\left[\sqrt{2}\delta_{F(1/2)}-\frac{1}{\sqrt{5}}\delta_{F(3/2)}\right]$$
$$=\left[\sqrt{2}\delta_{F(1/2)}-\frac{1}{\sqrt{5}}\delta_{F(3/2)}\right]\times 0.0630\ \mu\mathrm{eV}. \quad (46)$$

A comparison of our results (42)–(46) with earlier estimates in [16] shows that there is a significant difference of the order of tenths of μeV. For this reason we decided to perform additional validation of our results using a different method of the calculation. As was shown in [21] the vacuum polarization effects presented in Fig. 1 in first-order perturbation theory can be calculated in coordinate representation. The amplitude shown in Fig. 1(a) gives the following hyperfine interaction potential in coordinate space:

$$\Delta V^{\mathrm{HFS}}_{1\gamma,\mathrm{VP}}(r)=\frac{Z\alpha(1+\kappa_d)}{2m_1m_2r^3}\frac{\alpha}{3\pi}\int_1^\infty\rho(\xi)d\xi e^{-2m_e\xi r}\left\{\left(1+\frac{m_1\kappa_d}{m_2(1+\kappa_d)}\right)\right.$$
$$\times(\boldsymbol{L}\cdot\boldsymbol{s}_2)(1+2m_e\xi r)-(1+a_\mu)\big(4m_e^2\xi^2r^2[(\boldsymbol{s}_1\cdot\boldsymbol{s}_2)-(\boldsymbol{s}_1\cdot\boldsymbol{n})(\boldsymbol{s}_2\cdot\boldsymbol{n})]$$
$$\left.+(1+2m_e\xi r)[(\boldsymbol{s}_1\cdot\boldsymbol{s}_2)-3(\boldsymbol{s}_1\cdot\boldsymbol{n})(\boldsymbol{s}_2\cdot\boldsymbol{n})]\big)\right\}. \quad (47)$$

Averaging (47) over the Coulomb wave functions, we obtain an analytical expression for the vacuum polarization correction of order α^5 in the one-photon interaction:

$$\Delta E^{\mathrm{HFS}}_{1\gamma,\mathrm{VP}}(r)=\frac{\alpha^4\mu^3(1+\kappa_d)}{24m_1m_2r^3}\frac{\alpha}{6\pi}\int_1^\infty\rho(\xi)d\xi\int_0^\infty xdxe^{-x[1+2m_e\xi/W]}\left\{\left(1+\frac{m_1\kappa_d}{m_2(1+\kappa_d)}\right)\right.$$
$$\left.\times\overline{T_1}\left(1+\frac{2m_nj;e\xi}{W}x\right)-(1+a_\mu)\left[\frac{4m_e^2\xi^2x^2}{W^2}\overline{T_3}+\left(1+\frac{2m_e\xi}{W}x\right)\overline{T_2}\right]\right\}, \quad (48)$$

where we introduce the designations for operators T_i in (47):

$$T_1=(\boldsymbol{L}\cdot\boldsymbol{s}_2),\quad T_2=[(\boldsymbol{s}_1\cdot\boldsymbol{s}_2)-3(\boldsymbol{s}_1\cdot\boldsymbol{n})(\boldsymbol{s}_2\cdot\boldsymbol{n})],\quad T_3=[(\boldsymbol{s}_1\cdot\boldsymbol{s}_2)-(\boldsymbol{s}_1\cdot\boldsymbol{n})(\boldsymbol{s}_2\cdot\boldsymbol{n})]. \quad (49)$$

The coordinate integration in (48) is carried out analytically and numerically over the spectral parameter ξ. Numerical results for separate states include both diagonal and off-diagonal matrix elements:

$$\Delta E^{\mathrm{HFS}}_{j=1/2,\mathrm{VP}}(F=1/2)=-0.7145\ \mu\mathrm{eV},$$
$$\Delta E^{\mathrm{HFS}}_{j=1/2,\mathrm{VP}}(F=3/2)=0.3573\ \mu\mathrm{eV},$$
$$\Delta E^{\mathrm{HFS}}_{j=3/2,\mathrm{VP}}(F=1/2)=-0.0992\ \mu\mathrm{eV},$$
$$\Delta E^{\mathrm{HFS}}_{j=3/2,\mathrm{VP}}(F=3/2)=-0.0397\ \mu\mathrm{eV}, \quad (50)$$
$$\Delta E^{\mathrm{HFS}}_{j=3/2,\mathrm{VP}}(F=5/2)=0.0595\ \mu\mathrm{eV}.$$
$$\Delta E^{\mathrm{HFS}}_{(j=1/2\to j=3/2),\mathrm{VP}}(F=1/2)=-0.1111\ \mu\mathrm{eV},$$
$$\Delta E^{\mathrm{HFS}}_{(j=1/2\to j=3/2),\mathrm{VP}}(F=3/2)=-0.1757\ \mu\mathrm{eV}.$$

They evidently show that two of our approaches to the calculation of hyperfine structure in muonic deuterium P states lead to the same results. Two-loop vacuum polarization corrections shown in Fig. 1 are calculated in a similar way. They are included in Appendix C. Their numerical value is essentially smaller (see Table I).

For completeness, we analyze vacuum polarization corrections of order α^5 in second-order perturbation theory (SOPT), which are determined by the reduced Coulomb Green's function [34,35] [see the amplitude in Fig. 2(a)]:

$$G_{2P}(\boldsymbol{r},\boldsymbol{r}')=-\frac{\mu^2(Z\alpha)}{36z^2z'^2}\left(\frac{3}{4\pi}\boldsymbol{nn}'\right)e^{-(z+z')/2}g(z,z'),$$
$$g(z,z')=24z_<^3+36z_<^3z_>+36z_<^3z_>^2+24z_>^3+36z_<z_>^3$$

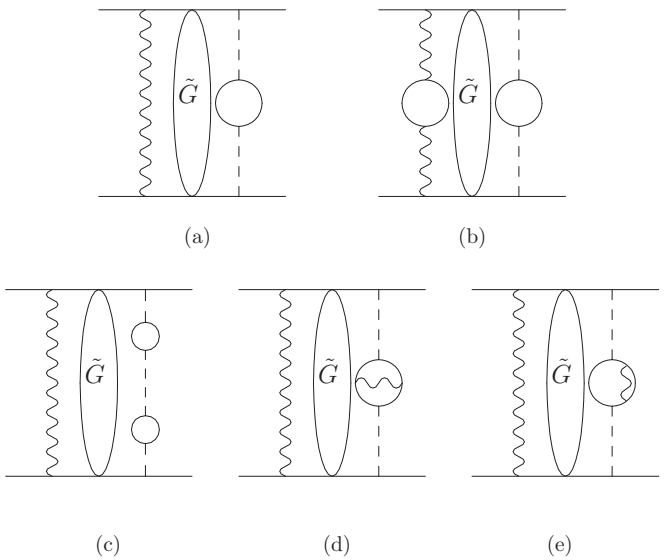

FIG. 2. Vacuum polarization effects in the second-order perturbation theory. Dashed and wavy lines represent correspondingly the Coulomb and hyperfine interactions.

$$+36z_<^2z_>^3+49z_<^3z_>^3-3z_<^4z_>^3$$
$$-12e^{z_<}(2+z_<+z_<^2)z_>^3-3z_<^3z_>^4+12z_<^3z_>^3$$
$$\times[-2C+\mathrm{Ei}(z_<)-\ln z_<-\ln z_>], \quad (51)$$

where $C=0.5772\ldots$ is the Euler constant, $z=\mathrm{Wr}, z_<=\min(z,z'), z_>=\max(z,z')$. Using (A1) and (51), we obtain the following integral expression for VP correction [21]:

$$\Delta E^{\mathrm{HFS}}_{\mathrm{VP,SOPT}}=\frac{\alpha^4\mu^3(1+\kappa_d)}{24m_1m_2}\frac{\alpha}{54\pi}\int_1^\infty\rho(\xi)d\xi\int_0^\infty dx\int_0^\infty\frac{e^{-x'}}{x'^2}dx'e^{-x(1+2m_e\xi/W)}\left[\overline{T_1}+\frac{m_1\kappa_d}{m_2(1+\kappa_d)}\overline{T_1}-(1+a_\mu)\overline{T_2}\right]. \quad (52)$$

Similarly, the correction of vacuum polarization and quadrupole interaction in second-order PT has the form:

$$\Delta E^{\mathrm{HFS}}_{\mathrm{VP},Q,\mathrm{SOPT}}=\frac{\alpha^5\mu^3Q_d}{2592\pi}\int_1^\infty\rho(\xi)d\xi\int_0^\infty dx\int_0^\infty\frac{e^{-x'}}{x'^2}dx'e^{-x(1+2m_e\xi/W)}g(x,x')\overline{[(\boldsymbol{s}_2\cdot\boldsymbol{s}_2)-3(\boldsymbol{s}_2\cdot\boldsymbol{n})(\boldsymbol{s}_2\cdot\boldsymbol{n})]}$$
$$=\begin{cases}\left(\delta_{F,1/2}-\frac{4}{5}\delta_{F,3/2}+\frac{1}{5}\delta_{F,5/2}\right)0.1120\ (\mu\mathrm{eV}), & j=j'=\frac{3}{2},\\ \left(\sqrt{2}\delta_{F,1/2}-\frac{1}{\sqrt{5}}\delta_{F,3/2}\right)0.1120\ (\mu\mathrm{eV}), & j=\frac{3}{2},j'=\frac{1}{2}.\end{cases} \quad (53)$$

The coordinate integration over x,x' is performed again analytically and numerically over ξ. Summary numerical values of contributions in the first and second orders of PT to the P-state energies are presented in Tables I and II separately for diagonal and off-diagonal matrix elements.

Based on the amplitudes (21)–(23) it is possible to find the nuclear structure correction (the index str designates this contribution) to hyperfine splittings. For this aim, we will introduce into them an additional factor $(-r_d^2\mathbf{k}^2/6)$ with the deuteron root-mean-square radius connected with the expansion of form factors and omit factors containing the deuteron magnetic moment. After evident simplifications we obtain the following contributions to hyperfine splitting potentials for states $2P_{1/2}$ and $2P_{3/2}$:

$$\overline{T_{1\gamma,\mathrm{str}}(\mathbf{p},\mathbf{q})}^{\mathrm{HFS}}_{j=1/2}(F=3/2;1/2)=\frac{Z\alpha r_d^2}{12}\left\{\frac{m_1}{m_2}\left[pq-\frac{(\mathbf{pq})^2}{pq}\right]-2\frac{(\mathbf{pq})^2}{pq}+2\left(1+\frac{a_\mu}{2}\right)\left[pq+\frac{(\mathbf{pq})^2}{pq}\right]\right\}, \quad (54)$$

$$\overline{T_{1\gamma,\mathrm{str}}(\mathbf{p},\mathbf{q})}^{\mathrm{HFS}}_{j=3/2}(F=3/2;1/2)=\frac{Z\alpha r_d^2}{12}\left\{\frac{m_1}{2m_2}\left[pq-\frac{(\mathbf{pq})^2}{pq}\right]-4\frac{(\mathbf{pq})^2}{pq}+\frac{2}{5}\left(1-\frac{a_\mu}{4}\right)\left[pq+7\frac{(\mathbf{pq})^2}{pq}\right]\right\}, \quad (55)$$

$$\overline{T_{1\gamma,\mathrm{str}}(\mathbf{p},\mathbf{q})}^{\mathrm{HFS}}_{j=3/2}(F=5/2;3/2)=\frac{Z\alpha r_d^2}{12}\left\{\frac{5m_1}{6m_2}\left[\frac{(\mathbf{pq})^2}{pq}-pq\right]+\frac{20}{3}\frac{(\mathbf{pq})^2}{pq}-\frac{2}{3}\left(1-\frac{a_\mu}{4}\right)\left[pq+7\frac{(\mathbf{pq})^2}{pq}\right]\right\}. \quad (56)$$

Further integration and consideration of the general normalization factor directly lead to the following splittings:

$$\Delta E^{\mathrm{HFS}}_{1\gamma,\mathrm{str}}(j=1/2,F=3/2;1/2)=\frac{\mu^5\alpha^6r_d^2}{16m_1m_2}\left(\frac{m_1}{m_2}+\frac{a_\mu}{2}\right)=0.0032\ \mu\mathrm{eV}, \quad (57)$$

$$\Delta E^{\mathrm{HFS}}_{1\gamma,\mathrm{str}}(j=3/2,F=3/2;1/2)=\frac{\mu^5\alpha^6r_d^2}{32m_1m_2}\left(\frac{m_1}{m_2}-a_\mu\right)=0.0016\ \mu\mathrm{eV}, \quad (58)$$

$$\Delta E^{\mathrm{HFS}}_{1\gamma,\mathrm{str}}(j=3/2,F=5/2;3/2)=-\frac{5\mu^5\alpha^6r_d^2}{96m_1m_2}\left(\frac{m_1}{m_2}-a_\mu\right)=-0.0026\ \mu\mathrm{eV}. \quad (59)$$

As expected, these corrections are very small and do not affect the comparison of theoretical results and planned experimental data. Other corrections of order α^6 are discussed in Appendixes B and C.

V. SUMMARY AND DISCUSSION

In this work we investigate the hyperfine structure of energy levels related to the P-wave states of muonic deuterium on the basis of the three-dimensional quasipotential approach in quantum electrodynamics. To increase the accuracy of the calculation we take into account the leading-order contribution and several basic corrections of order α^5 and α^6. These corrections are connected with the vacuum polarization effect, quadrupole interaction, nuclear structure, and relativistic effects. Some corrections are obtained in analytical form, but the biggest part of the contributions to the energy spectrum is presented first in integral form, and then calculated numerically. All results are presented in Tables I–III giving the values of diagonal and off-diagonal matrix elements and the positions of the P-energy levels.

We would like to point out the three main results obtained in this work.

(1) An approach based on the use of a special type of projection operators on the states with definite quantum numbers of atomic angular momentum F and total muon angular momentum j is developed. It allows us to simplify essentially the construction of the particle interaction operator

through the use of computer methods for calculating Feynman amplitudes. In particular, this method can be useful when working with different loop corrections.

(2) We have increased the accuracy of the calculation of P-wave hyperfine splittings primarily due to the correct account of the corrections of the fifth order over α. To this end, the contributions have been built into the operator of the interaction of particles that are connected to the vacuum polarization and quadrupole interactions. We check the obtained results in two ways: in the formulated framework of tensor projection operators in momentum representation and the more traditional method for the calculation of corrections in the energy spectrum in the coordinate representation. Moreover, in our calculation we take into account the contributions not only of the first- but also the second-order perturbation theory.

(3) Higher-order $O(\alpha^6)$ corrections are calculated. These corrections, although small numerically and so do not affect the comparison with future experimental data, clarify the structure of the perturbation series for the hyperfine splittings.

Let us present more detailed comparison of the results with previous calculations in [16,22]. Being different in the method of obtaining corrections of leading order $O(\alpha^4)$ our results coincide with [16,22]. We mean both the spin-orbit, spin-spin contributions of order $O(\alpha^4)$ [16,22] and quadrupole corrections of the same order [16]. But we obtain the fifth order in α corrections which differ significantly from the results of [16]. In [16] the vacuum polarization corrections to the hyperfine part of the Breit Hamiltonian are determined by the following modification of the potential with $l > 0$:

$$\frac{1}{r}\frac{dV}{dr} = \frac{Z\alpha}{r^3}\left[1 + \frac{\alpha}{3\pi}\int_1^\infty \rho(\xi)d\xi(1 + 2m_e\xi r)e^{-2m_e\xi r}\right]. \tag{60}$$

This leads to the appearance of a special factor of the form $(1 + \varepsilon_{2P})$ with numerical value $\varepsilon_{2P} = 0.000\,391$ for the quadrupole correction and

$$\varepsilon_{2P} = \frac{\alpha}{3\pi}\int_1^\infty \rho(\xi)d\xi\left(\frac{1}{(1+a\xi)^2} + \frac{2az}{(1+a\xi)^3}\right) \tag{61}$$

for the Uehling correction to the Breit Hamiltonian. Numerically, the coefficient in (61) is equal to the same value, $\varepsilon_{2P} = 0.000\,391$. In our calculation we demonstrate that the vacuum polarization corrections to P states are determined by different potentials [compare (60) with our formula (47)] and have a different form for states with various quantum numbers F and j. In contrast to [16] we have performed exact construction of corresponding potentials for different P states and obtained through them numerical results that cannot be reduced to a factor (61). Our results are checked by two independent methods. As an example, we give a comparison of our vacuum polarization plus quadrupole interaction contributions to hyperfine splittings of the level $2P_{3/2}$ with the results of [16]. In [16] these contributions are equal to $\Delta\tilde{E}^{\rm HFS}_{j=3/2}(F = 3/2; 1/2) = -3\mu^3\alpha^4 Q_d\varepsilon_{2p}/80 = -0.3058\ \mu$eV, $\Delta\tilde{E}^{\rm HFS}_{j=3/2}(F = 5/2; 3/2) = \mu^3\alpha^4 Q_d\varepsilon_{2p}/48 = 0.1699\ \mu$eV and differ essentially from our corresponding values $(-0.4394)\ \mu$eV and $0.2441\ \mu$eV. The same situation occurs for other VP corrections. The only significant error of our calculations is associated with the error of the quadrupole moment of the deuteron, so it is presented in Tables I–III.

Summing all diagonal and off-diagonal matrix elements we obtain the following energy matrix:

$$M = \begin{array}{c} \\ 2\,^2P_{1/2} \\ 2\,^4P_{1/2} \\ 2\,^2P_{3/2} \\ 2\,^4P_{3/2} \\ 2\,^6P_{3/2} \end{array} \begin{array}{c} \begin{array}{ccccc} 2\,^2P_{1/2} & 2\,^4P_{1/2} & 2\,^2P_{3/2} & 2\,^4P_{3/2} & 2\,^6P_{3/2} \end{array} \\ \begin{pmatrix} -1381.5765 & 0 & 487.5360 & 0 & 0 \\ 0 & 690.7897 & 0 & -393.5918 & 0 \\ 487.5360 & 0 & 8596.2539 & 0 & 0 \\ 0 & -393.5918 & 0 & 8235.7070 & 0 \\ 0 & 0 & 0 & 0 & 9371.8295 \end{pmatrix} \end{array} \mu\text{eV}. \tag{62}$$

Its diagonalization leads directly to the position of the energy levels $2P$ (see Table III) and hyperfine splitting intervals which can be measured in the experiment. Accounting for the accuracy of the calculation, we have added one extra decimal place in our results in Table III.

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APPENDIX A: BASIC CONTRIBUTIONS TO HYPERFINE STRUCTURE IN COORDINATE REPRESENTATION

Basic contribution to hyperfine structure is determined by the hyperfine part of the Breit Hamiltonian [36]:

$$\Delta V_B^{\rm HFS}(r) = \frac{Z\alpha(1+\kappa_d)}{2m_1m_2r^3}\left[\left[1 + \frac{m_1\kappa_d}{m_2(1+\kappa_d)}\right](\boldsymbol{L}\boldsymbol{s}_2) - \frac{Z\alpha(1+\kappa_d)(1+a_\mu)}{2m_1m_2r^3}[(\boldsymbol{s}_1\boldsymbol{s}_2) - 3(\boldsymbol{s}_1\boldsymbol{n})(\boldsymbol{s}_2\boldsymbol{n})], \tag{A1}$$

where m_1, m_2 are the muon and deuteron masses, κ_d, a_μ are the deuteron and muon anomalous magnetic moments, $\boldsymbol{s}_1$ and $\boldsymbol{s}_2$ are the spin operators of muon and deuteron, $\boldsymbol{n} = \boldsymbol{r}/r$. The operator (A1) does not commute with the muon total angular

momentum $\mathbf{J} = \mathbf{L} + \mathbf{s}_1$. As a result there is the mixing between energy levels $2P_{1/2}$ and $2P_{3/2}$.

For the calculation of diagonal matrix elements $\langle 2P_{1/2} \,|\, \Delta V_B^{\rm HFS} \,|\, 2P_{1/2}\rangle$ and $\langle 2P_{3/2} \,|\, \Delta V_B^{\rm HFS} \,|\, 2P_{3/2}\rangle$ we use the Coulomb wave function of the $2P$ state in coordinate representation:

$$\Psi_{2P}(\boldsymbol{r}) = \frac{1}{2\sqrt{6}} W^{5/2} r e^{-Wr/2} Y_{1m}(\theta,\phi), \quad W = \mu Z\alpha. \tag{A2}$$

The angle averaging in (A1) can be carried out by means of the following replacements [36]:

$$\boldsymbol{s}_1 \to \boldsymbol{J}\frac{\overline{(\boldsymbol{s}_1\cdot\boldsymbol{J})}}{J^2}, \quad \boldsymbol{L} \to \boldsymbol{J}\frac{\overline{(\boldsymbol{L}\cdot\boldsymbol{J})}}{J^2}, \tag{A3}$$

which give the eigenvalues of the corresponding operators:

$$\begin{aligned} \overline{(\boldsymbol{s}_1\cdot\boldsymbol{J})} &= \tfrac{1}{2}\big[j(j+1) - l(l+1) + \tfrac{3}{4}\big], \\ \overline{(\boldsymbol{L}\cdot\boldsymbol{J})} &= \tfrac{1}{2}\big[j(j+1) + l(l+1) - \tfrac{3}{4}\big], \end{aligned} \tag{A4}$$

$$\langle \delta_i j - 3n_i n_j \rangle = -\tfrac{1}{5}(4\delta_{ij} - 3L_iL_j - 3L_jL_i). \tag{A5}$$

The diagonal matrix elements have the general form

$$E_B^{\rm HFS} = \frac{\alpha^4\mu^3(1+\kappa_d)}{48 m_1 m_2}\left[\overline{T_1} + \frac{m_1\kappa_d}{m_2(1+\kappa_d)}\overline{T_1} - (1+a_\mu)\overline{T_2}\right], \tag{A6}$$

where the operators T_i are defined in (49). Substituting here $\overline{T_1}$ and $\overline{T_2}$ for definite quantum numbers F and j, we obtain the leading-order contributions to the hyperfine structure of $2P_{1/2}$ and $2P_{3/2}$ states:

$$\begin{aligned} {}^2E_{1/2}^{\rm HFS} &= -\frac{\alpha^4\mu^3(1+\kappa_d)}{18 m_1 m_2}\left[1 + \frac{m_1\kappa_d}{2m_2(1+\kappa_d)} + \frac{a_\mu}{2}\right] \\ &= -1380.3360\ \mu\text{eV}, \end{aligned} \tag{A7}$$

$$\begin{aligned} {}^4E_{1/2}^{\rm HFS} &= \frac{\alpha^4\mu^3(1+\kappa_d)}{36 m_1 m_2}\left[1 + \frac{m_1\kappa_d}{2m_2(1+\kappa_d)} + \frac{a_\mu}{2}\right] \\ &= 690.1680\ \mu\text{eV}, \end{aligned} \tag{A8}$$

$$\begin{aligned} {}^2E_{3/2}^{\rm HFS} &= -\frac{\alpha^4\mu^3(1+\kappa_d)}{72 m_1 m_2}\left[2 + \frac{5m_1\kappa_d}{2m_2(1+\kappa_d)} - \frac{a_\mu}{2}\right] \\ &= 8162.2889\ \mu\text{eV}, \end{aligned} \tag{A9}$$

$$\begin{aligned} {}^4E_{3/2}^{\rm HFS} &= -\frac{\alpha^4\mu^3(1+\kappa_d)}{36 m_1 m_2}\left[\frac{2}{5} + \frac{m_1\kappa_d}{2m_2(1+\kappa_d)} - \frac{a_\mu}{10}\right] \\ &= 8583.2315\ \mu\text{eV}, \end{aligned} \tag{A10}$$

$$\begin{aligned} {}^6E_{3/2}^{\rm HFS} &= -\frac{\alpha^4\mu^3(1+\kappa_d)}{24 m_1 m_2}\left[\frac{2}{5} + \frac{m_1\kappa_d}{2m_2(1+\kappa_d)} - \frac{a_\mu}{10}\right] \\ &= 9284.8027\ \mu\text{eV}, \end{aligned} \tag{A11}$$

where we take into account the fine-structure interval $\Delta E_{\rm FS} = 8.863\,86$ meV calculated in [16,37]. All expressions (A7)–(A11) contain the correction to the anomalous magnetic moment of the muon.

Off-diagonal matrix elements $\langle 2P_{1/2} \,|\, \Delta V^{\rm HFS} \,|\, 2P_{3/2}\rangle^{F=1/2}$ and $\langle 2P_{1/2} \,|\, \Delta V^{\rm HFS} \,|\, 2P_{3/2}\rangle^{F=3/2}$ are essential to achieve a high accuracy of the calculation. They differ by the value of atomic angular momentum. The angular averaging by means of (A5) leads to $\overline{T}_1 = 2\overline{T}_2$. For the calculation $\overline{(\mathbf{L}\mathbf{s}_2)}$, we use the general formula for the matrix elements of the scalar product of two irreducible tensor operators:

$$\begin{aligned} &\langle j' s_2 F \,|\, (T^1 T^2) \,|\, j s_2 F\rangle \\ &\quad = (-1)^{s_2+J'-F} W(j s_2 j' s_2; F1) \big\langle j' \,\|\, T^1 \,\|\, j\big\rangle \big\langle s_2 \,\|\, T^2 \,\|\, s_2\big\rangle, \end{aligned} \tag{A12}$$

where $W(j s_2 j' s_2; F1)$ is the Racah coefficient. Applying (A12) to $\overline{(\mathbf{L}\mathbf{s}_2)}$ we find

$$\begin{aligned} &\langle j' s_2 F \,|\, (\boldsymbol{L}\cdot\boldsymbol{s}_2) \,|\, j s_2 F\rangle \\ &\quad = (-1)^{-j-F-s_2+L+3/2+j'}\sqrt{(2j'+1)(2j+1)} \\ &\qquad \times\sqrt{(2s_2+1)(s_2+1)s_2(2L+1)(L+1)L} \\ &\qquad \times \begin{Bmatrix} j & s_2 & F \\ s_2 & j' & 1 \end{Bmatrix} \begin{Bmatrix} l & j' & \frac{1}{2} \\ j & l & 1 \end{Bmatrix}. \end{aligned} \tag{A13}$$

Two off-diagonal matrix elements of the operator T_1 have the form

$$\begin{aligned} \left\langle \frac{1}{2},1,\frac{1}{2}\middle|(\boldsymbol{L}\cdot\boldsymbol{s}_2)\middle|\frac{3}{2},1,\frac{1}{2}\right\rangle &= -\frac{\sqrt{2}}{3}, \left\langle \frac{1}{2},1,\frac{3}{2}\middle|(\boldsymbol{L}\cdot\boldsymbol{s}_2)\middle|\frac{3}{2},1,\frac{3}{2}\right\rangle \\ &= -\frac{\sqrt{5}}{3}, \end{aligned} \tag{A14}$$

where the $6j$ symbols are taken from [30].

Using (A14), we obtain the leading-order contributions to off-diagonal matrix elements of the Breit Hamiltonian (A1):

$$\begin{aligned} E_{F=1/2}^{\rm HFS,off\text{-}diag} &= \frac{\alpha^4\mu^3(1+\kappa_d)}{48 m_1 m_2}\left(-\frac{\sqrt{2}}{6}\right)\left[1 + \frac{2m_1\kappa_d}{m_2(1+\kappa_d)} - a_\mu\right] \\ &= -126.0372\ \mu\text{eV}, \end{aligned} \tag{A15}$$

$$\begin{aligned} E_{F=3/2}^{\rm HFS,off\text{-}diag} &= \frac{\alpha^4\mu^3(1+\kappa_d)}{48 m_1 m_2}\left(-\frac{\sqrt{5}}{6}\right)\left[1 + \frac{2m_1\kappa_d}{m_2(1+\kappa_d)} - a_\mu\right] \\ &= -199.2824\ \mu\text{eV}. \end{aligned} \tag{A16}$$

There exist higher-order corrections to (A15) and (A16) which are related to additional interactions and examined above.

APPENDIX B: RELATIVISTIC CORRECTIONS TO HYPERFINE STRUCTURE

Relativistic corrections of order α^6 can be calculated by means of the Dirac equation [38,39]. We present here only a sketch of the output of the final formula for the numerical estimate. In the Dirac theory the hyperfine part of the relativistic Hamiltonian has the form

$$\Delta H^{\rm HFS} = e g_N \mu_N \boldsymbol{s}_2 \frac{[\boldsymbol{r}\times\boldsymbol{\alpha}]}{r^3}, \tag{B1}$$

where μ_N is the nuclear magneton, g_N is the deuteron gyromagnetic factor. To find the expectation value of (B1) over atomic wave functions we should use the Wigner-Eckart theorem expressing the initial matrix element through the reduced matrix elements:

$$\Delta E^{\rm HFS}_{\rm rel} = e g_N \mu_N (-1)^{s_2+j'-F} W(j s_2 j' s_2; F1) \langle s_2 \| \boldsymbol{s_2} \| s_2 \rangle \times \left\langle j' \left\| \frac{[\boldsymbol{r}\times\boldsymbol{\alpha}]}{r^3} \right\| j \right\rangle. \tag{B2}$$

Calculating the first reduced matrix element we can simplify (B2) as follows:

$$\Delta E^{\rm HFS}_{\rm rel} = e g_N \mu_N (-1)^{s_2+j'-F} \sqrt{(2s_2+1)(s_2+1)s_2} \times \sqrt{(2j'+1)(j'+1)j'} W(j s_2 j' s_2; F1) \times \left\langle j'\mu \left| \left(\frac{[\boldsymbol{r}\times\boldsymbol{\alpha}]}{r^3} \right)_z \right| j\mu \right\rangle \mu^{-1}. \tag{B3}$$

In the case of the diagonal matrix element we have

$$\left\langle j\mu \left| \left(\frac{[\boldsymbol{r}\times\boldsymbol{\alpha}]}{r^3} \right)_z \right| j\mu \right\rangle = -i A_{kk} R_{kk},$$
$$R_{kk} = 2\int_0^\infty g_k(r) f_k(r) dr, \tag{B4}$$
$$-i A_{kk} = \frac{4k}{4k^2-1}.$$

The radial matrix elements are calculated analytically with the use of exact Dirac radial wave functions. After their expansion over α we find [39]

$$R(2P_{1/2}) = \frac{(Z\alpha)^3}{12}\left(1+\frac{47}{24}(Z\alpha)^2\right)m_1^2,$$
$$R(2P_{3/2}) = -\frac{(Z\alpha)^3}{24}\left(1+\frac{7}{24}(Z\alpha)^2\right)m_1^2. \tag{B5}$$

As a result, general expressions for relativistic corrections to diagonal matrix elements take the form

$$E^{\rm HFS}_{\rm rel}(2P_{1/2}) = \frac{\alpha^6(1+\kappa_d)\mu^3}{48 m_1 m_2}\frac{m_1^3}{\mu^3}\frac{47}{9}\frac{1}{2} \times [F(F+1)-J(J+1)-I(I+1)], \tag{B6}$$

$$E^{\rm HFS}_{\rm rel}(2P_{3/2}) = \frac{\alpha^6(1+\kappa_d)\mu^3}{48 m_1 m_2}\frac{m_1^3}{\mu^3}\frac{7}{45}\frac{1}{2} \times [F(F+1)-J(J+1)-I(I+1)]. \tag{B7}$$

Numerical results for separate P states are presented in Table I. Relativistic corrections to off-diagonal matrix elements are evaluated in a similar way. The radial and angular integrals in this case take the form

$$R_{kk} = \int_0^\infty [g_{1/2}(r) f_{3/2}(r) + g_{3/2}(r) f_{1/2}(r)] dr,$$
$$-i A_l = \frac{[(l+1/2)^2-\mu^2]^{1/2}}{2l+1} = \frac{\sqrt{2}}{3}, \tag{B8}$$

where the indexes near radial wave functions designate the values of muon total angular momentum j. Radial integrations lead to analytical formulas and corresponding numerical results:

$$E^{\rm HFS,off\text{-}diag}_{{\rm rel},F=1/2} = -\frac{\alpha^6(1+\kappa_d)\mu^3}{48 m_1 m_2}\frac{m_1^3}{\mu^3}\frac{3\sqrt{2}}{32} = -0.0043\ \mu{\rm eV}, \tag{B9}$$

$$E^{\rm HFS,off\text{-}diag}_{{\rm rel},F=3/2} = -\frac{\alpha^6(1+\kappa_d)\mu^3}{48 m_1 m_2}\frac{m_1^3}{\mu^3}\frac{3\sqrt{5}}{32} = -0.0067\ \mu{\rm eV}. \tag{B10}$$

Although their size is extremely small compared with other corrections we have included them in Table II by inserting numerical values with an accuracy 0.0001 μeV for definiteness. It shows the relative numerical value of obtained corrections.

APPENDIX C: TWO-LOOP VACUUM POLARIZATION CORRECTIONS TO HYPERFINE STRUCTURE

Two-loop vacuum polarization corrections presented in Figs. 1(b)–1(d) have the order α^6. We divide them into two parts: loop after loop contribution (VP-VP) and two-loop contribution to polarization operator (two-loop VP). For their calculation we use corresponding potentials in coordinate representation constructed in the same way as in [21]:

$$\Delta V^{\rm HFS}_{1\gamma,\text{VP-VP}}(r) = \frac{Z\alpha(1+\kappa_d)}{2m_1 m_2 r^3}\left(\frac{\alpha}{3\pi}\right)^2 \int_1^\infty \rho(\xi)d\xi \int_1^\infty \rho(\eta)d\eta \frac{1}{\xi^2-\eta^2} \times \left[\left(1+\frac{m_1\kappa_d}{m_2(1+\kappa_d)}\right)(\boldsymbol{L}\cdot\boldsymbol{s}_2)[\xi^2(1+2m_e\xi r)e^{-2m_e\xi r} - \eta^2(1+2m_e\eta r)e^{-2m_e\eta r}] - (1+a_\mu)\big(4m_e^2 r^2[\xi^4 e^{-2m_e\xi r} - \eta^4 e^{-2m_e\eta r}][(\boldsymbol{s}_1\cdot\boldsymbol{s}_2)-(\boldsymbol{s}_1\cdot\boldsymbol{n})(\boldsymbol{s}_2\cdot\boldsymbol{n})] + [\xi^2(1+2m_e\xi r)e^{-2m_e\xi r} - \eta^2(1+2m_e\eta r)e^{-2m_e\eta r}][(\boldsymbol{s}_1\cdot\boldsymbol{s}_2)-3(\boldsymbol{s}_1\cdot\boldsymbol{n})(\boldsymbol{s}_2\cdot\boldsymbol{n})]\big)\right], \tag{C1}$$

$$\Delta V^{\rm HFS}_{\text{two-loop VP}}(r) = \frac{Z\alpha(1+\kappa_d)}{2m_1 m_2 r^3}\frac{2}{3}\left(\frac{\alpha}{\pi}\right)^2 \int_0^1 \frac{f(v)dv}{1-v^2} e^{-2m_e r/\sqrt{1-v^2}} \left\{\left(1+\frac{m_1\kappa_d}{m_2(1+\kappa_d)}\right)\left[1+\frac{2m_e r}{\sqrt{1-v^2}}\right](\boldsymbol{L}\cdot\boldsymbol{s}_2) - (1+a_\mu)\left[\frac{4m_e^2 r^2}{1-v^2}[(\boldsymbol{s}_1\cdot\boldsymbol{s}_2)-(\boldsymbol{s}_1\cdot\boldsymbol{n})(\boldsymbol{s}_2\cdot\boldsymbol{n})] + \left(1+\frac{2m_e r}{\sqrt{1-v^2}}\right)[(\boldsymbol{s}_1\cdot\boldsymbol{s}_2)-3(\boldsymbol{s}_1\cdot\boldsymbol{n})(\boldsymbol{s}_2\cdot\boldsymbol{n})]\right]\right\}. \tag{C2}$$

Averaging (C1) and (C2) over the Coulomb wave functions we obtain their numerical values in the hyperfine structure which are presented in Tables I and II. The muon vacuum polarization correction is evaluated by means of a replacement $m_e \to m_1$ in (48). Its numerical value also is included in Tables I and II.

For the calculation of contributions in the second-order PT we should use in the basic expression

$$\Delta E^{\rm HFS}_{\rm SOPT,VP} = 2\langle\psi|\Delta V^{(1),C}_{\rm VP}\tilde{G}\Delta V^{(2),\rm HFS}_{B,\rm VP}|\psi\rangle, \qquad \text{(C3)}$$

the potential $\Delta V^{(2),\rm HFS}_{B,\rm VP}$ corresponding to pure hyperfine interaction or to hyperfine interaction corrected by the vacuum polarization effect. Aa a second perturbation we use the Coulomb potential of one-loop or two-loop order. All resulting matrix elements are calculated analytically in a standard way in the integration over the coordinates of the particles and numerically by spectral parameters. Other details of their calculation can be founded in our previous papers [17,18,21].

The two-loop vacuum polarization contribution to hyperfine structure of order α^6 is determined also by the third-order PT. In this case we should use the following expression:

$$\begin{aligned}\Delta E^{\rm HFS}_{\rm TOPT,VP} = {} & \langle\psi_n\,|\,\Delta V^C_{\rm VP}\tilde{G}\Delta V^{\rm HFS}\tilde{G}\Delta V^C_{\rm VP}\,|\,\psi_n\rangle \\ & + 2\langle\psi_n\,|\,\Delta V^C_{\rm VP}\tilde{G}V^C_{\rm VP}\tilde{G}\Delta V^{\rm HFS}\,|\,\psi_n\rangle \\ & - \langle\psi_n\,|\,\Delta V^{\rm HFS}\,|\,\psi_n\rangle\langle\psi_n\,|\,\Delta V^C_{\rm VP}\tilde{G}\tilde{G}\Delta V^C_{\rm VP}\,|\,\psi_n\rangle \\ & - 2\langle\psi_n\,|\,\Delta V^C_{\rm VP}\,|\,\psi_n\rangle\langle\psi_n|\Delta V^C_{\rm VP}\tilde{G}\tilde{G}\Delta V^{\rm HFS}|\psi_n\rangle. \end{aligned} \qquad \text{(C4)}$$

Using further exact perturbation potential (A1), modification of the Coulomb potential ΔV^C, and the Coulomb Green's function $\tilde{G}$ (51), we obtain numerical values of corresponding corrections which are written in Table I as a separate line. Numerically the vacuum polarization contributions of order α^6 are extremely small and will not have a significant impact on the comparison with future experimental data.

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